Supplementary Information for

Azirine-containing dipeptides and depsipeptides: synthesis, transformations and antibacterial activity

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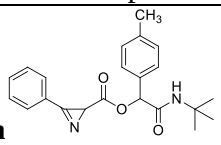
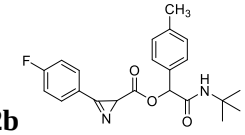
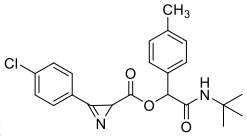
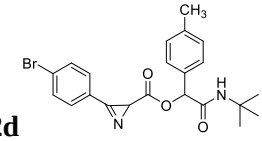
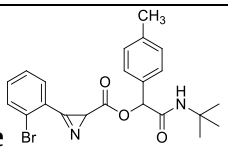
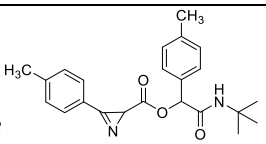
Table of Contents

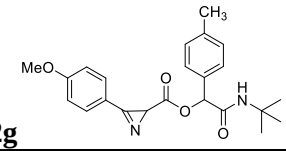
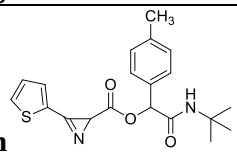
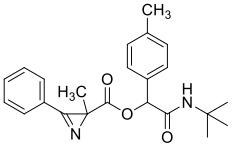
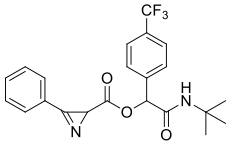
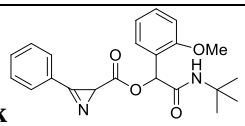
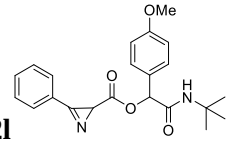
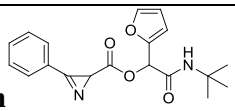
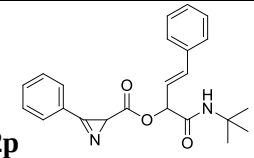
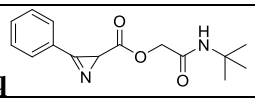
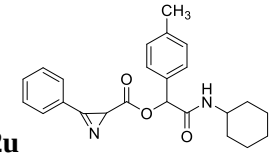
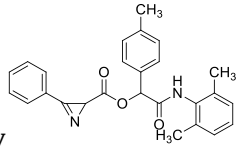
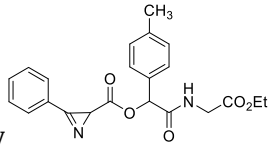
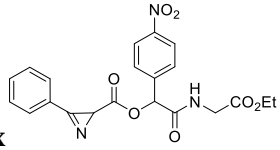
1. Determination of antibacterial activity *in vitro*

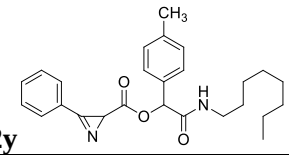
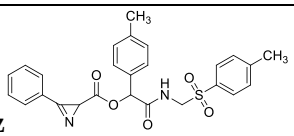
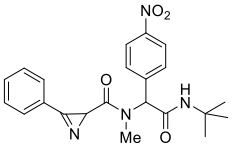
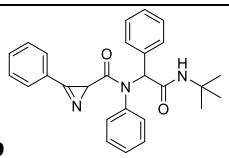
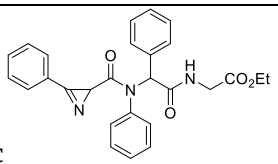
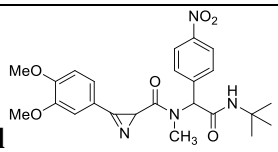
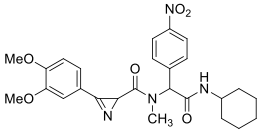
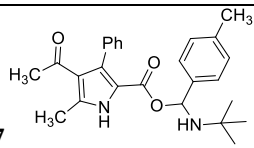
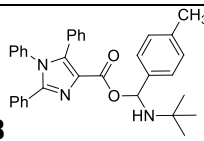
Disk diffusion method

Testing of the susceptibility of several microorganisms (*Enterococcus faecium*, *Staphylococcus aureus*, *Pseudomonas aeruginosa*, *Enterobacter cloacae*) to compounds **2a**–**m**,**p**,**q**,**u**–**z**,**za**–**ze**,**7**,**8** as well as Sulfamethoxazole (positive control) was performed using the conventional Kirby-Bauer disk diffusion test[1] under the Standard Operating Procedure of The European Committee on Antimicrobial Susceptibility Testing (EUCAST).[2] Disks containing 5 μg of Sulfamethoxazole were used. The tested compound (1 mg) was dissolved in dimethyl sulfoxide (10 μL) and diluted to a volume of 1 mL with deionized water. To a Petri dish containing Muller-Hilton agar inoculated with a bacterial suspension (McFarland OD = 0.5) 5 μL of this solution were added. After drying of the compound solution, the Petri dish was incubated at 37 °C for 24 h. The susceptibility to a drug was assessed by measuring the bacterial growth inhibition zone diameter around the disc with Sulfamethoxazole or the tested compound dried solution circular spot.

Table S-1. Screening results of antibacterial activity by the disk diffusion method (DDM)

Compound	*E. faecium ATCC® 29212*	*S. aureus ATCC® 23235*	*P. aeruginosa ATCC® 27853*	*E. cloacae ATCC® 13047*
 **2a**	0	0	0	7
 **2b**	7	5	0	6
 **2c**	0	3	0	0
 **2d**	7	5	0	0
 **2e**	7	7	0	7
 **2f**	6	6	6	6

2g 	6	7	0	0
2h 	7	0	0	7
2i 	6	6	6	0
2j 	6	5	0	0
2k 	0	7	0	0
2l 	6	8	0	0
2m 	0	6	6	0
2p 	9	11	0	0
2q 	0	6	0	0
2u 	0	6	0	0
2v 	6	5	0	0
2w 	6	5	0	0
2x 	6	4	0	0

 **2y**	0	6	0	0
 **2z**	6	9	6	0
 **2za**	0	5	0	0
 **2zb**	0	0	0	0
 **2zc**	0	0	0	0
 **2zd**	0	6	0	0
 **2ze**	0	6	0	0
 **7**	0	0	0	0
 **8**	0	0	0	0

Determination of the minimum inhibitory concentration (MIC)

The test was performed under the Standard Operating Procedure of The European Committee on Antimicrobial Susceptibility Testing (EUCAST)[3] at a final volume of 0.2 mL in a 96-well sterile immunology plate with sterile lids. The nutrient medium for this method is the Muller – Hinton medium. A standard microbial suspension equivalent to 0.5 according to the Mcfarland standard was used for inoculation, diluted 100 times on a nutrient broth, after which the concentration of the microorganism in it was approximately 10^6 CFU/ml.

The working solution of the antibiotic compound was prepared from the basic solution using a liquid nutrient medium. The first concentration was the maximum. In all wells of the plate 100 μL of nutrient medium were placed. Then 100 μL of the maximum concentration solution of the compound were placed in the first well of the horizontal row of the plate. The contents of the well were mixed and 100 μL from the first well of the first horizontal row was transferred to the second well of the first horizontal row. So it was continued to the well number 10, from which 100 μL of the contents were removed after mixing. Thus, a number of wells with a solution of antibacterial compound was obtained, the concentrations of which differed in neighboring tubes by 2 times. Then, in the first 10 wells 100 μL of the prepared suspension of bacteria was placed. Wells 11 and 12 were controls. Well 11 was a control of bacteria, it contained 100 μL of the nutrient medium and 100 μL of the bacteria suspension, which was used in the first horizontal row. Well 12 was a control of the broth, it contained 200 μL of the nutrient medium.

Each horizontal row of the plate corresponded to a separate antibacterial compound or a separate microorganism. One or two rows of the plate were used to establish controls of the respective antibiotics selected as reference for the compound under study with each microorganism.

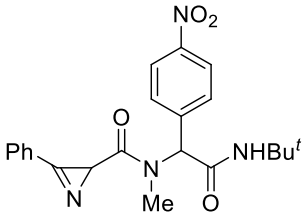
The plates were incubated at +37 °C in the thermostat during 18–24 h. The results were taken into account visually, comparing the growth of microorganisms in the presence of an antibacterial compound with the growth of culture in the cell without it. The minimum concentration providing complete suppression of the visible growth of the studied strain was used for MIC value.

2. Calculation details

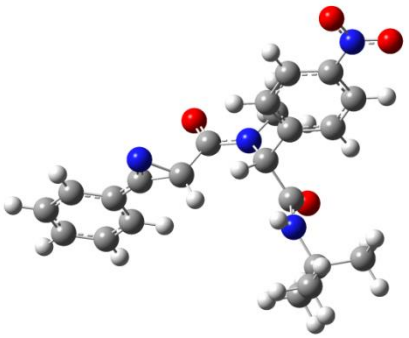
All calculations were performed by using the Gaussian 09 suite of quantum chemical programs.[4] Geometry optimizations of compounds **2za**, **2zf**, **2za**-enol, and **2zf**-enol were performed at the DFT B3LYP/6-31+G(d,p) level using PCM model for methanol (298 K).

Table S-2. Energies (au) and cartesian coordinates of stationary points for compounds **2za**, **2zf**, **2za**-enol, and **2zf**-enol.

Compound **2za**

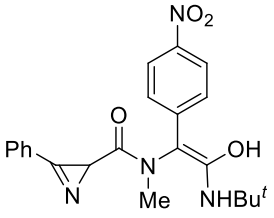


(E_0 + ZPE) = -1372,251278, E = -1372,222152,
H = -1372,221208, G = -1372,316336.
Imaginary frequency = 0.



C	2.40991653	0.69858058	-0.23020746
N	1.60747653	1.34069158	-0.96385046
C	1.03230953	0.27665558	0.00522854
C	3.81319253	0.53561358	0.08044154
C	0.33332553	0.80218258	1.22953354
N	-0.89634447	0.30446558	1.56101454
O	0.89704453	1.65093158	1.93783254
C	-1.72457847	-0.49016842	0.64379154
C	-1.46768747	0.71002058	2.85098654
C	-1.70484147	-1.99895342	1.02127054
C	-3.14414047	0.07842658	0.54309954
N	-1.97085047	-2.82559442	-0.01340246
O	-1.46679747	-2.36778942	2.17488254
C	-4.22725447	-0.47570142	1.23976754
C	-5.50110447	0.07914558	1.13449954
C	-5.67820847	1.19847758	0.32126354
C	-4.62015347	1.77426258	-0.38535646
C	-3.35636647	1.20441458	-0.26868146
C	4.21058653	-0.41523342	1.03506254
C	5.56474653	-0.57943042	1.32794854
C	6.52121953	0.20211558	0.67114954
C	6.12695753	1.15101758	-0.28190746
C	4.77709953	1.32062358	-0.58010046

Compound **2za**-enol



(E_0 + ZPE) = -1372,228049, E = -1372,198948,
H = -1372,198004, G = -1372,290624.
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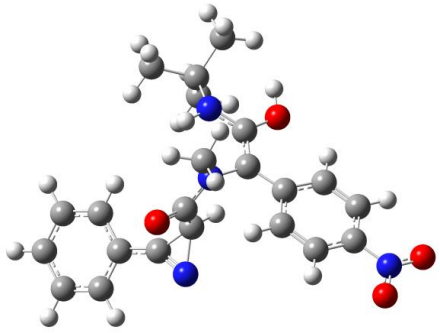

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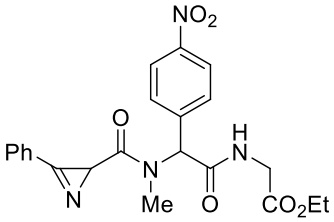
N	-0.76437881	-3.32198564	-0.29809356
C	-0.69443881	-1.78772664	-0.08680056
C	-3.27203281	-2.79837064	-0.48507056
C	-0.40816081	-1.33987864	1.31707944
N	0.40565819	-0.24562564	1.48625644
O	-0.90611581	-1.93009364	2.28539544
C	1.19800619	0.32878636	0.42510544
C	0.68348419	0.18286636	2.87012244
C	0.67612419	1.50485036	-0.11942256
C	2.46953919	-0.29275664	0.11335744
N	-0.47718081	2.06088836	0.32360244
O	1.34259919	2.12607336	-1.11000756
C	3.38691919	0.17796836	-0.87476356
C	4.58484519	-0.46806864	-1.12154356
C	4.92580719	-1.62083164	-0.39705456
C	4.05111319	-2.12085964	0.57920544
C	2.85633019	-1.46951264	0.82244844
C	-4.09411281	-1.66180164	-0.41321856
C	-5.47440881	-1.79256364	-0.56972356
C	-6.03467581	-3.05377564	-0.79801556
C	-5.21632381	-4.18923564	-0.87110756
C	-3.83768081	-4.06671464	-0.71557556

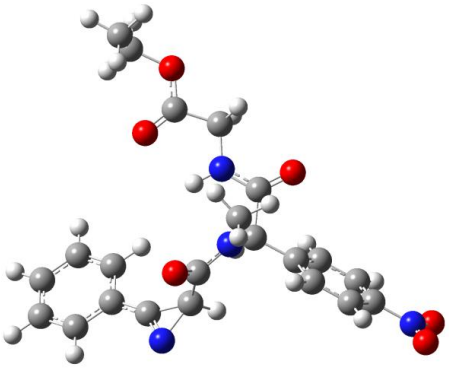
N	-7.01543347	1.78677658	0.20269554
O	-7.15508647	2.78007158	-0.51797046
O	-7.94283147	1.26327658	0.82831854
H	0.67629653	-0.63386142	-0.46609346
H	-0.66173747	0.80707158	3.57751454
H	-1.98729147	1.67144458	2.77398554
H	-2.16226947	-0.05649642	3.18904054
H	-2.14218047	-2.39703442	-0.91426846
H	-4.08685347	-1.34515642	1.87299654
H	-6.34043547	-0.34473642	1.67076154
H	-4.78816447	2.64074658	-1.01200546
H	-2.52634147	1.64213958	-0.81474946
H	3.45907953	-1.01465142	1.53945754
H	5.87362453	-1.31308142	2.06574654
H	7.57468253	0.07332958	0.90062654
H	6.87286853	1.75483958	-0.78915646
H	4.46171153	2.05275258	-1.31704846
H	-1.29299547	-0.38796942	-0.35175846
C	-2.06933047	-4.31243242	0.02828954
C	-0.71679747	-4.91233942	0.45428654
H	-0.44493847	-4.58996442	1.46160654
H	-0.77863647	-6.00537842	0.44381554
H	0.07427653	-4.60652442	-0.23814746
C	-2.41130547	-4.75586542	-1.40310146
H	-2.49282347	-5.84538542	-1.44225246
H	-3.36752247	-4.33273242	-1.73059846
H	-1.63164247	-4.44910442	-2.10924746
C	-3.19078647	-4.74139242	0.99160854
H	-2.97906947	-4.41429242	2.01174554
H	-4.15101647	-4.31870442	0.67864054
H	-3.27994147	-5.83251442	0.98876854

N	6.16827119	-2.28824364	-0.65522256
O	6.45248719	-3.30753764	0.00289244
O	6.92792919	-1.82854264	-1.52971456
H	-0.26248481	-1.22080264	-0.90460756
H	-0.23943981	0.17916536	3.45221844
H	1.40200619	-0.48477764	3.35867044
H	1.09868919	1.19058836	2.84121244
H	-0.92580981	1.52047336	1.05177044
H	1.03016919	3.03494336	-1.22994156
H	3.15379019	1.05808936	-1.45314456
H	5.26273619	-0.08795964	-1.87584156
H	4.31461219	-3.01119564	1.13655944
H	2.20348019	-1.87851864	1.58273744
H	-3.64810481	-0.68875564	-0.23332956
H	-6.11092581	-0.91525564	-0.51301456
H	-7.10907981	-3.15415564	-0.91884756
H	-5.65596881	-5.16574164	-1.04835856
H	-3.19548181	-4.94031164	-0.76952556
C	-1.36135981	3.06756736	-0.34223156
C	-0.67910581	4.45050036	-0.42139756
H	0.10897719	4.51974636	-1.18240956
H	-1.42137881	5.20182536	-0.70562756
H	-0.25333181	4.73153136	0.54554244
C	-2.59098981	3.18366936	0.57527944
H	-2.30548581	3.53708636	1.57124744
H	-3.30323781	3.89501836	0.15022944
H	-3.09812281	2.21819036	0.67645944
C	-1.79702981	2.57731336	-1.73742356
H	-0.94894581	2.45084436	-2.41652156
H	-2.31981081	1.61956736	-1.66034356
H	-2.47798881	3.30668336	-2.18682456

Compound **2zf**

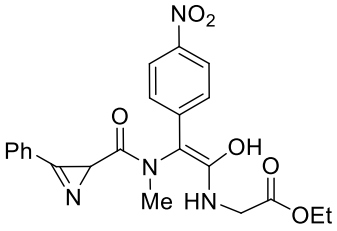


(E_0 + ZPE) = -1521,520257, E = -1521,489712,
H = -1521,488767, G = -1521,588530.
Imaginary frequency = 0.

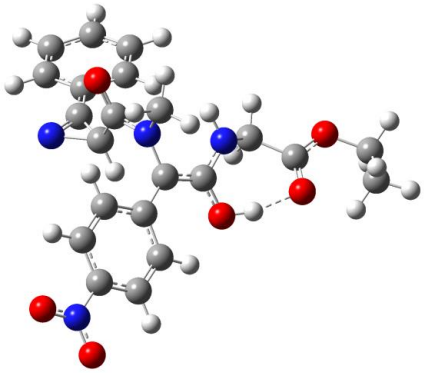


C	1.53925753	4.58675507	0.47461990
N	0.68536253	5.07510407	1.26428290
C	0.44749653	3.64766107	0.72706590

Compound **2zf**-enol



(E_0 + ZPE) = -1521,503007, E = -1521,472836,
H = -1521,471892, G = -1521,569000.
Imaginary frequency = 0.



C	-1.43516141	-3.82507582	-0.00647802
N	-0.26051841	-4.28177182	-0.05556402
C	-0.45650641	-2.79397182	0.33303598

C	2.79203353	4.86081407	-0.19519910	C	-2.82467041	-4.18331982	-0.19461902
C	0.60718553	2.55284207	1.75033990	C	-0.21050241	-2.46876082	1.77833998
N	0.10189153	1.31005507	1.46266990	N	0.30231659	-1.23017082	2.07731598
O	1.14992353	2.78030107	2.83765190	O	-0.47296741	-3.28850782	2.66888298
C	-0.38657547	0.91371507	0.13843090	C	0.76288759	-0.29402782	1.08000698
C	0.12802953	0.30732007	2.53914890	C	0.58036259	-0.93959982	3.49685798
C	0.19698953	-0.48226593	-0.25349610	C	-0.16053741	0.67180018	0.69864098
C	-1.90266947	0.96136707	-0.01908010	C	2.14736259	-0.38985582	0.64693198
N	1.54341953	-0.54461193	-0.23232610	N	-1.38977241	0.78224918	1.29520898
O	-0.51516347	-1.43572093	-0.57190410	O	0.11042859	1.55261018	-0.26946002
C	2.26372353	-1.76418493	-0.53944110	C	-2.58801041	1.27282418	0.61813498
C	-2.45844447	0.77733307	-1.29659610	C	2.78015359	0.53415318	-0.23527302
C	-3.83275047	0.83751407	-1.49382910	C	4.10622059	0.39217118	-0.60507902
C	-4.65605447	1.08645607	-0.39202110	C	4.85842559	-0.68585482	-0.11525002
C	-4.13474147	1.28334307	0.88585190	C	4.27352559	-1.61949182	0.75123298
C	-2.75303547	1.22234807	1.06209590	C	2.94834659	-1.46827582	1.12023298
C	3.33590553	3.91277607	-1.07762610	C	-3.82726841	-3.21844382	-0.00284302
C	4.54017853	4.18223307	-1.72851510	C	-5.16643241	-3.56260182	-0.18992402
C	5.20150853	5.39333807	-1.49970110	C	-5.50604341	-4.86556182	-0.56889702
C	4.66059353	6.34065807	-0.61970810	C	-4.50733841	-5.82978582	-0.76162102
C	3.45813753	6.08007607	0.03269590	C	-3.16844441	-5.49414382	-0.57595702
C	3.74835153	-1.54172493	-0.31621810	C	-2.63247441	2.79136618	0.50426998
O	4.22657853	-0.48231493	0.05345090	O	-1.64179741	3.46508018	0.22458798
O	4.43870853	-2.64998993	-0.58437710	O	-3.84420941	3.27965118	0.69247898
C	5.89156253	-2.62156393	-0.40667610	C	-4.06067141	4.72265618	0.51047498
C	6.27157853	-3.01602193	1.00983090	C	-4.41769041	5.03198118	-0.93173602
N	-6.10524747	1.15090707	-0.58715810	N	6.23477459	-0.83454482	-0.50384102
O	-6.82023947	1.37559207	0.39534190	O	6.88842859	-1.78838182	-0.04355002
O	-6.55136947	0.97694107	-1.72643610	O	6.72959259	-0.00450682	-1.28822402
H	-0.35769347	3.56146907	0.00298190	H	-0.15121241	-2.06957682	-0.41423102
H	-0.20677047	0.76265607	3.47206290	H	-0.28190041	-1.20811682	4.11064198
H	-0.54376247	-0.51201893	2.28085590	H	1.44623859	-1.50497382	3.85824098
H	1.13619153	-0.09057193	2.69050090	H	0.78433959	0.12672718	3.59443798
H	2.10320253	0.24984407	0.05636890	H	-1.56445541	0.11319418	2.03190298
H	2.10155153	-2.07234893	-1.57878510	H	-0.45787241	2.36660518	-0.16194202
H	1.92639853	-2.59174693	0.09458890	H	-3.45689641	0.92581118	1.17549098
H	-1.81261947	0.58552607	-2.14685810	H	-2.66779841	0.87463718	-0.40319902
H	-4.26391847	0.69769807	-2.47679910	H	2.22066059	1.36846218	-0.62938702
H	-4.79455047	1.48292007	1.72044890	H	4.56679759	1.10999118	-1.27253802
H	-2.34451147	1.39098807	2.05114690	H	4.85749259	-2.45110282	1.12546398
H	2.81312453	2.97705607	-1.24921310	H	2.52144059	-2.20189682	1.79228698
H	4.96159853	3.45108407	-2.41094310	H	-3.55185941	-2.21026682	0.29055198
H	6.13919453	5.60113907	-2.00621010	H	-5.94229941	-2.81833682	-0.04109802
H	5.17807553	7.27875507	-0.44542610	H	-6.54860641	-5.13183182	-0.71449402
H	3.03106653	6.80698907	0.71652990	H	-4.77589041	-6.83957782	-1.05570702
H	6.25608853	-3.34305793	-1.13897910	H	-2.38763241	-6.23396882	-0.72260802
H	6.25158253	-1.62474193	-0.66605710	H	-4.88332841	4.94246718	1.19111498
H	7.36303453	-3.05074193	1.09120690	H	-3.16191341	5.24612418	0.83832698
H	5.89766253	-2.29115693	1.73822390	H	-4.63718541	6.10089118	-1.02077102
H	5.87790553	-4.00588193	1.25863090	H	-3.59054541	4.79628018	-1.60695602
H	0.04116653	1.60342307	-0.59501810	H	-5.30443641	4.47307418	-1.24408002

3. References

1. A. W. Bauer, W. M. Kirby, J. C. Sherris and M. Turck, *Am. J. Clin. Pathol.*, 1966, **45**, 493–496.
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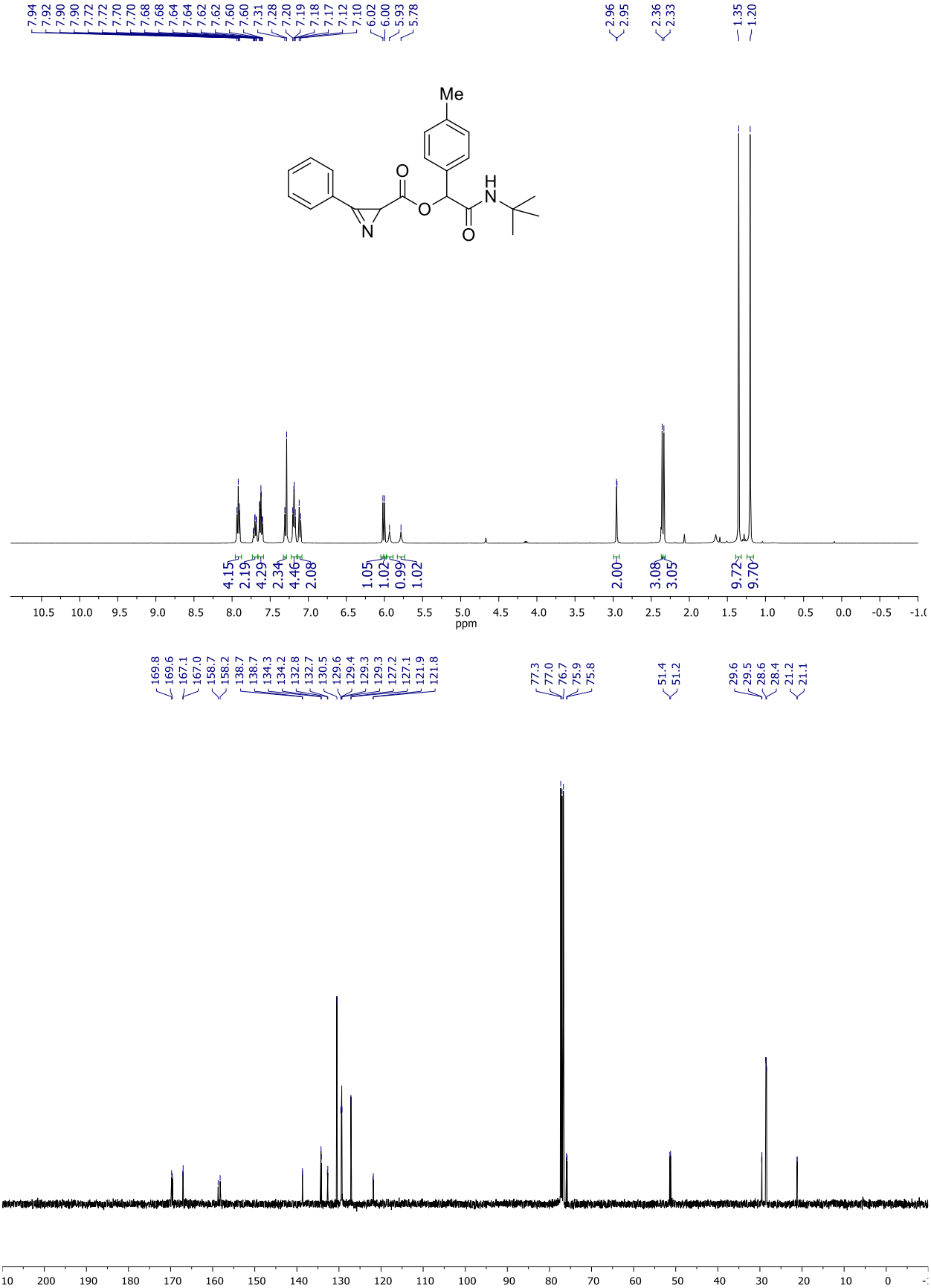
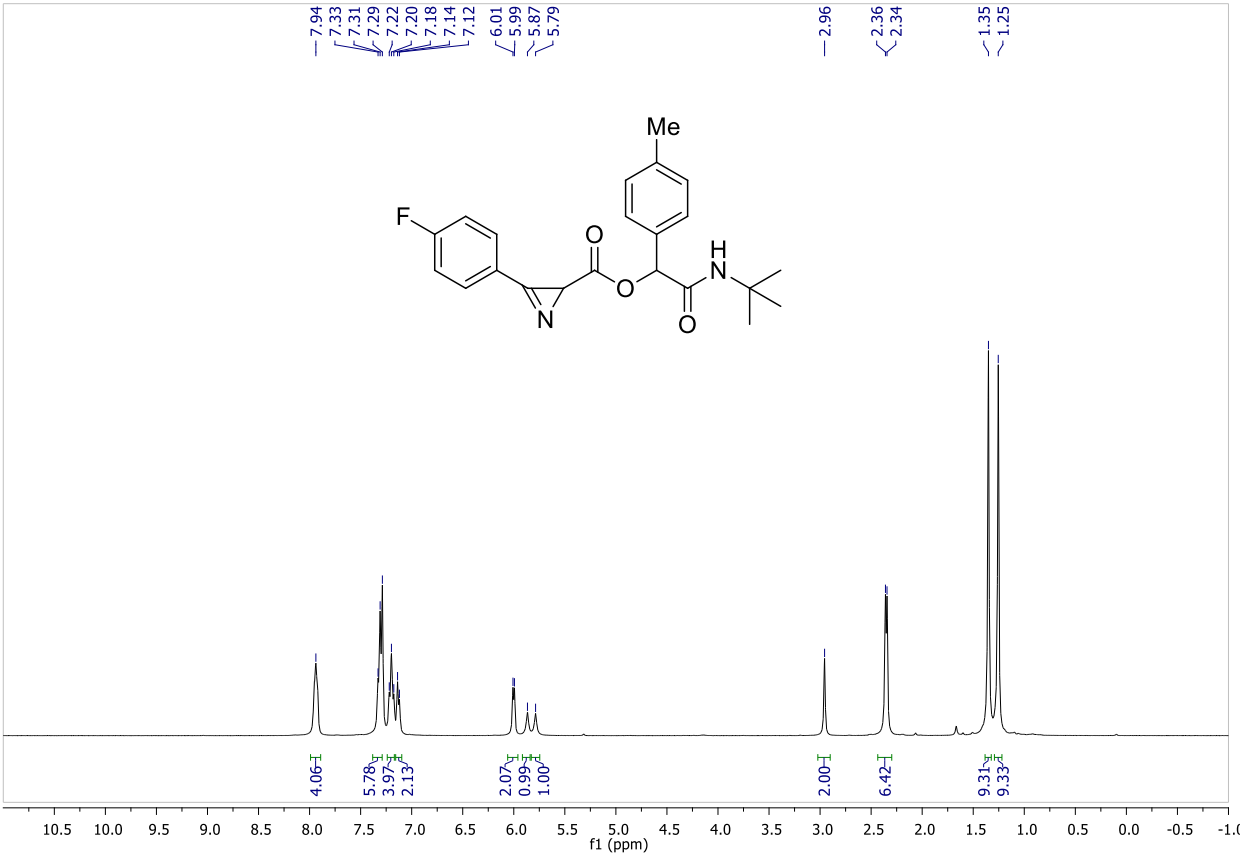
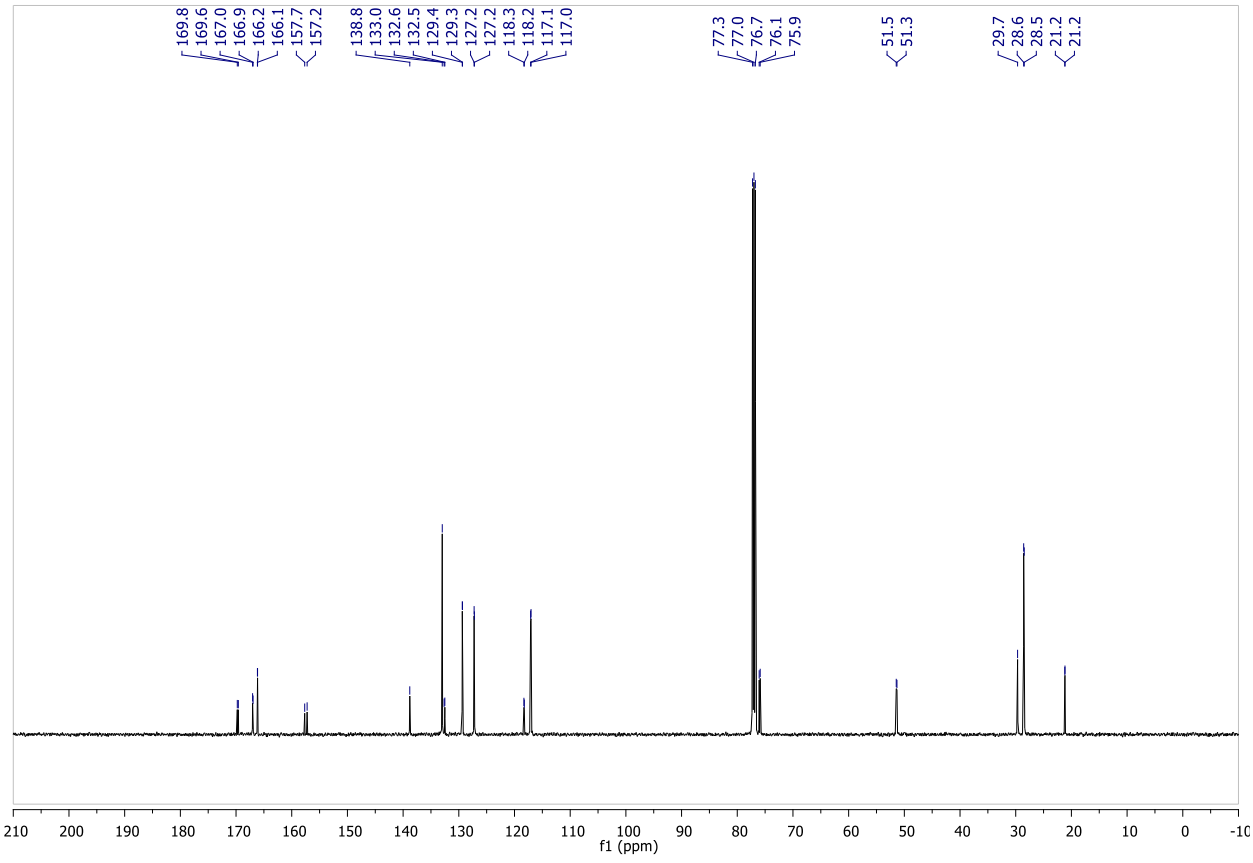
4. NMR spectra of new compounds

^{1}H and ^{13}C NMR spectra of compound **2a**

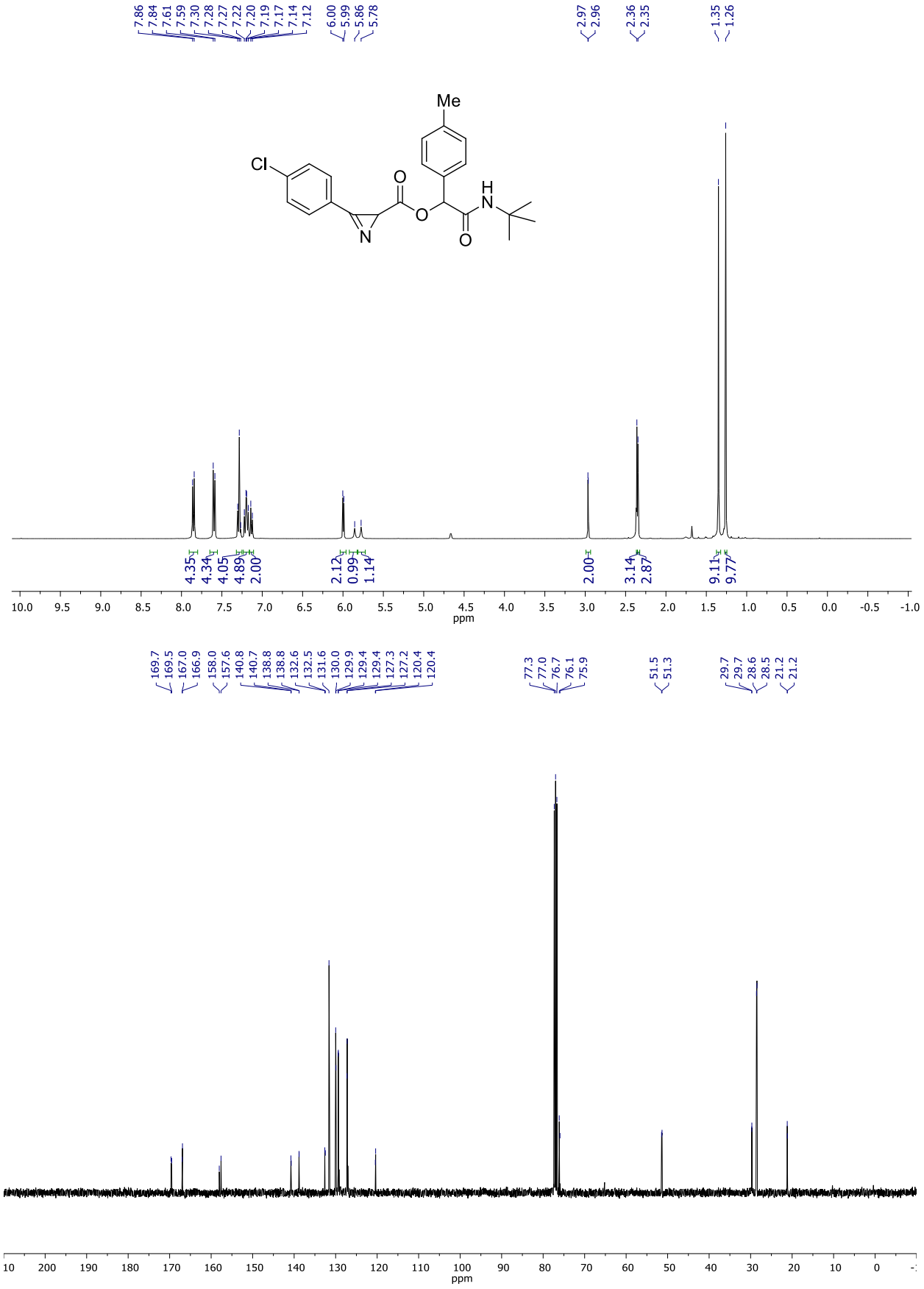


^{1}H and ^{13}C NMR spectra of compound **2b**

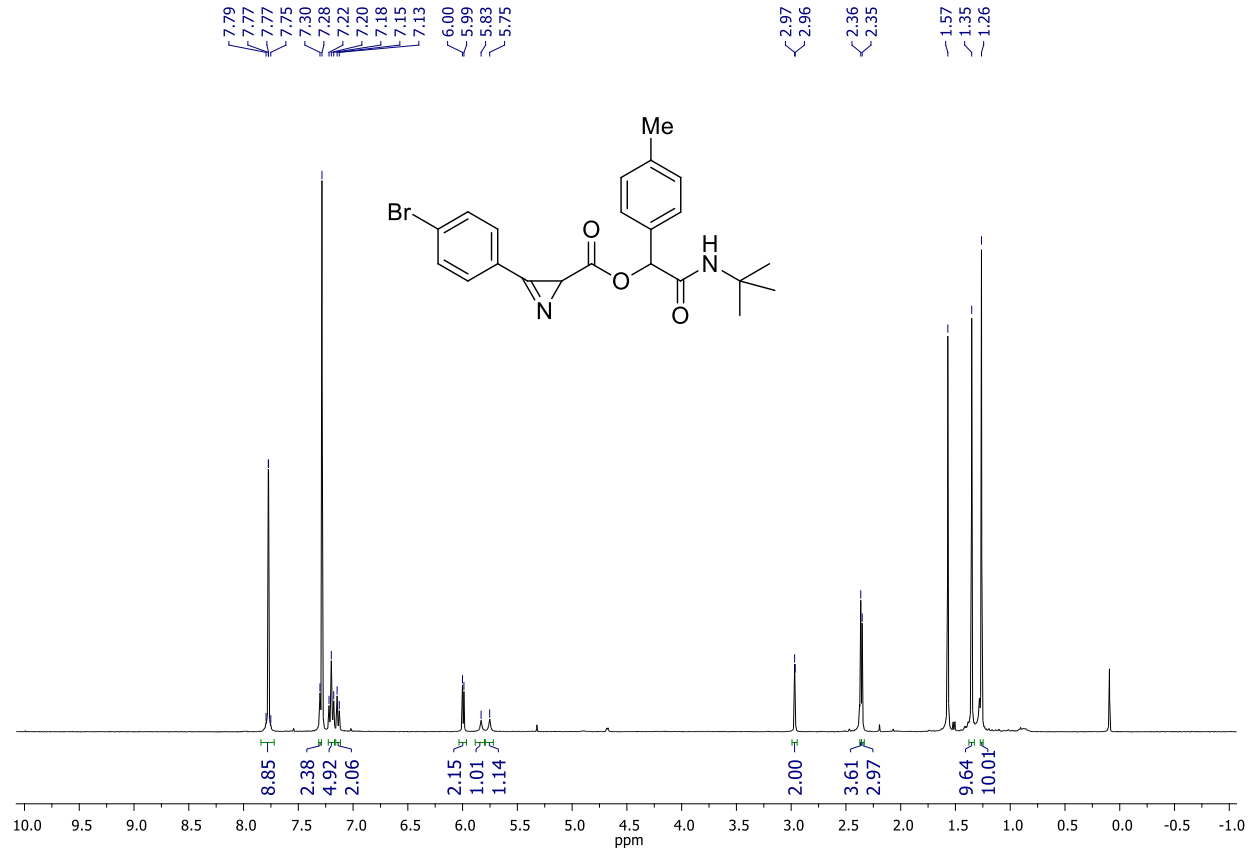


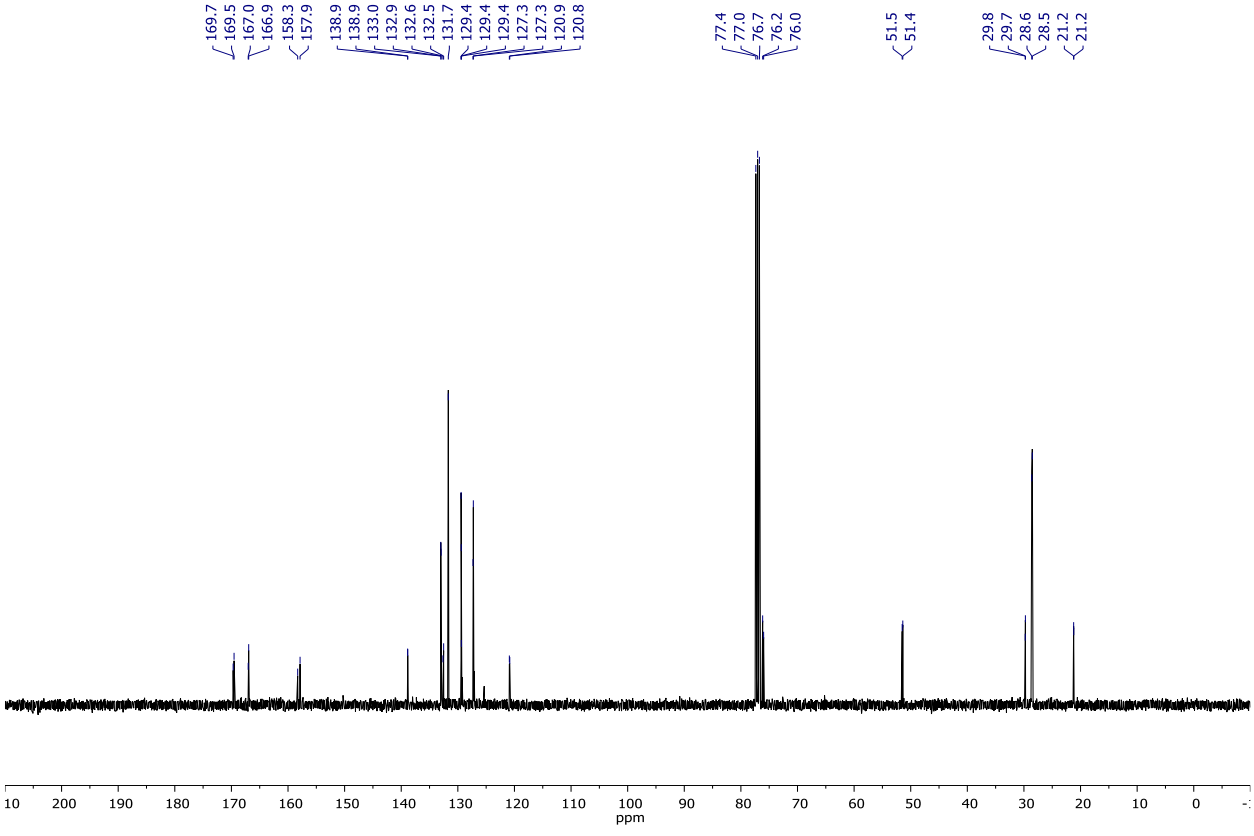


^{1}H and ^{13}C NMR spectra of compound **2c**

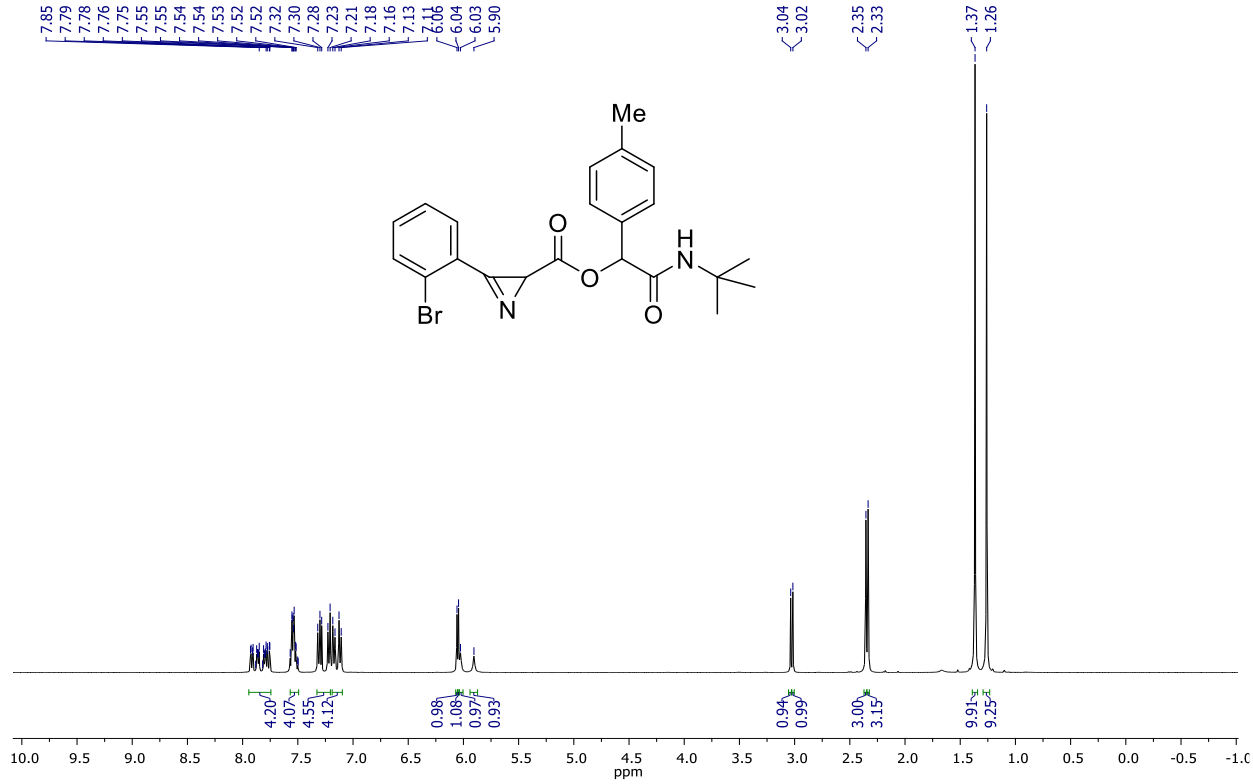


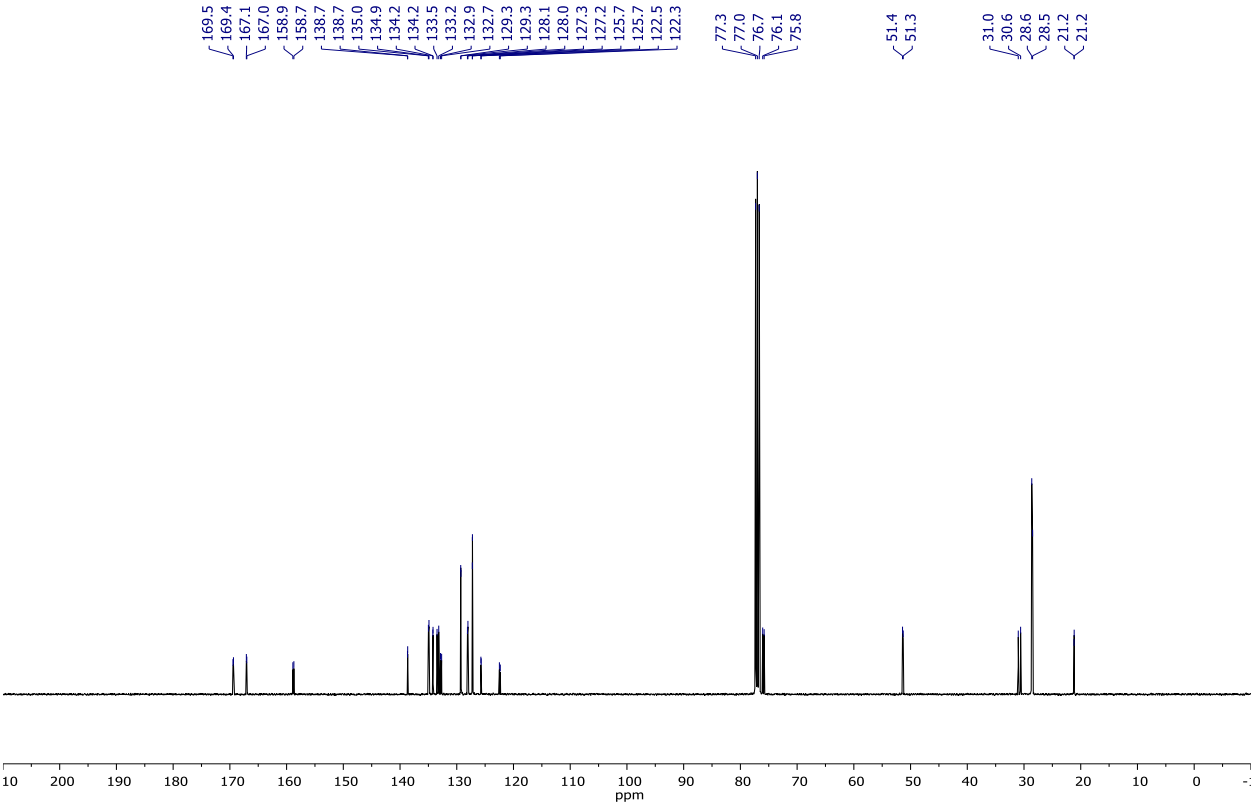
^{1}H and ^{13}C NMR spectra of compound **2d**



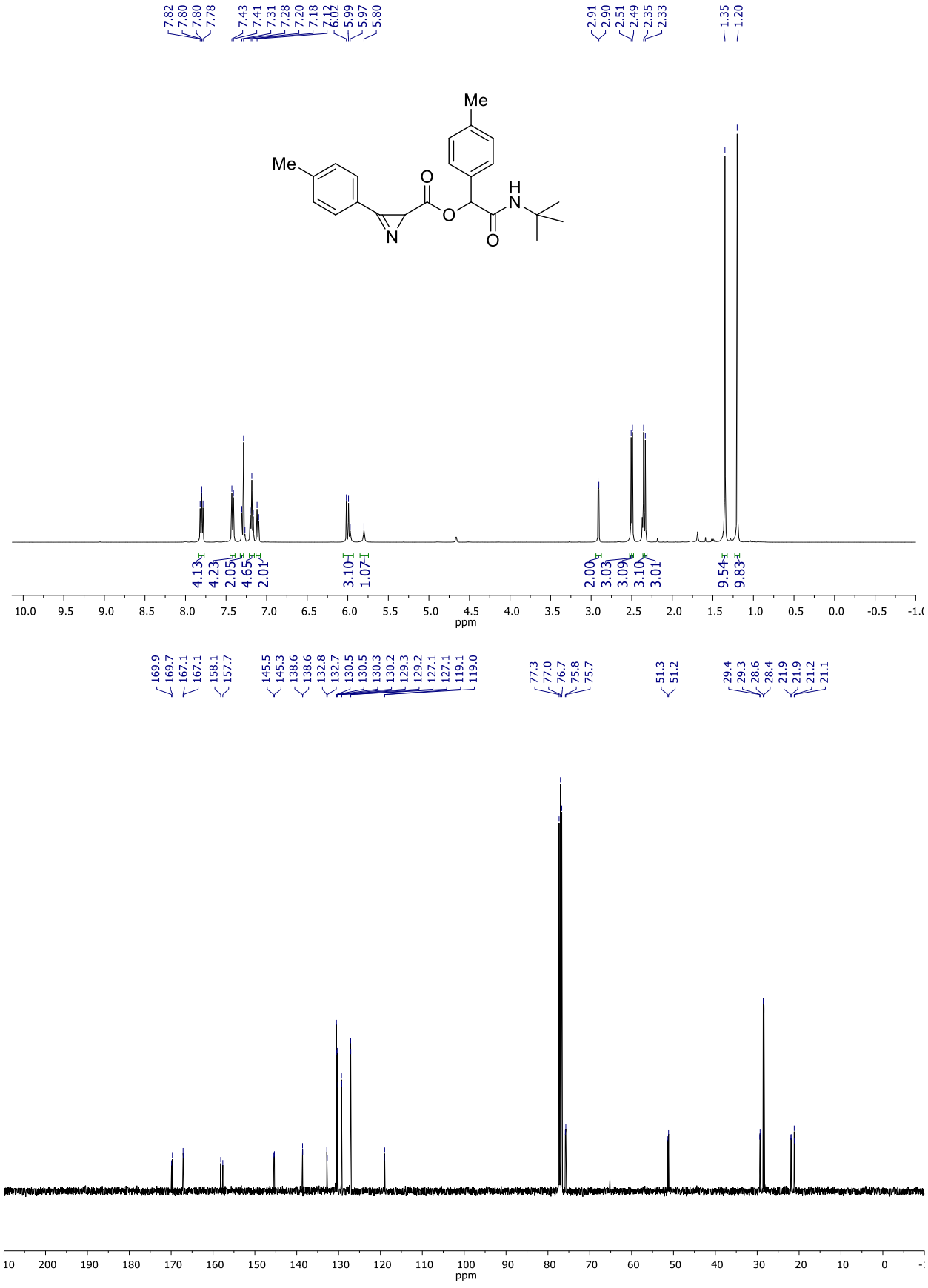


^{1}H and ^{13}C NMR spectra of compound **2e**

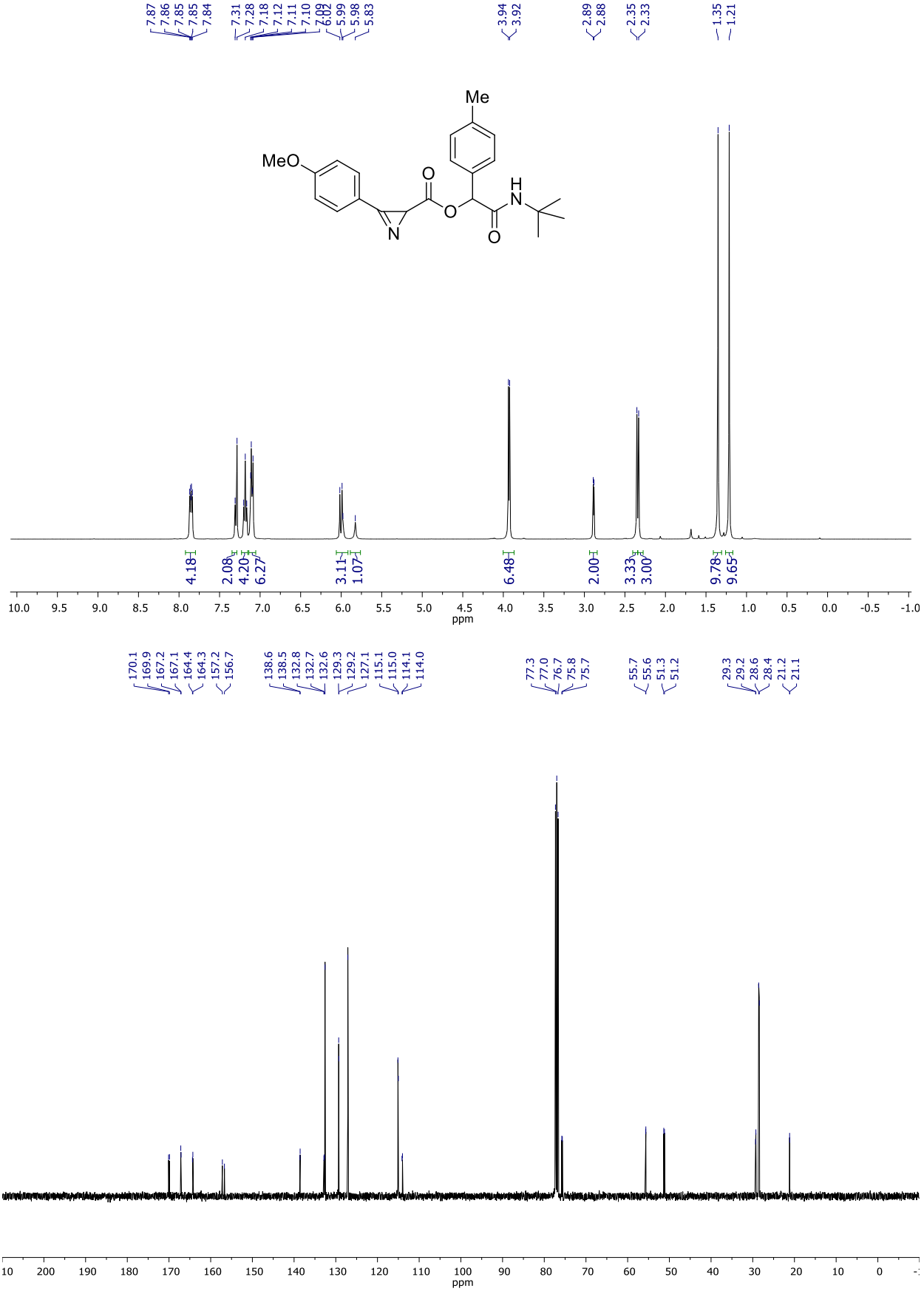




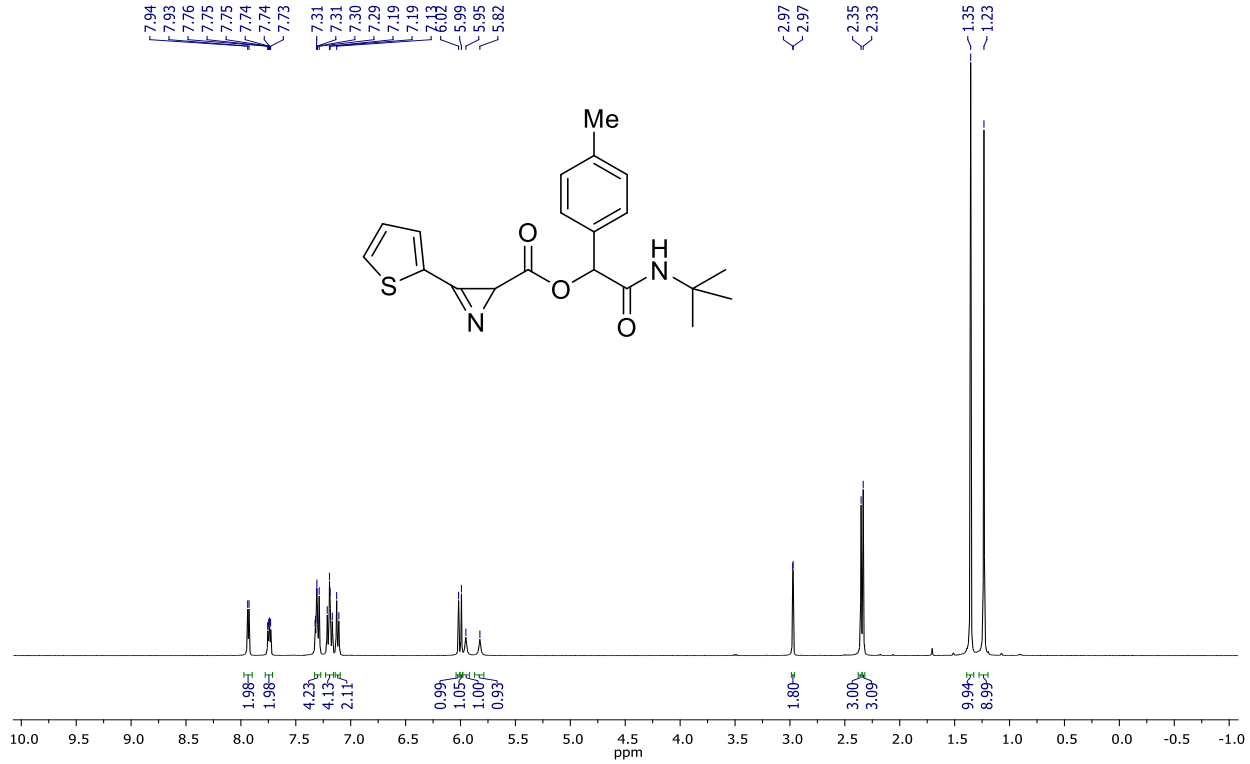
^{1}H and ^{13}C NMR spectra of compound **2f**

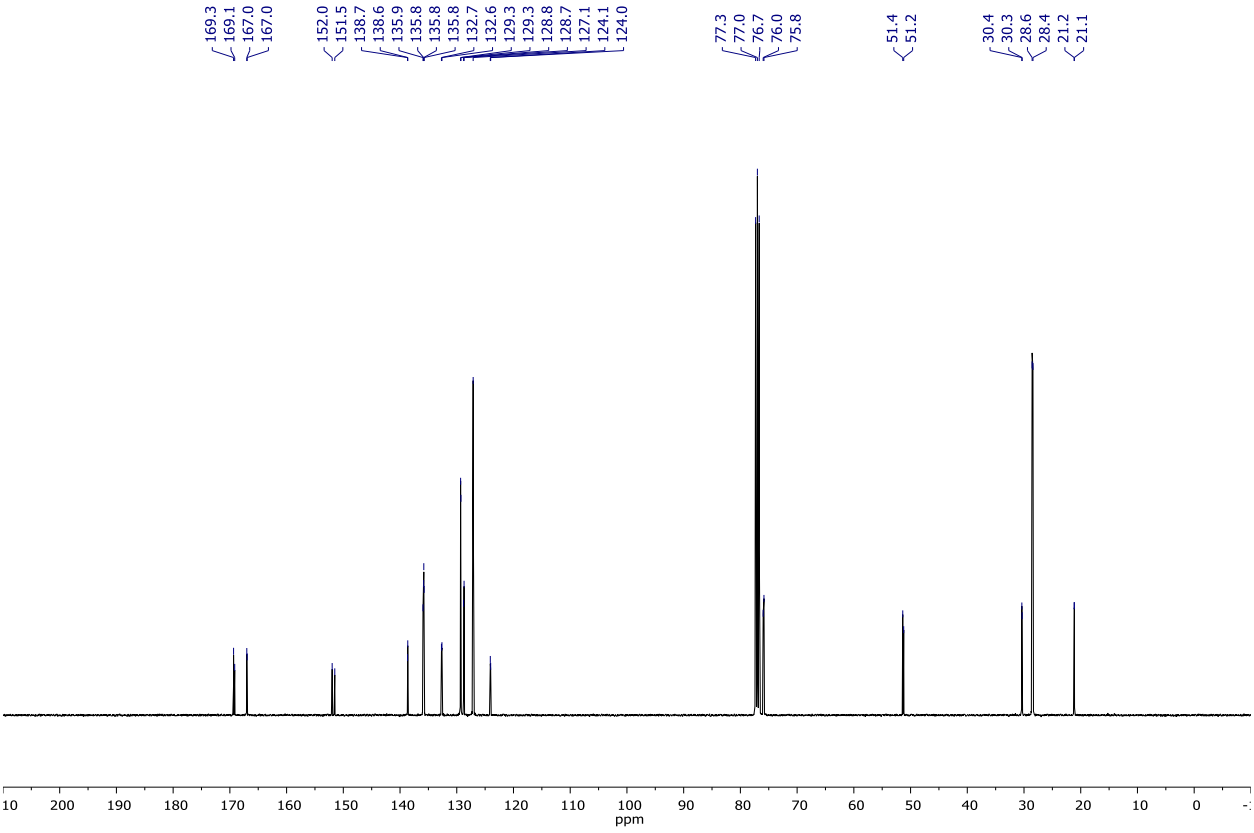


^{1}H and ^{13}C NMR spectra of compound **2g**

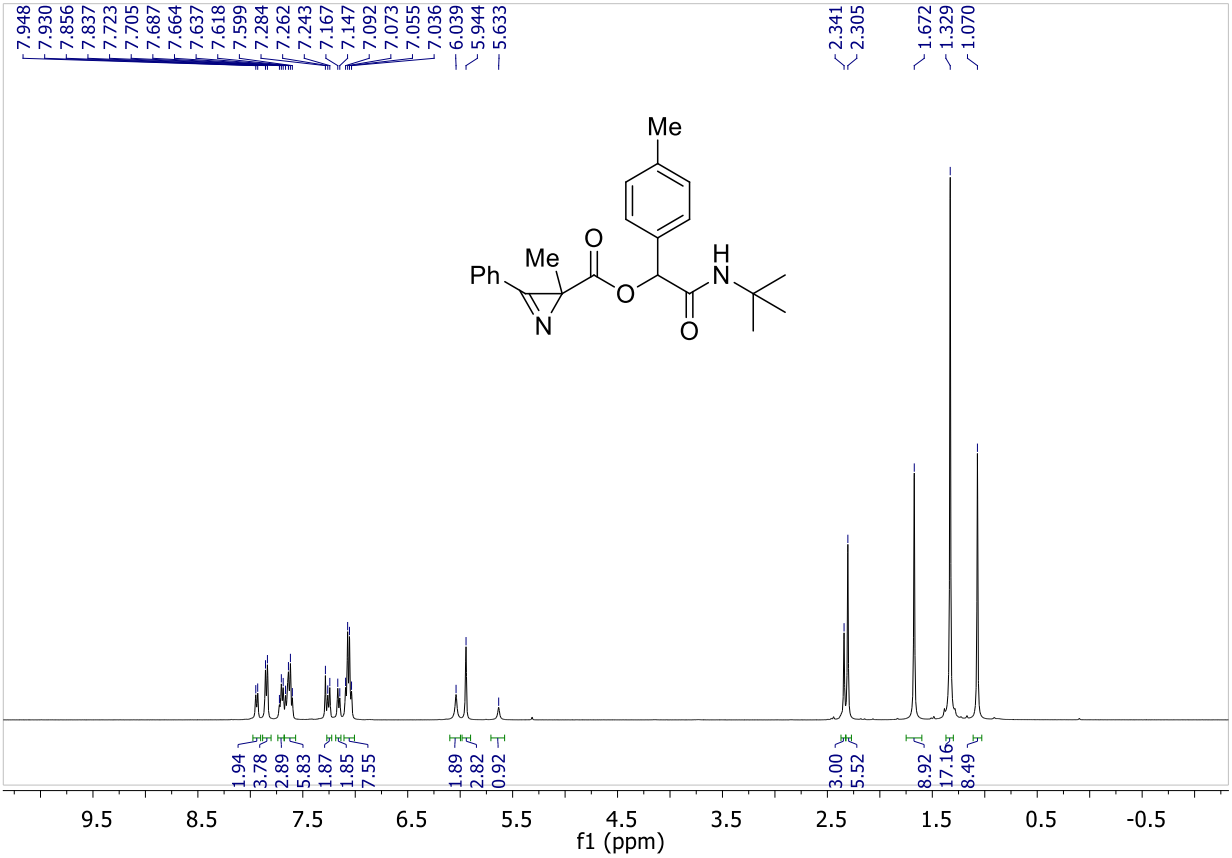


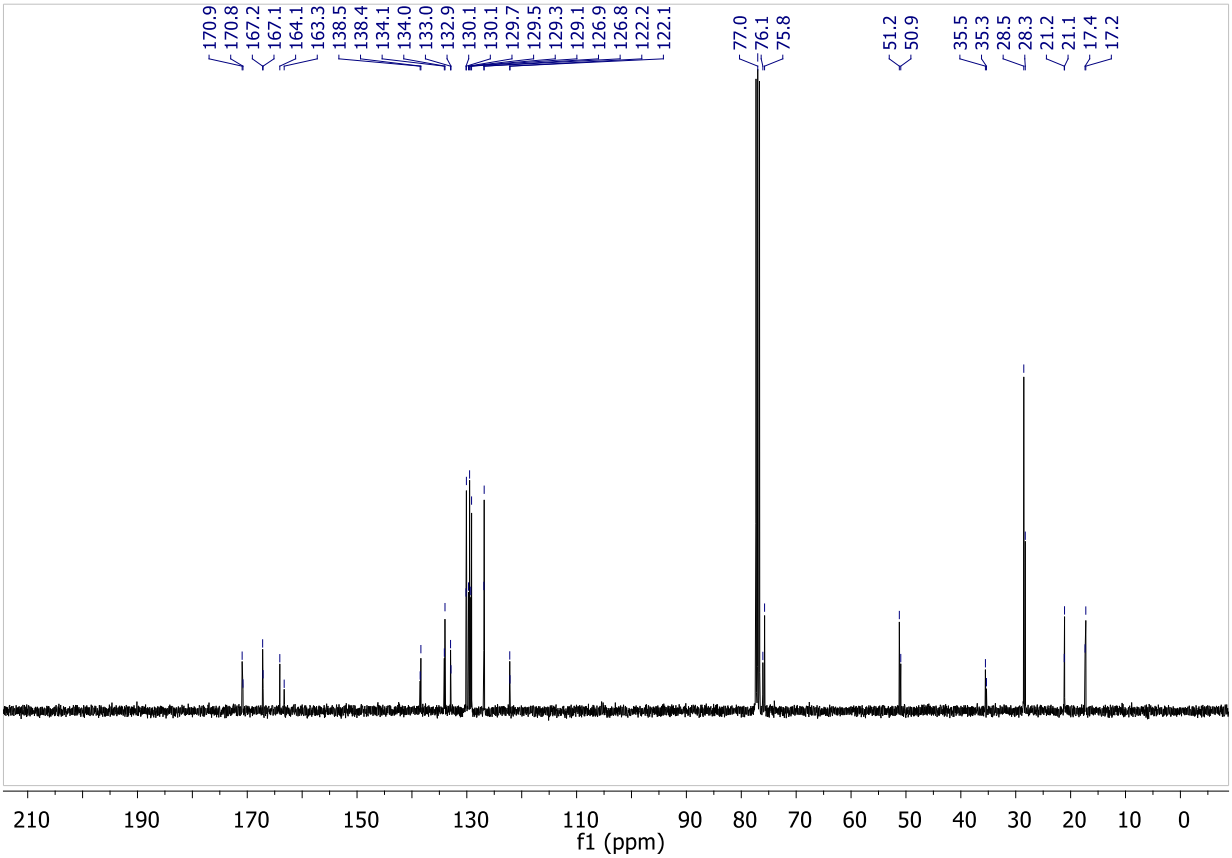
^{1}H and ^{13}C NMR spectra of compound **2h**



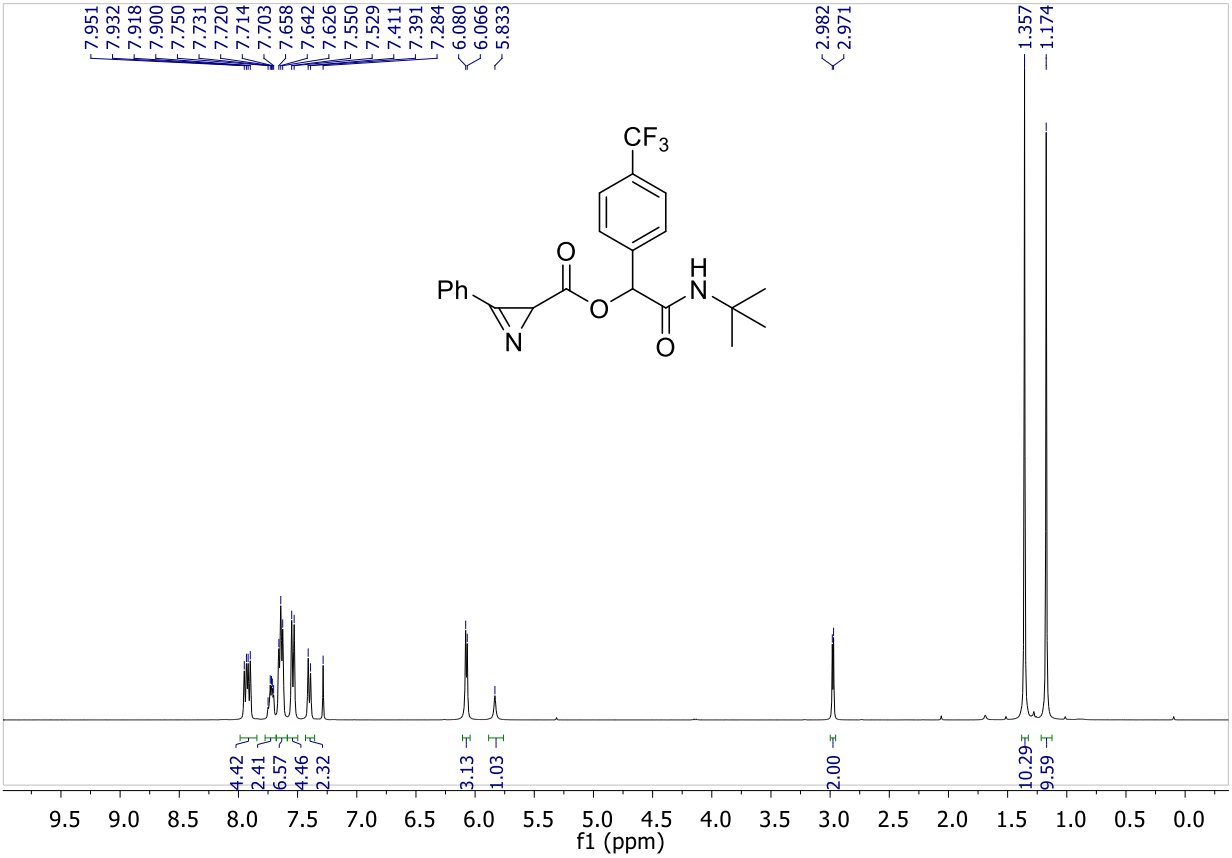


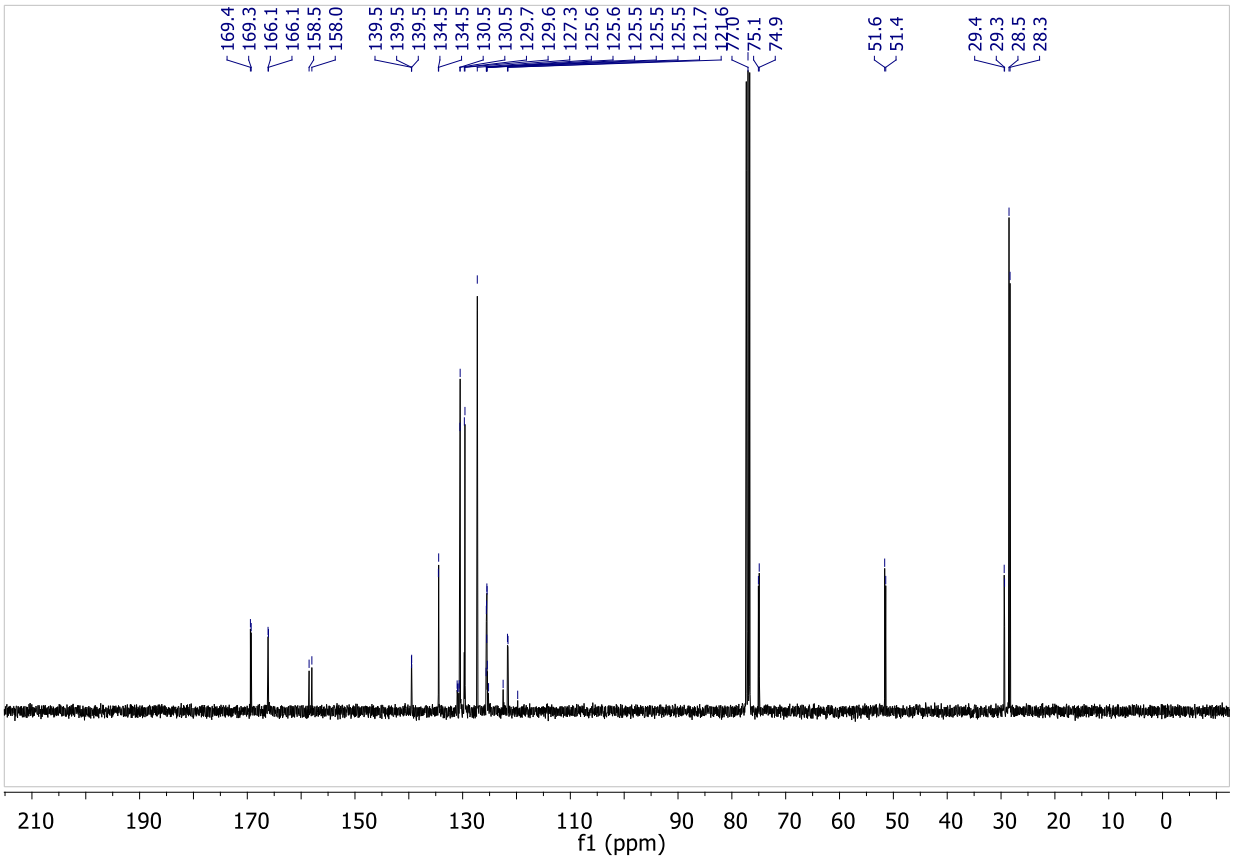
^{1}H and ^{13}C NMR spectra of compound **2i**



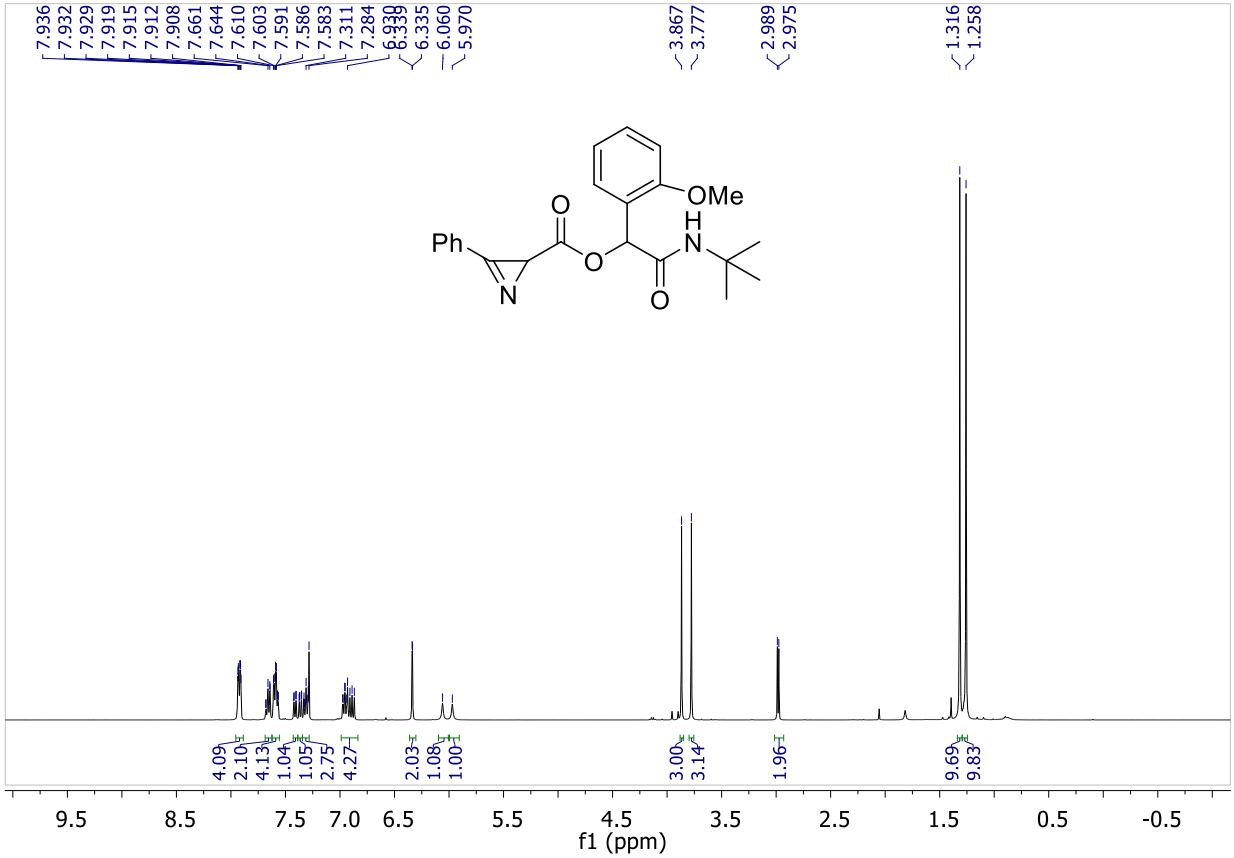


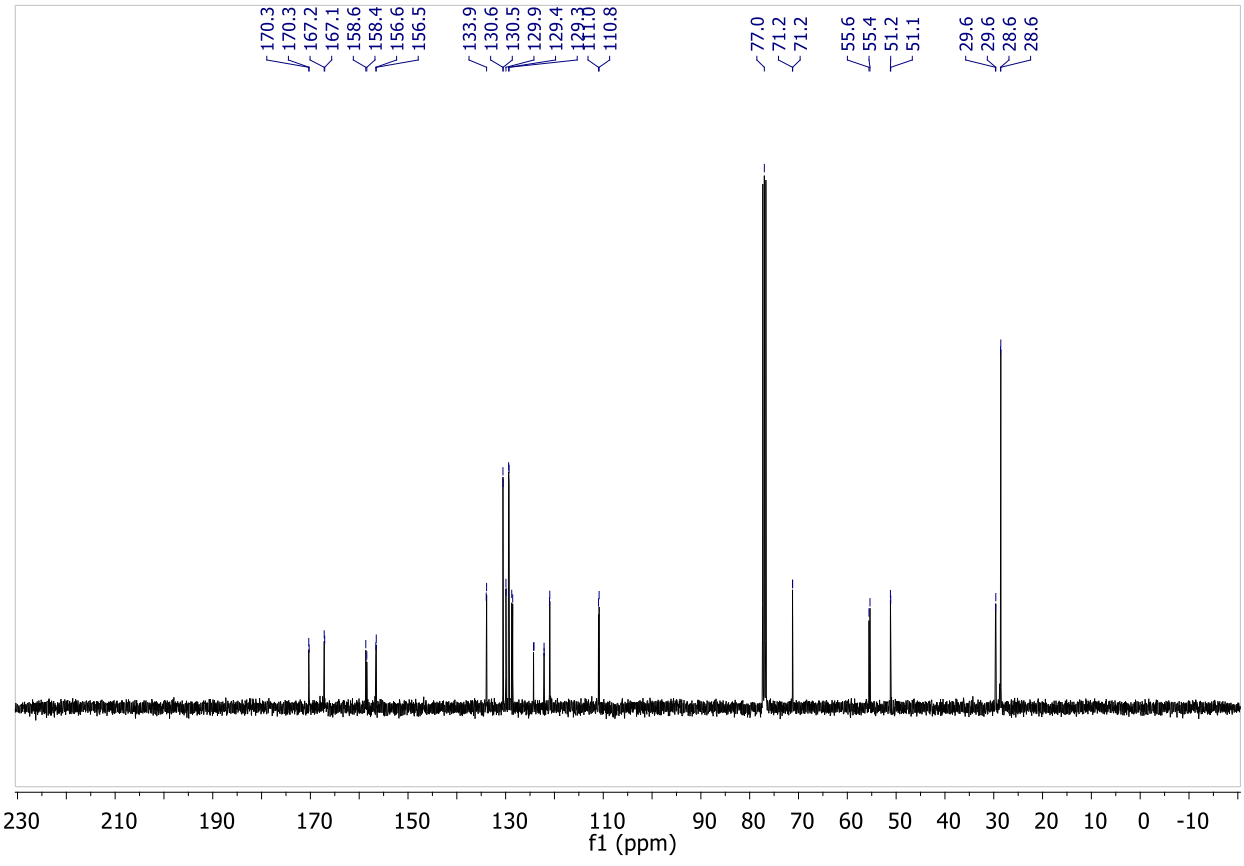
^{1}H and ^{13}C NMR spectra of compound **2j**



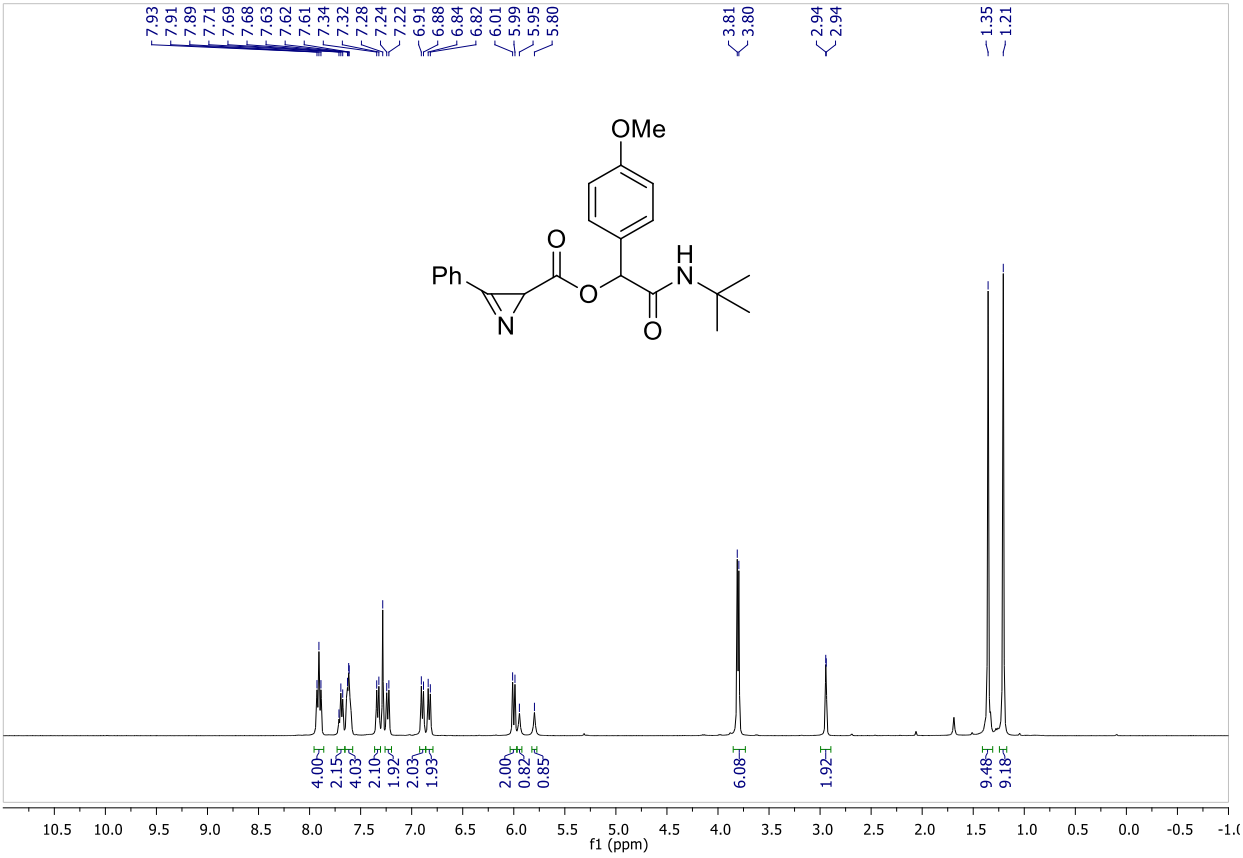


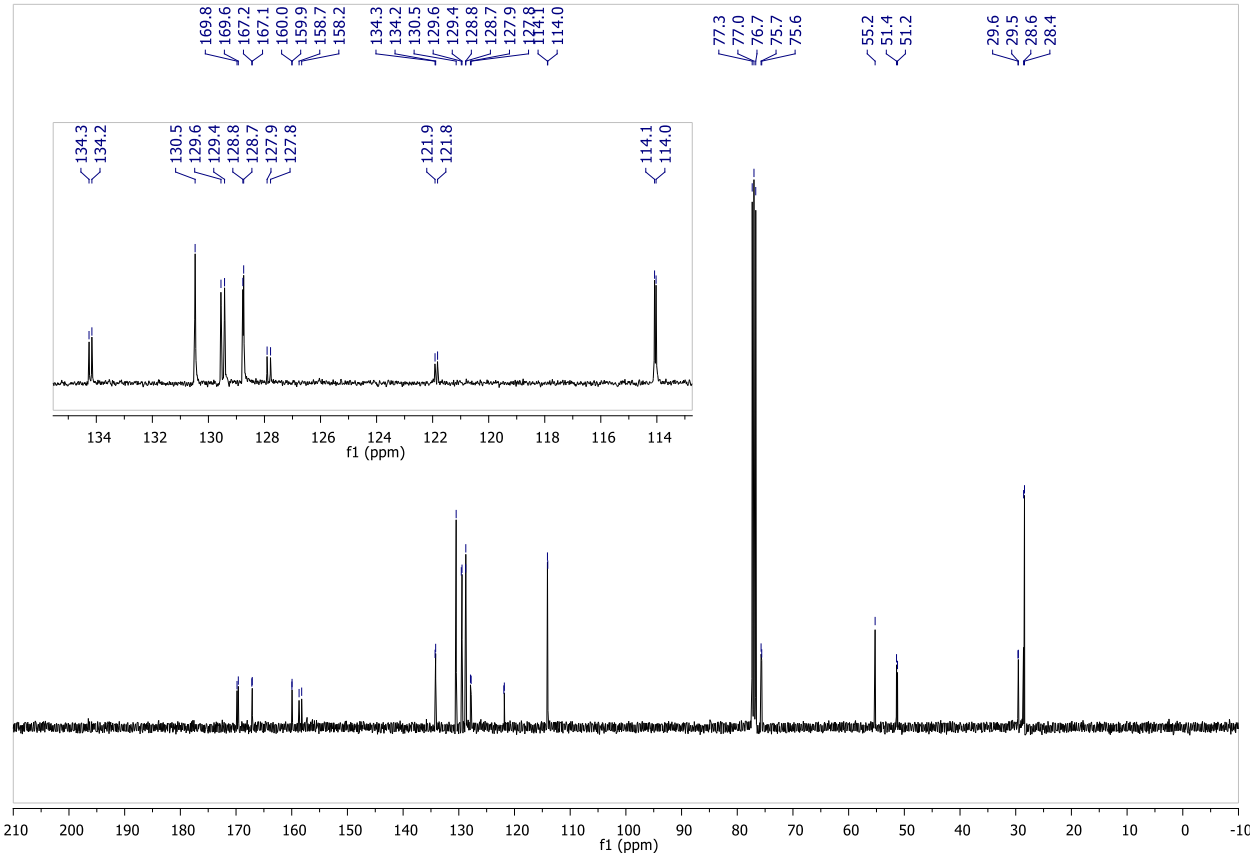
^{1}H and ^{13}C NMR spectra of compound **2k**



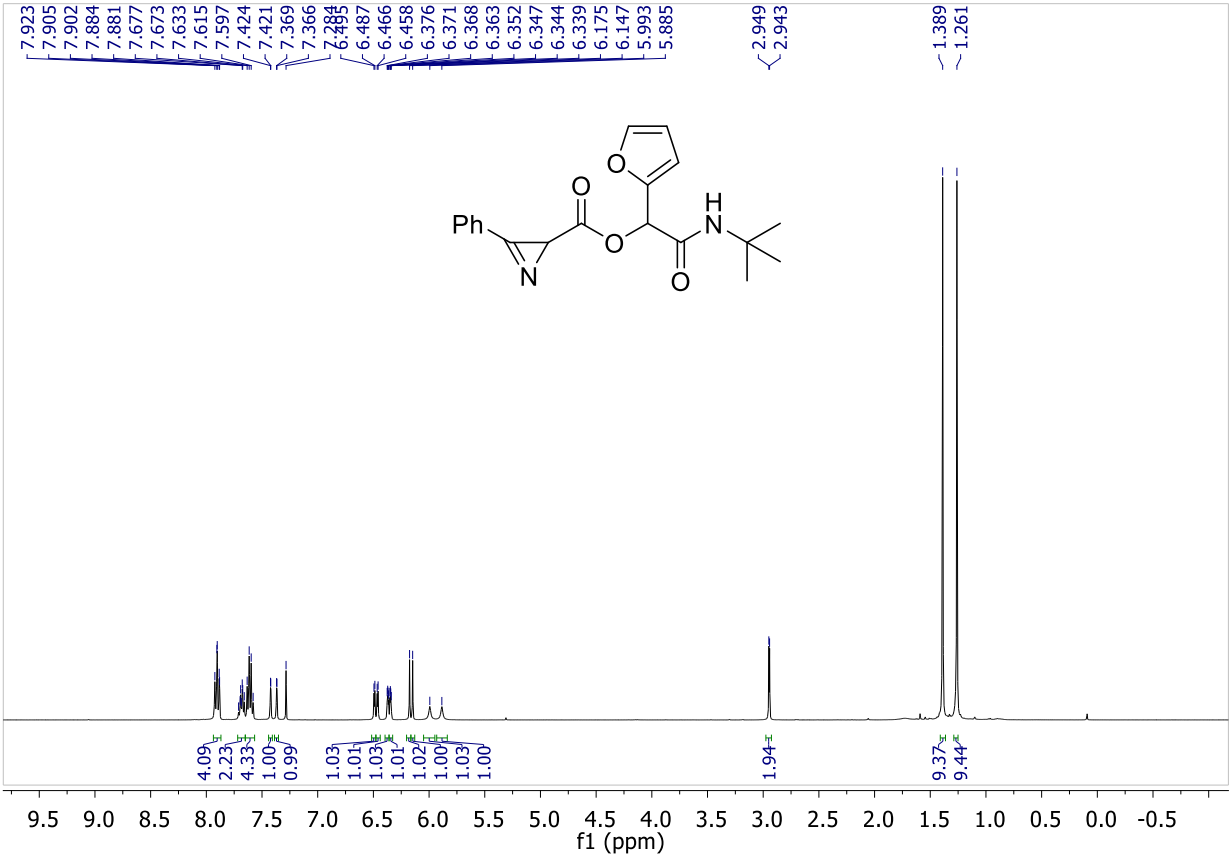


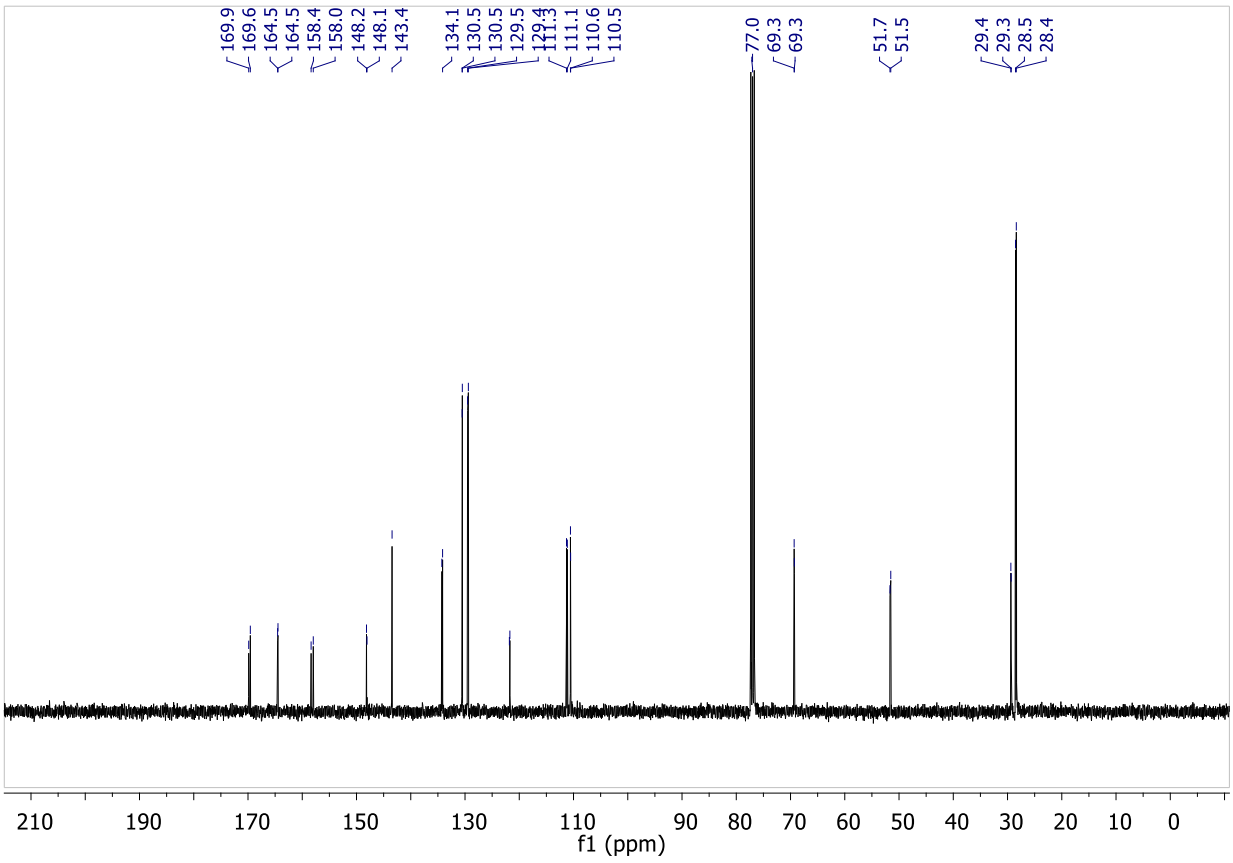
^{1}H and ^{13}C NMR spectra of compound **2l**



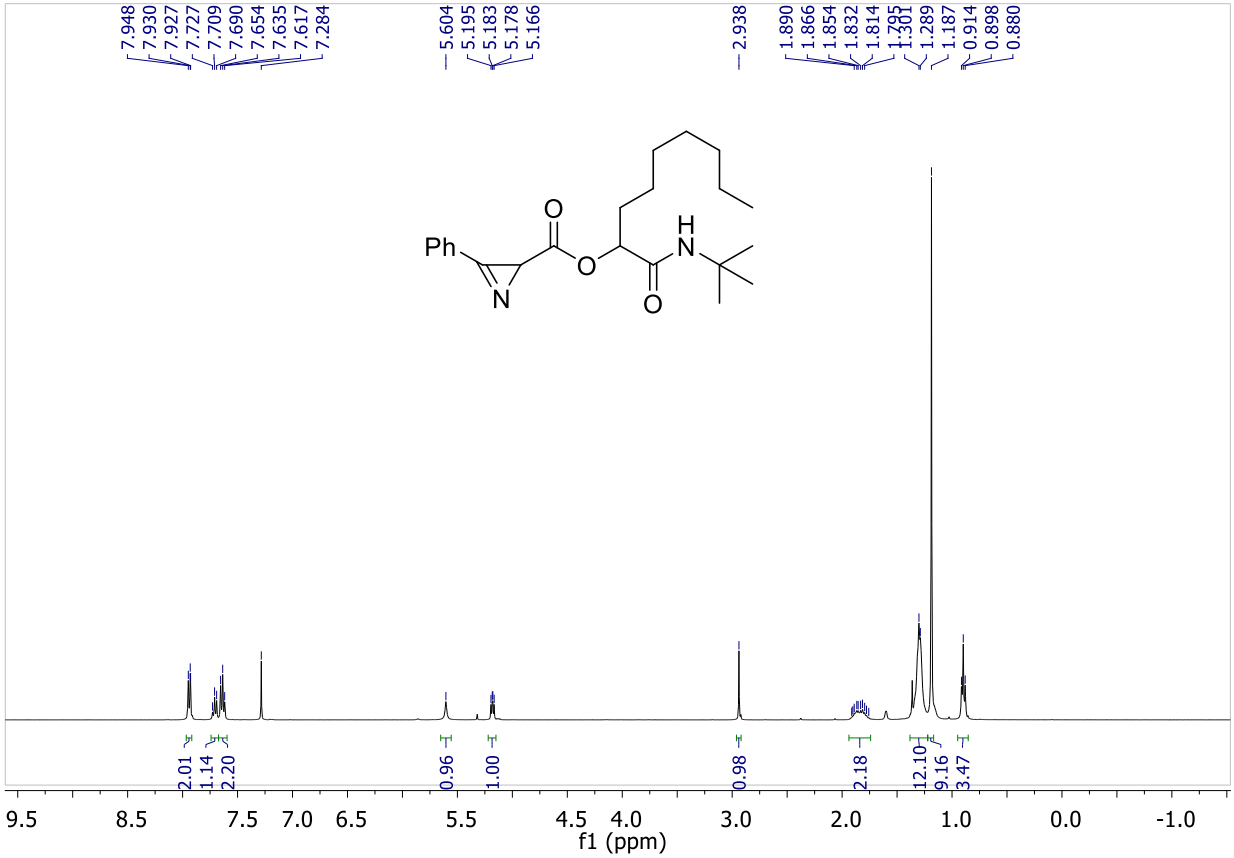


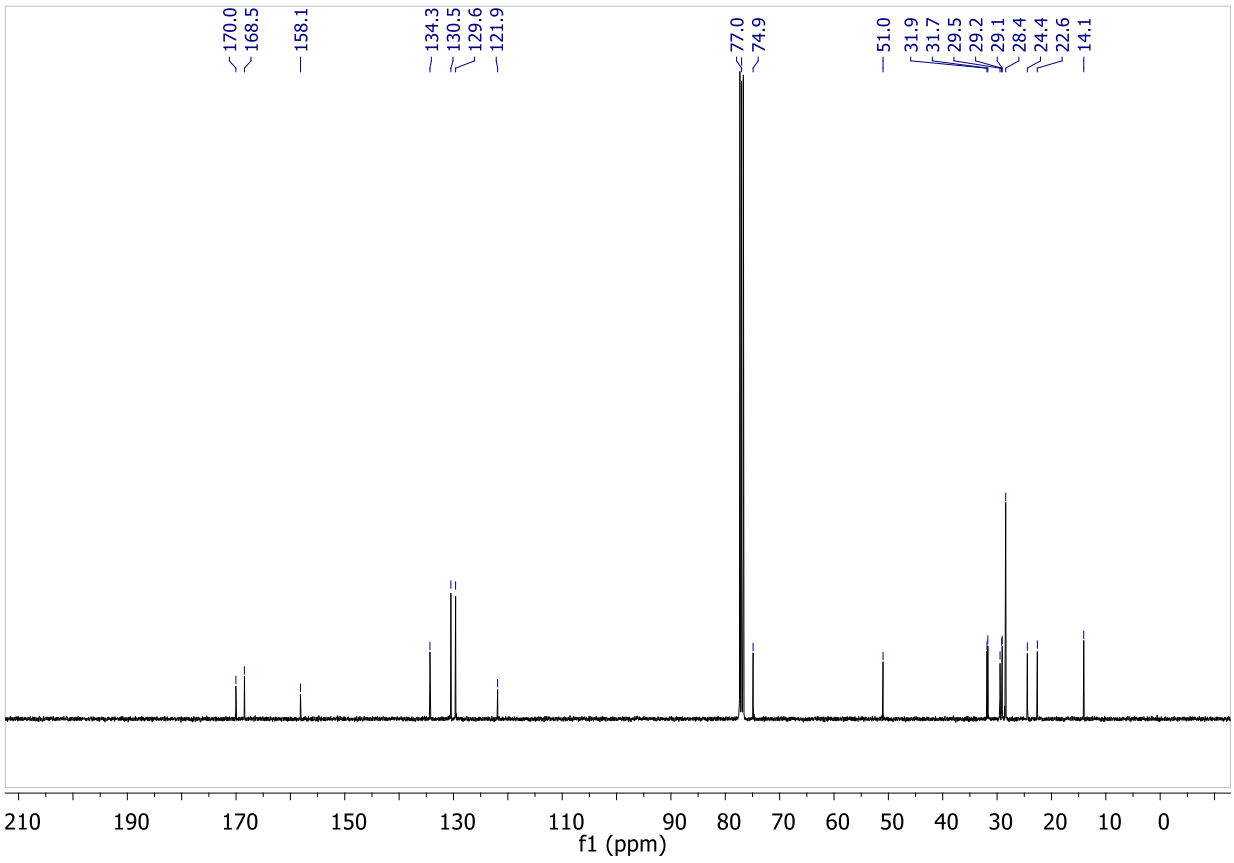
^{1}H and ^{13}C NMR spectra of compound **2m**



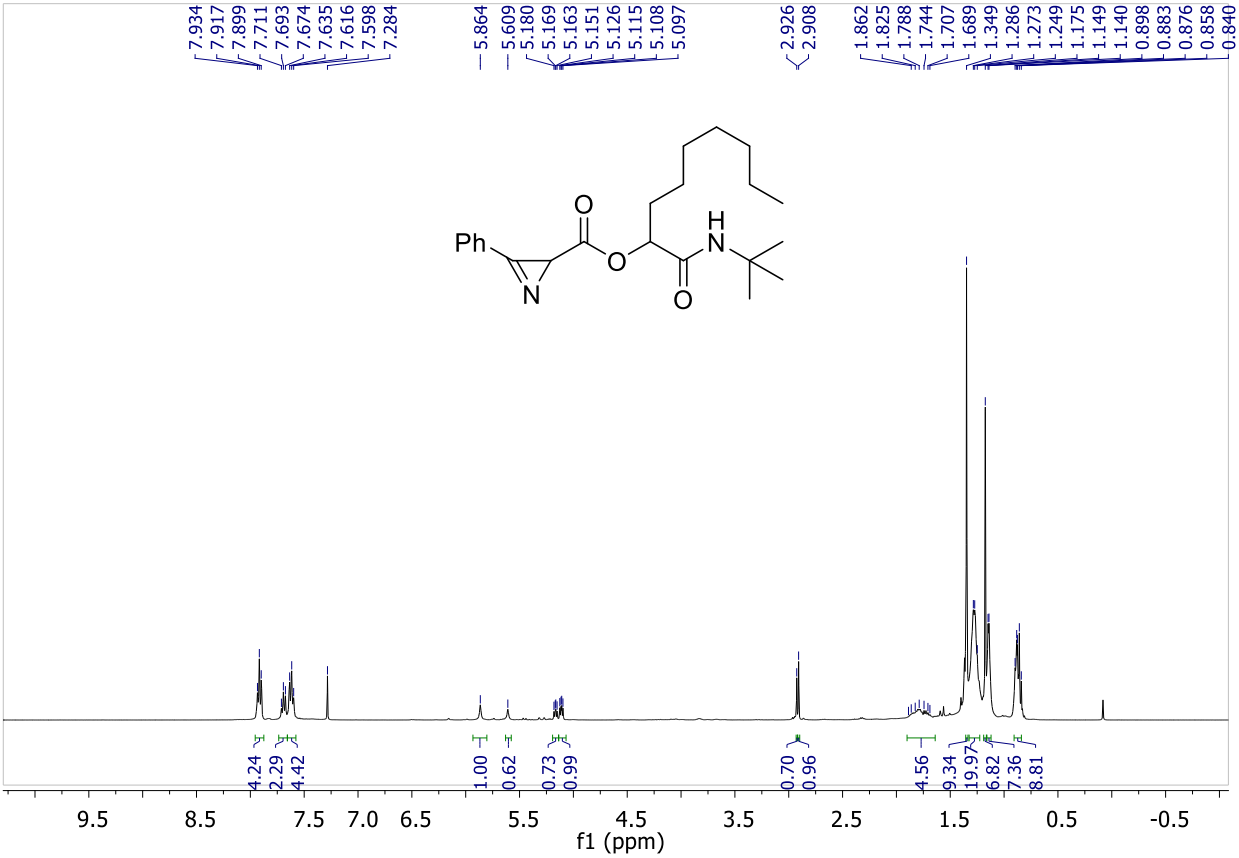


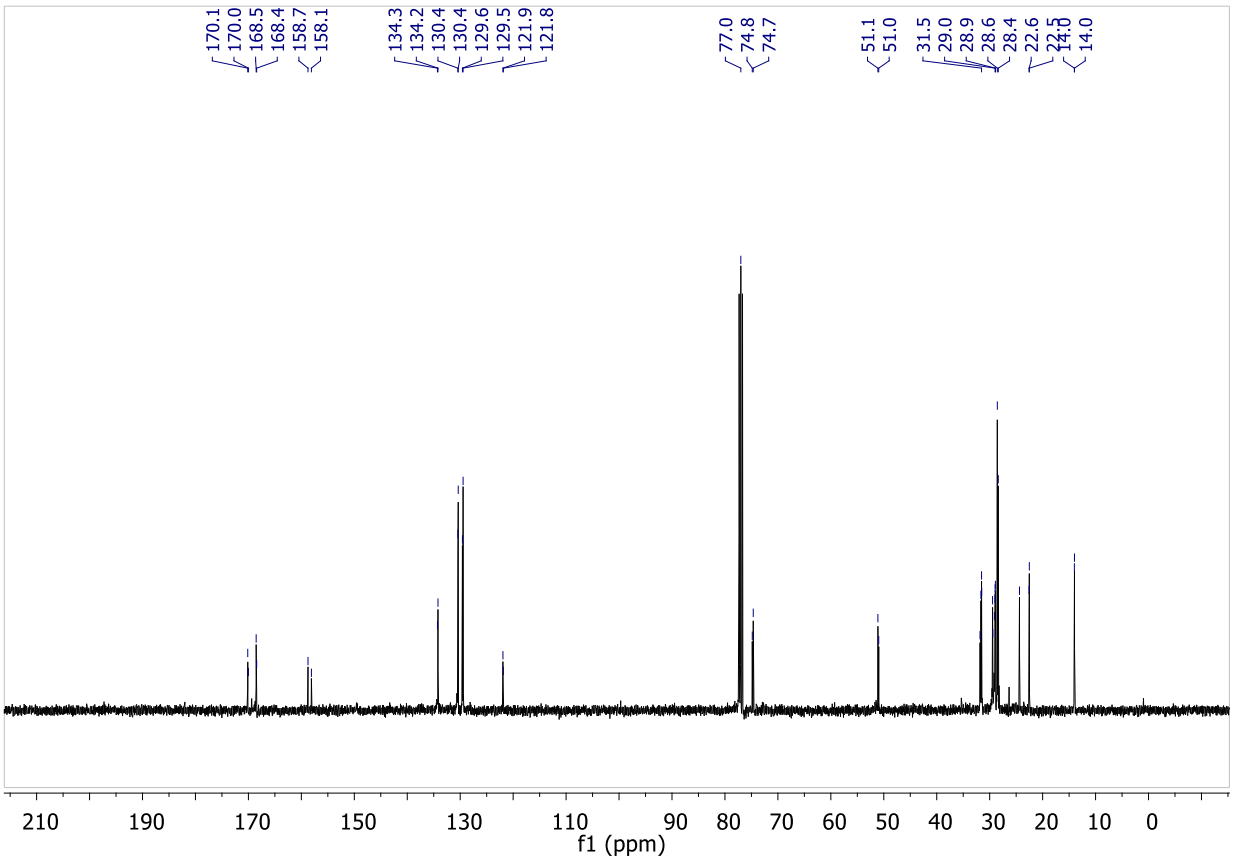
^{1}H and ^{13}C NMR spectra of compound **2n** (separated diastereomer)



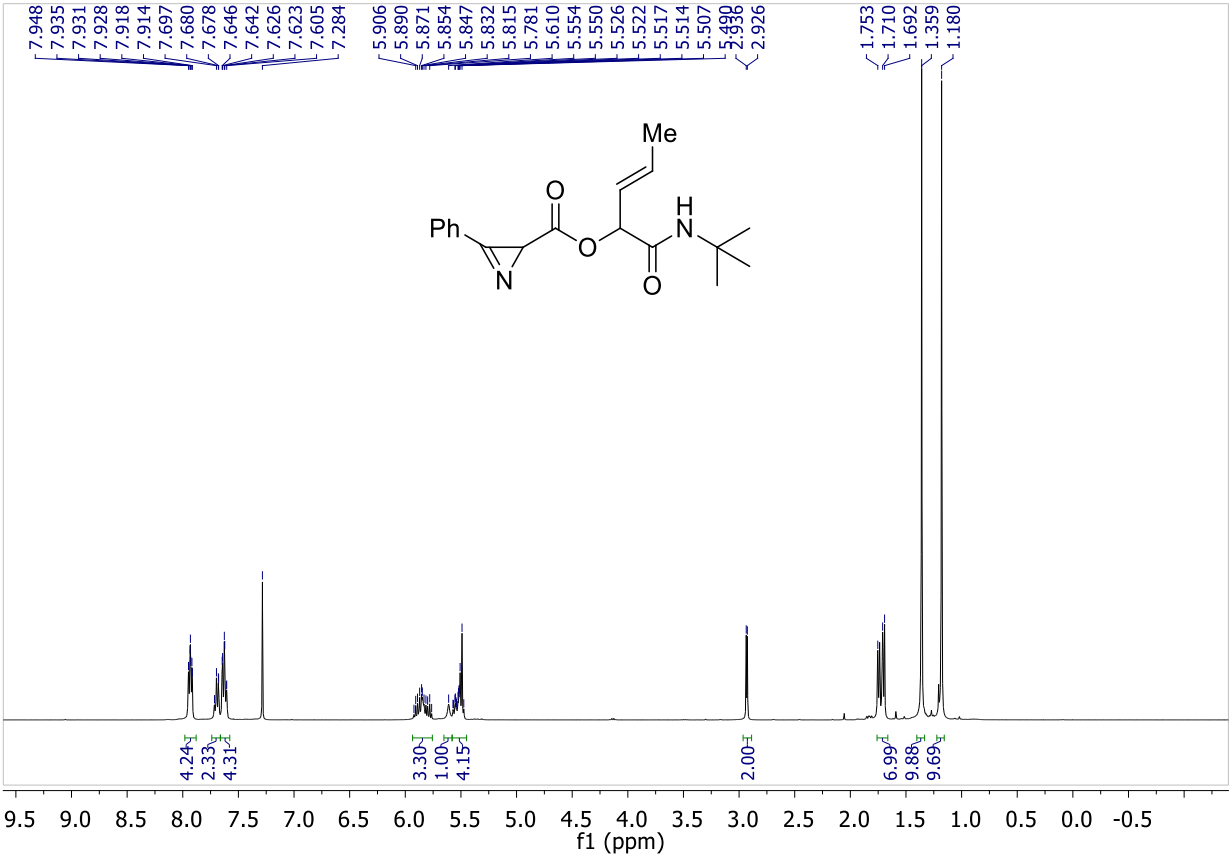


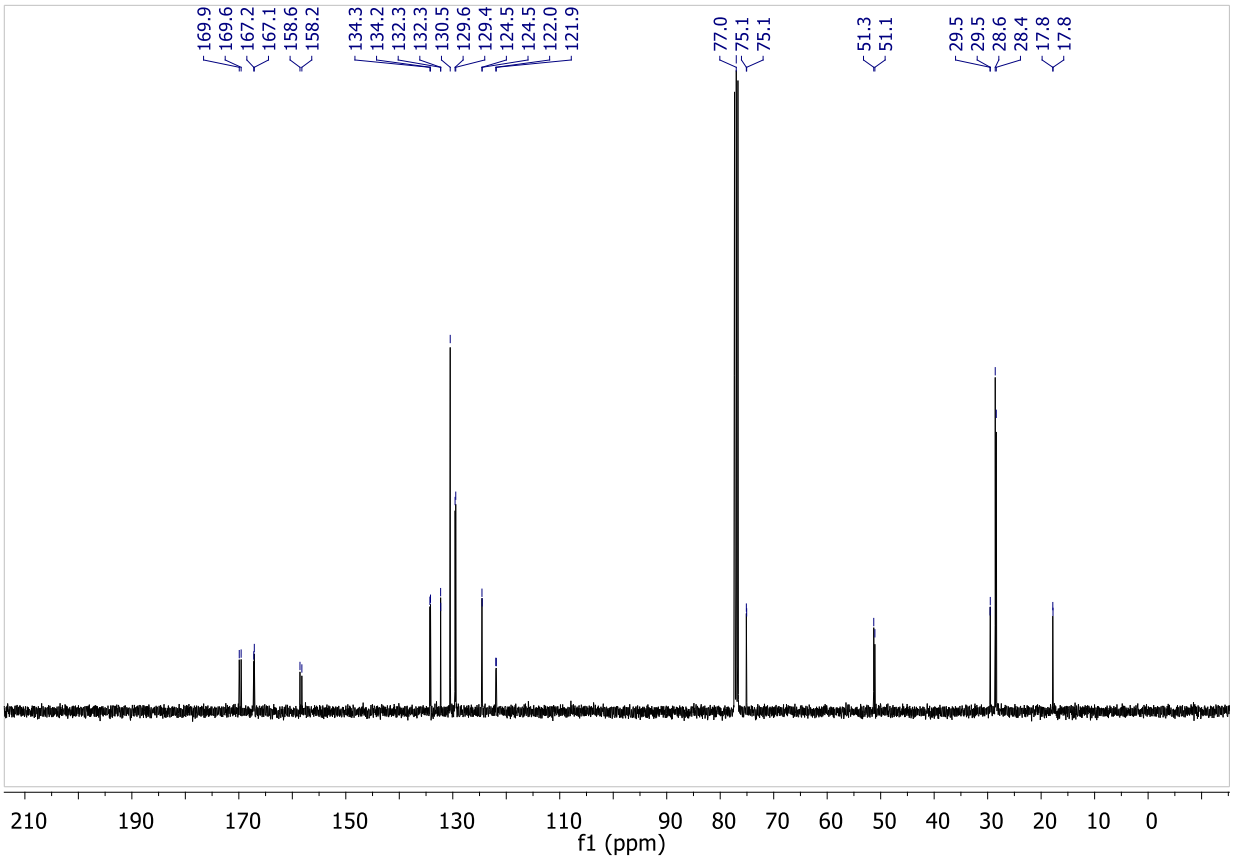
^{1}H and ^{13}C NMR spectra of compound **2n** (mixture of diastereomers)



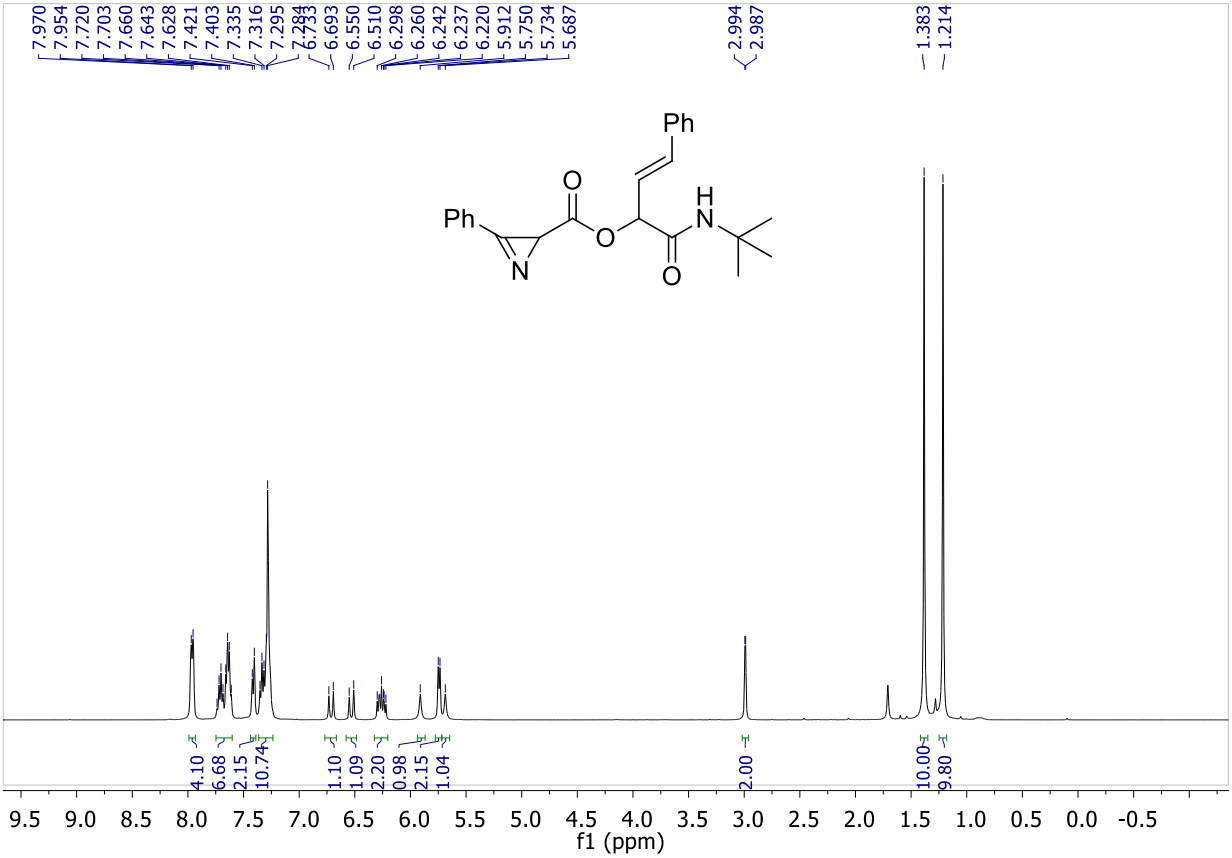


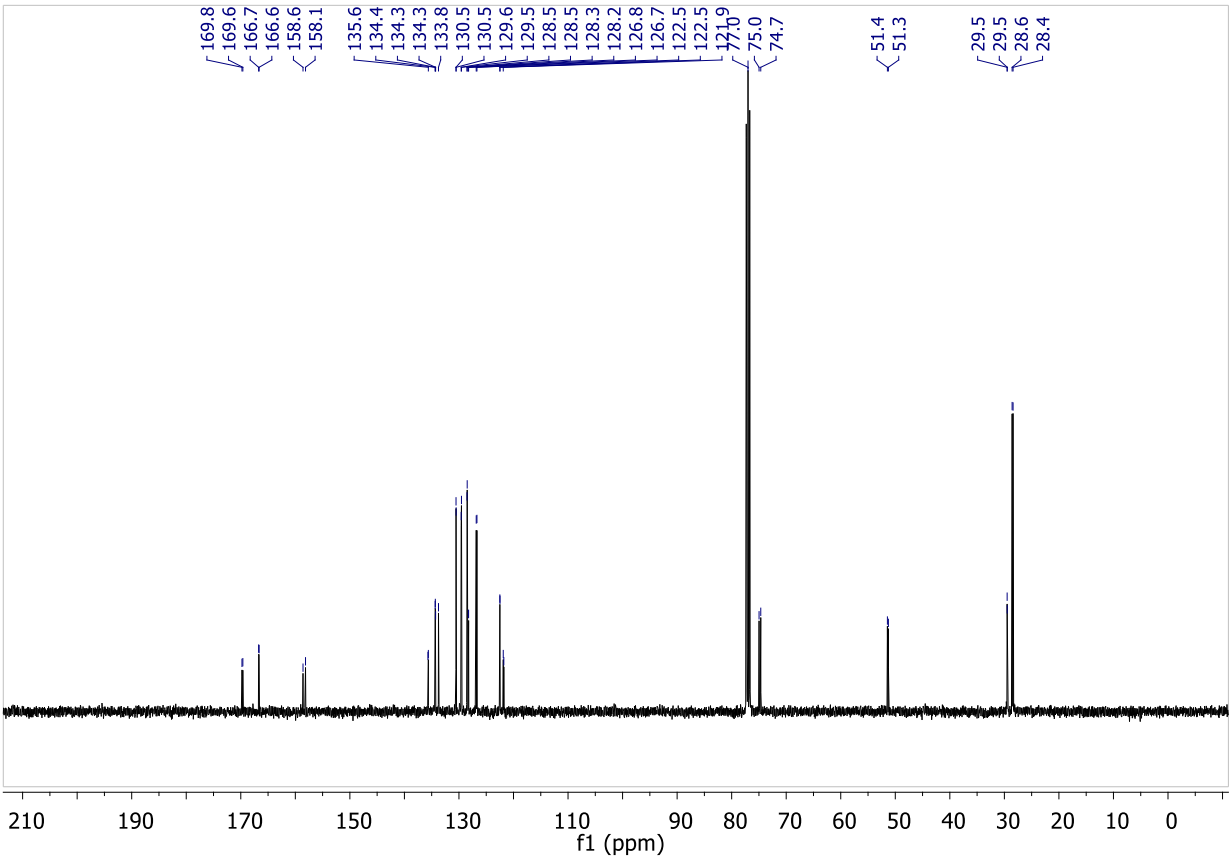
^{1}H and ^{13}C NMR spectra of compound **2o**



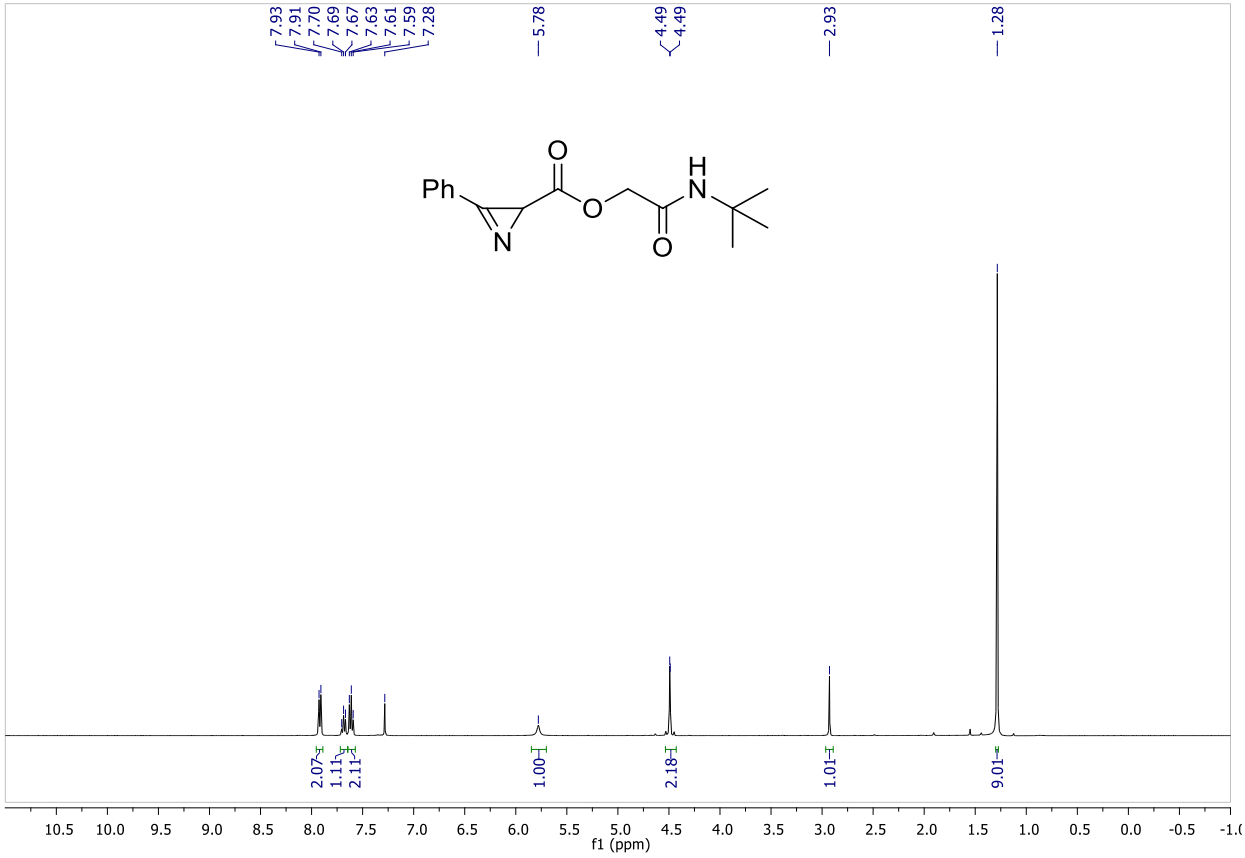


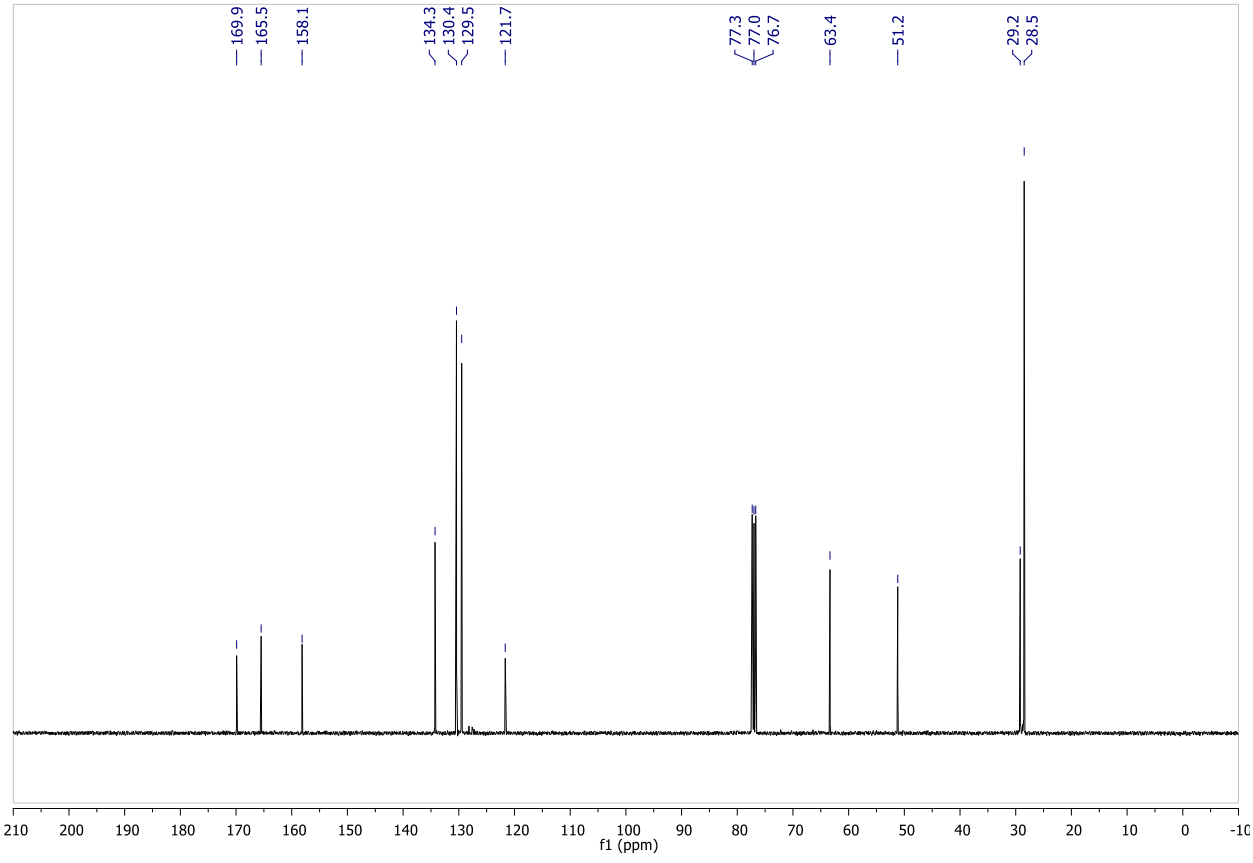
^{1}H and ^{13}C NMR spectra of compound **2p**



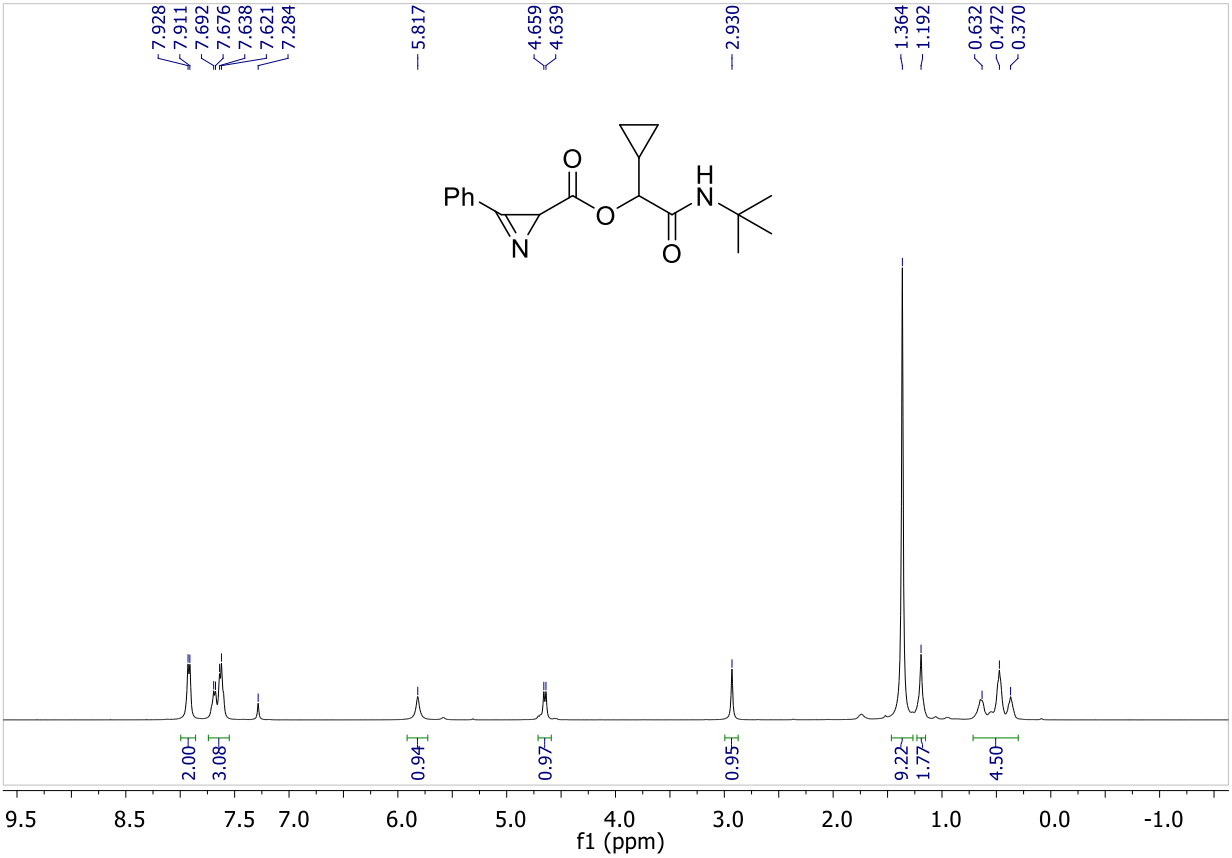


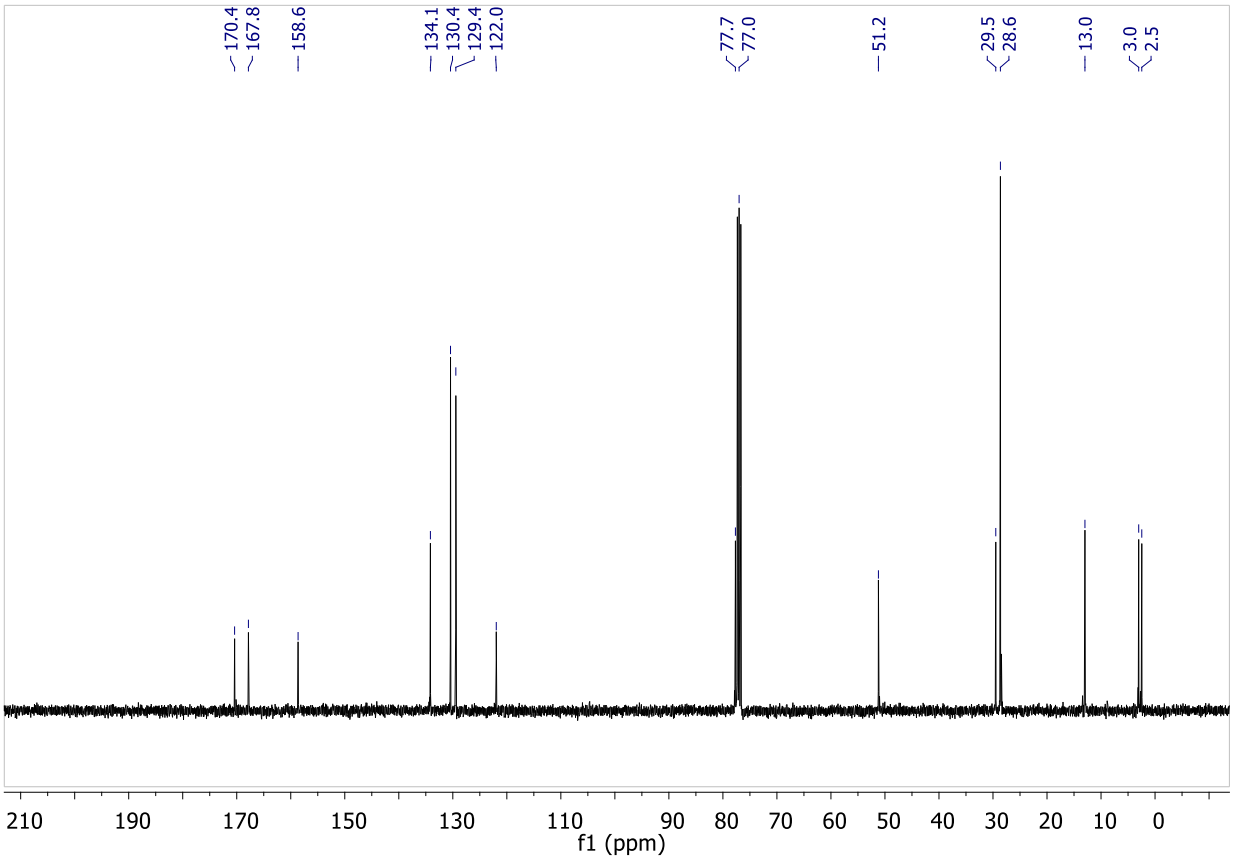
^{1}H and ^{13}C NMR spectra of compound **2q**



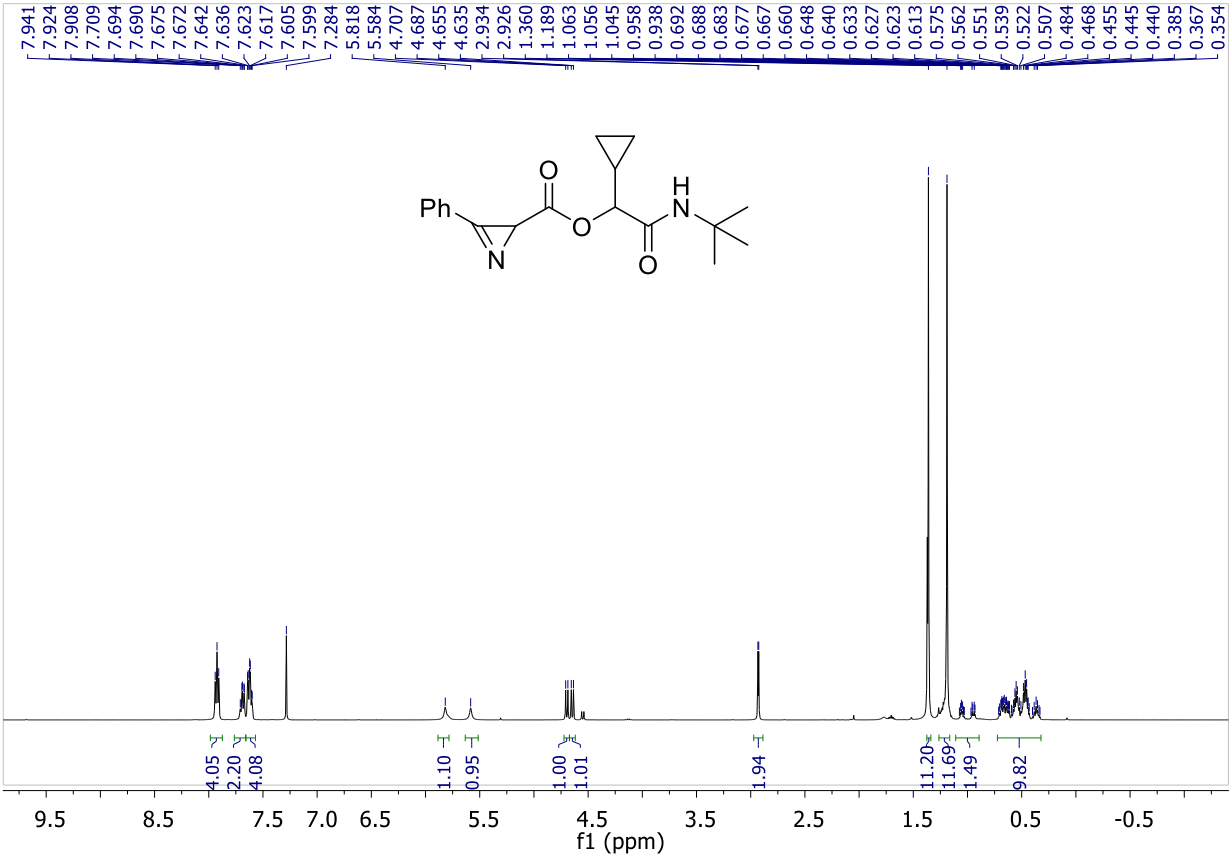


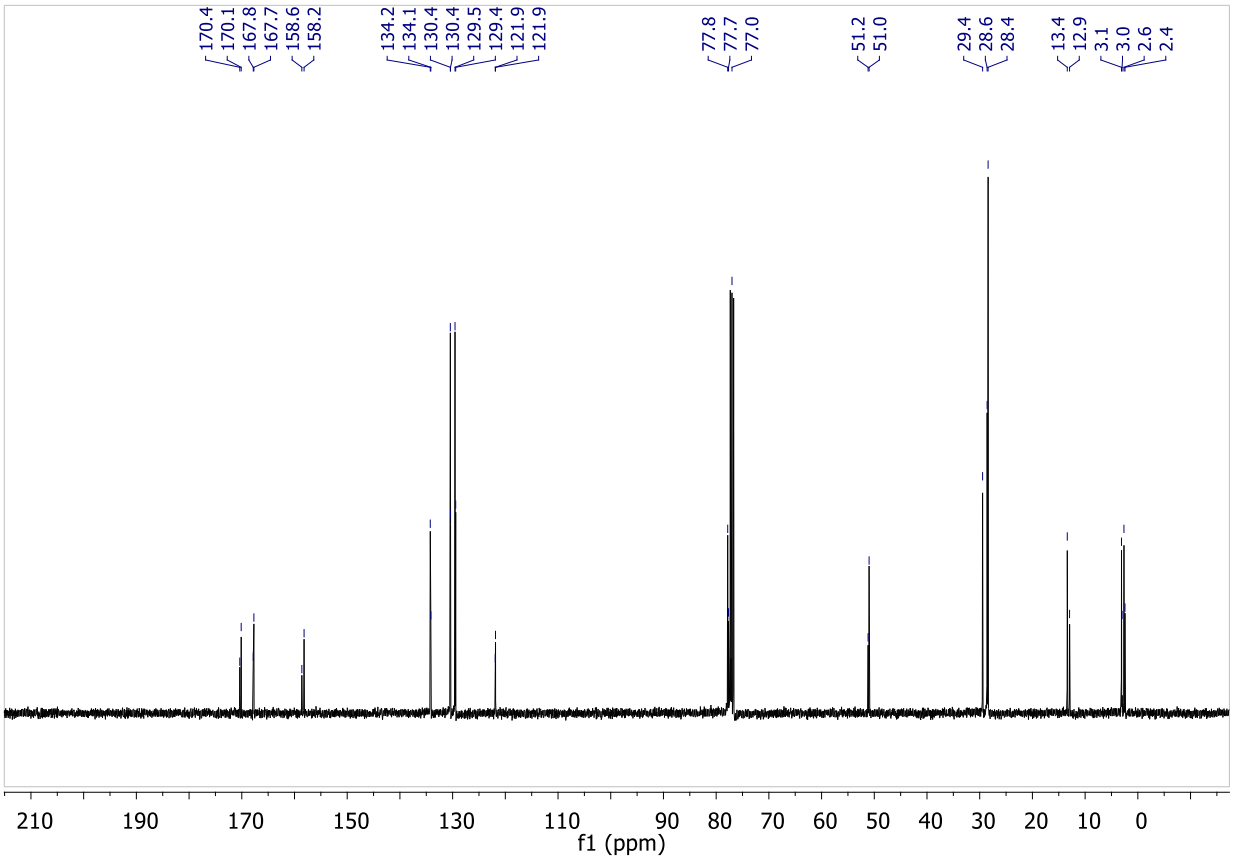
^{1}H and ^{13}C NMR spectra of compound **2r** (separated diastereomer)



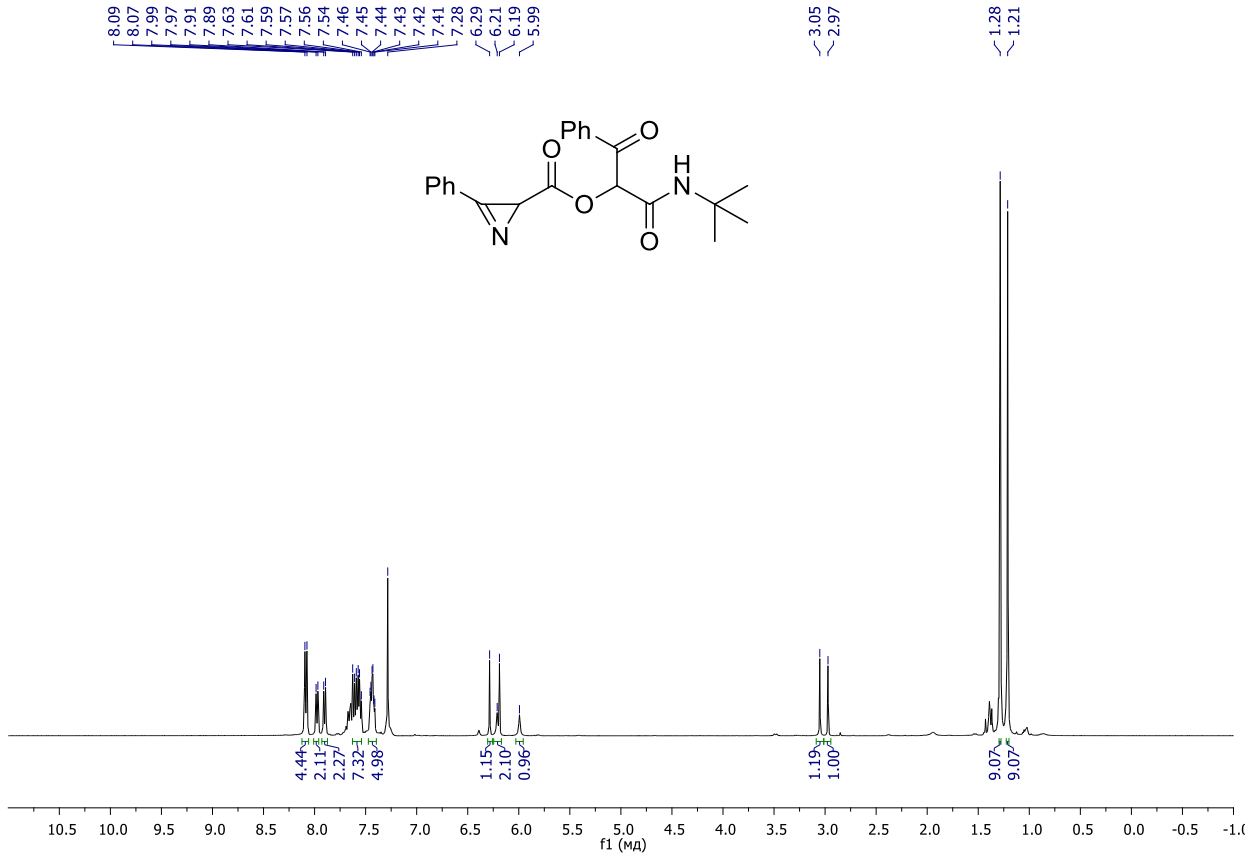


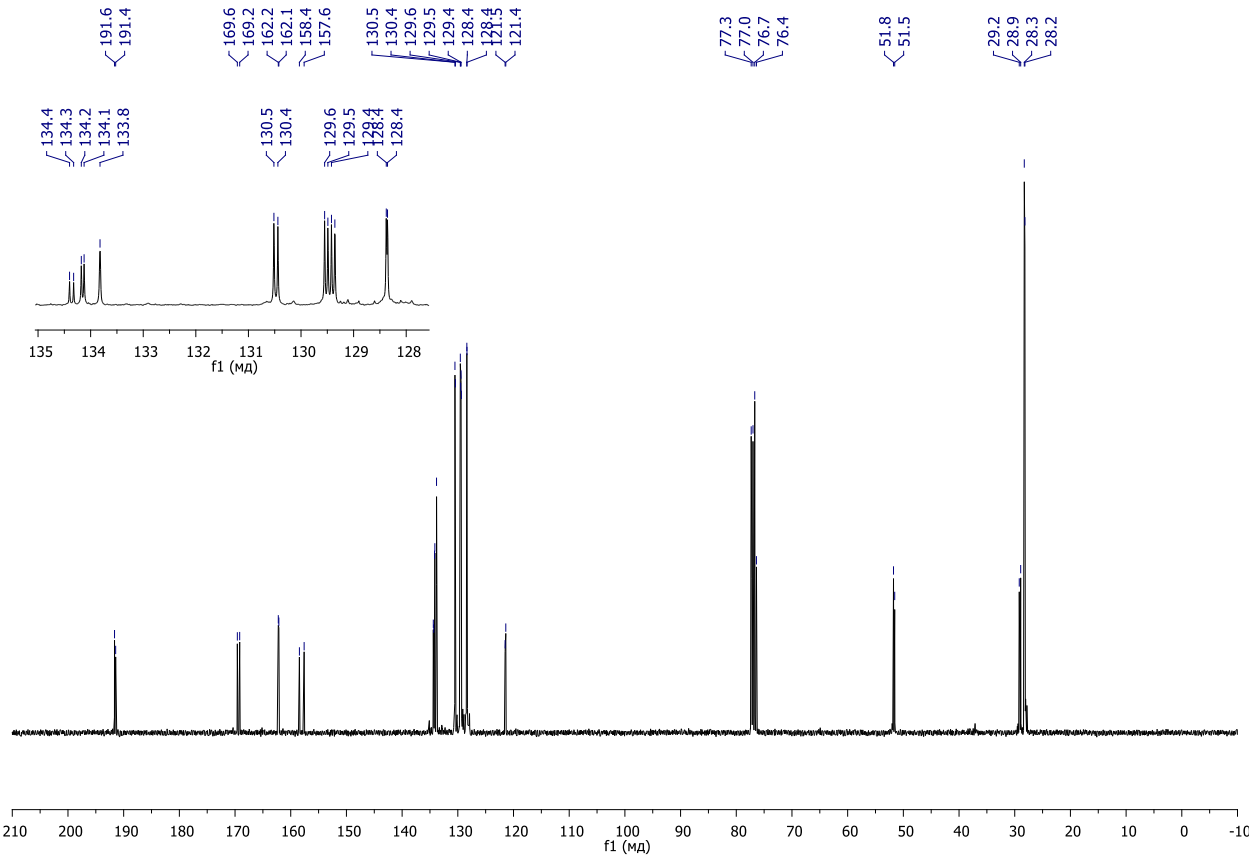
^{1}H and ^{13}C NMR spectra of compound **2r** (mixture of diastereomers)



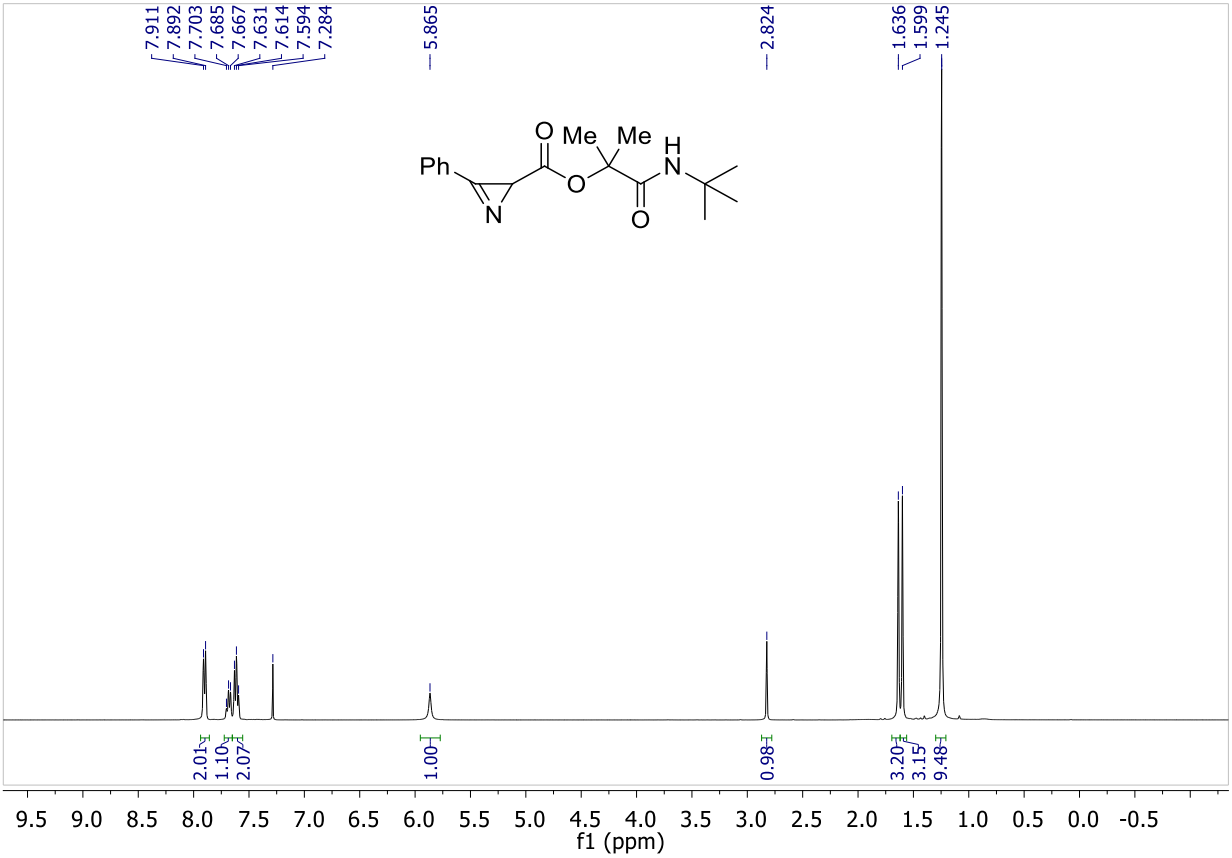


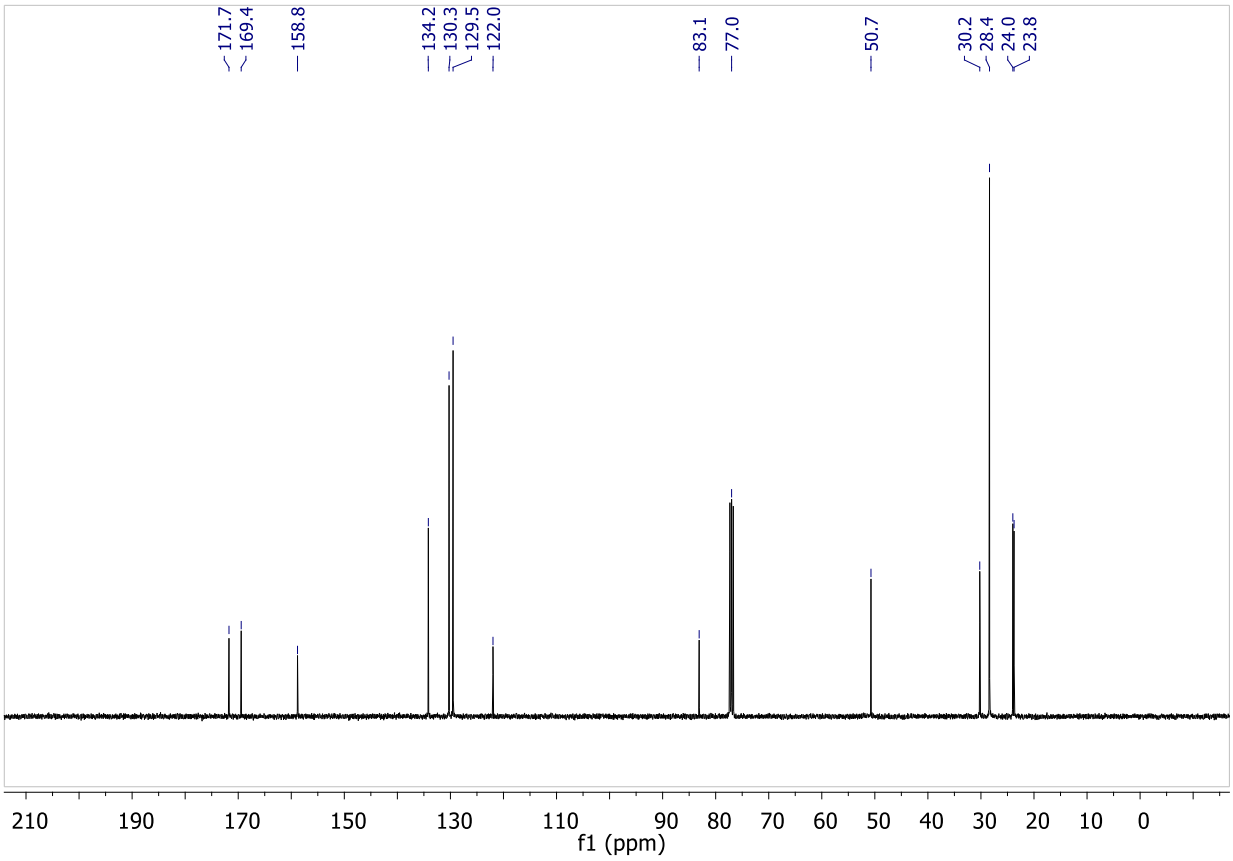
^{1}H and ^{13}C NMR spectra of compound **2s**



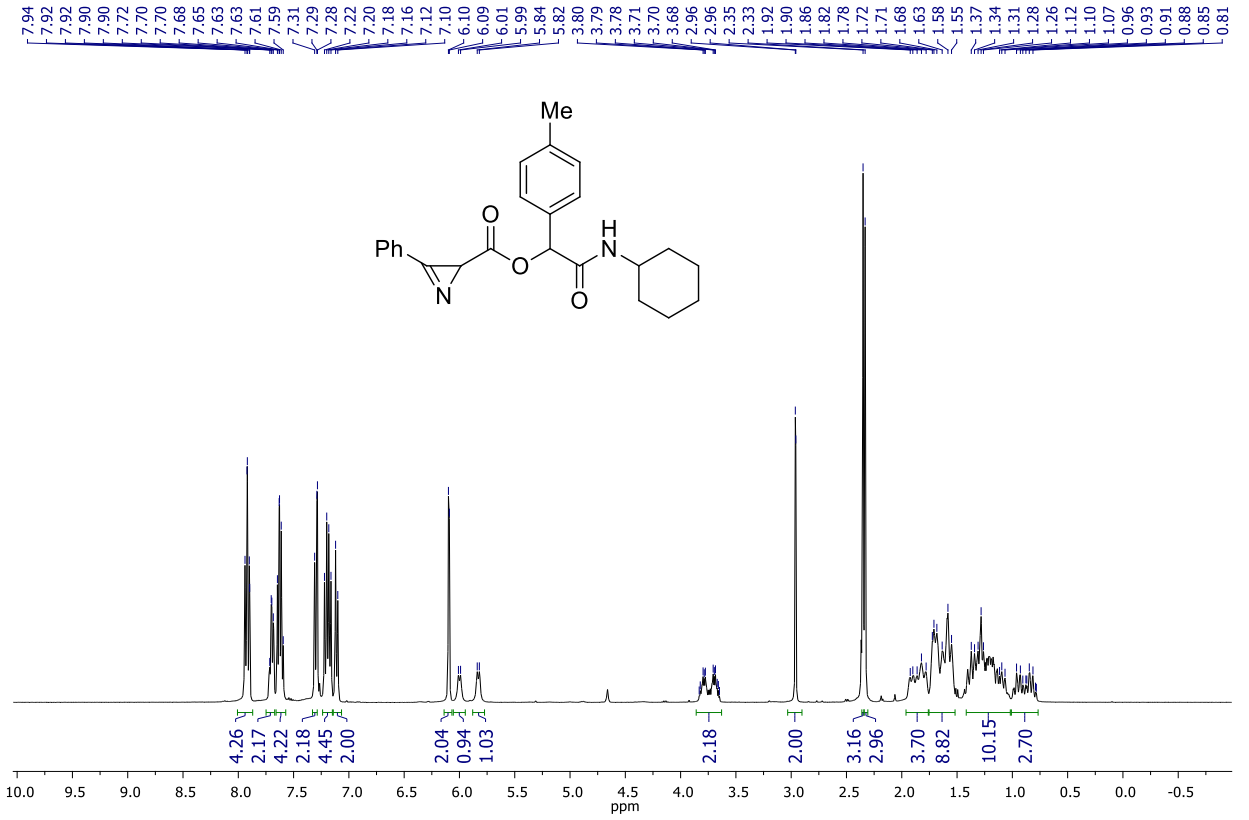


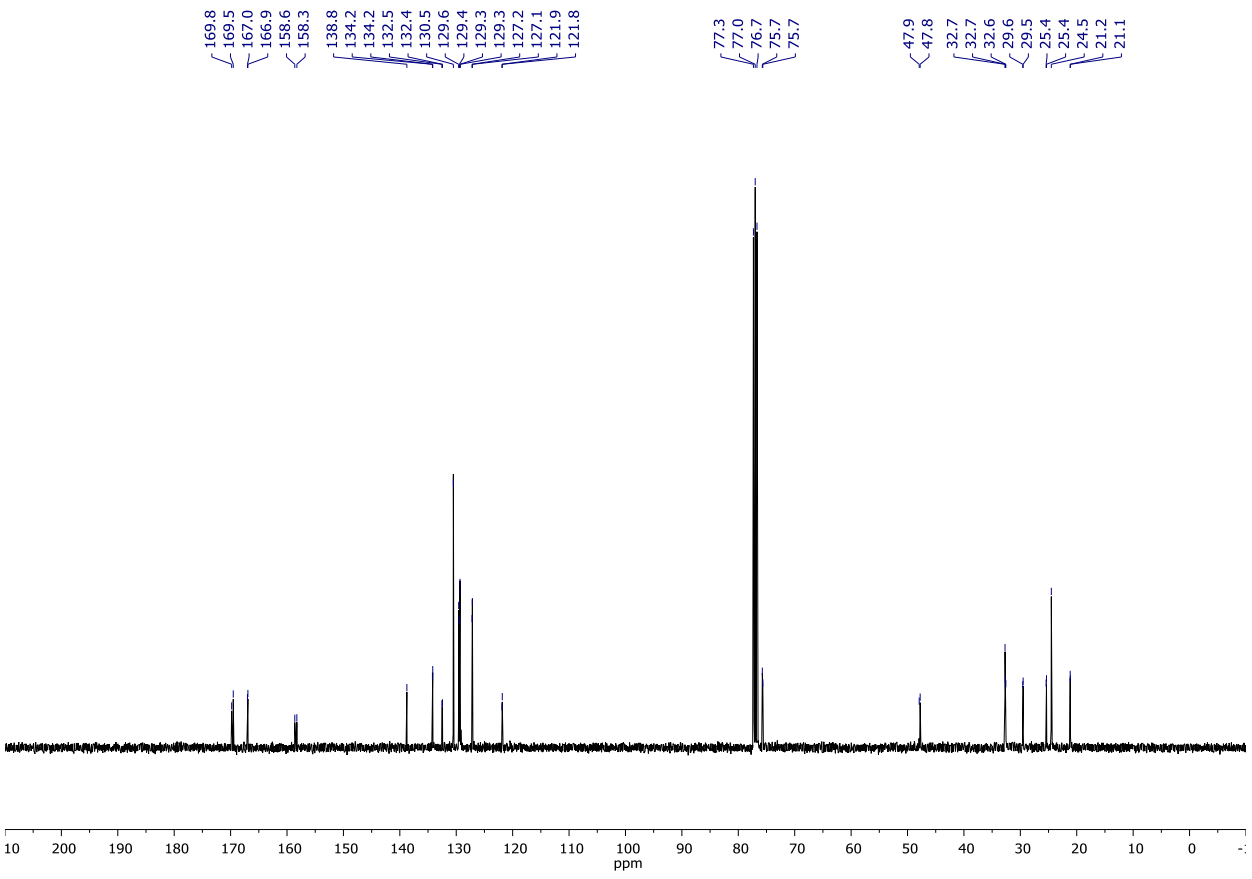
^{1}H and ^{13}C NMR spectra of compound **2t**



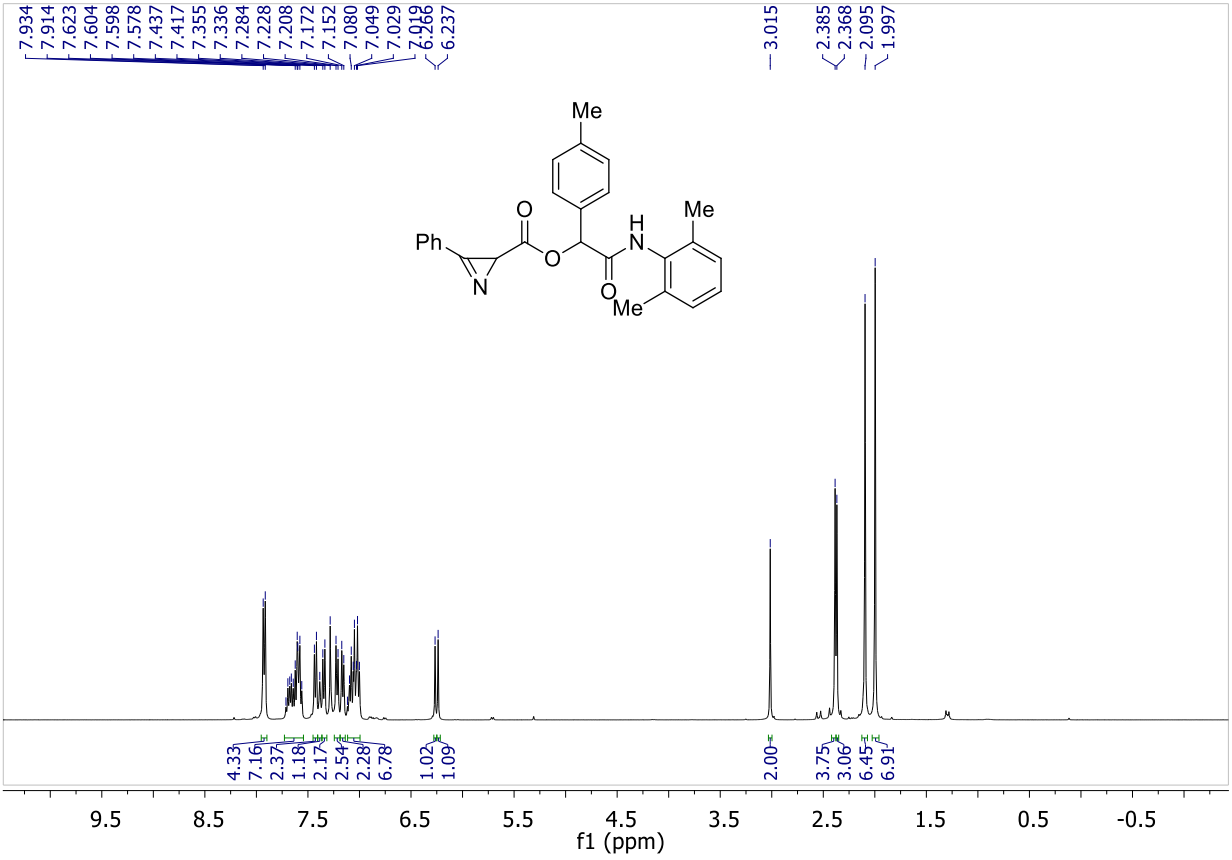


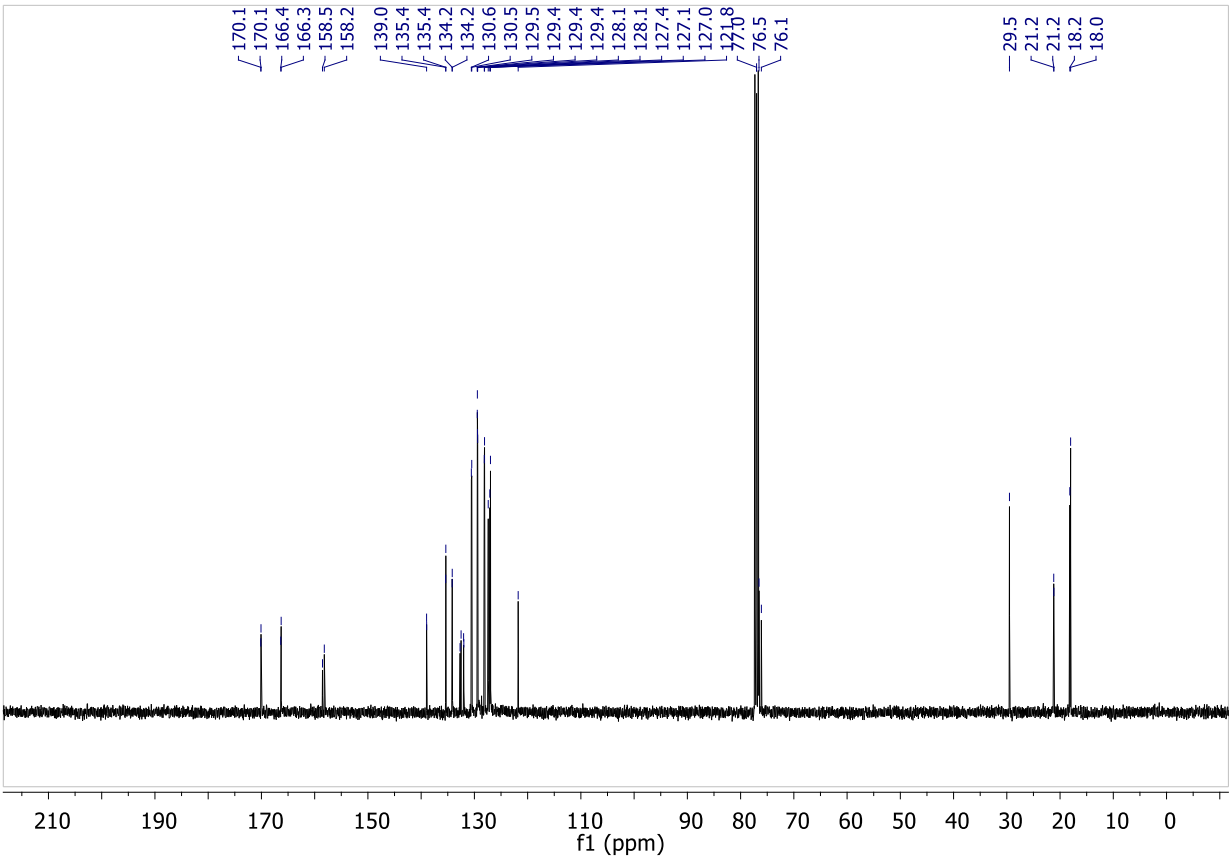
^{1}H and ^{13}C NMR spectra of compound **2u**



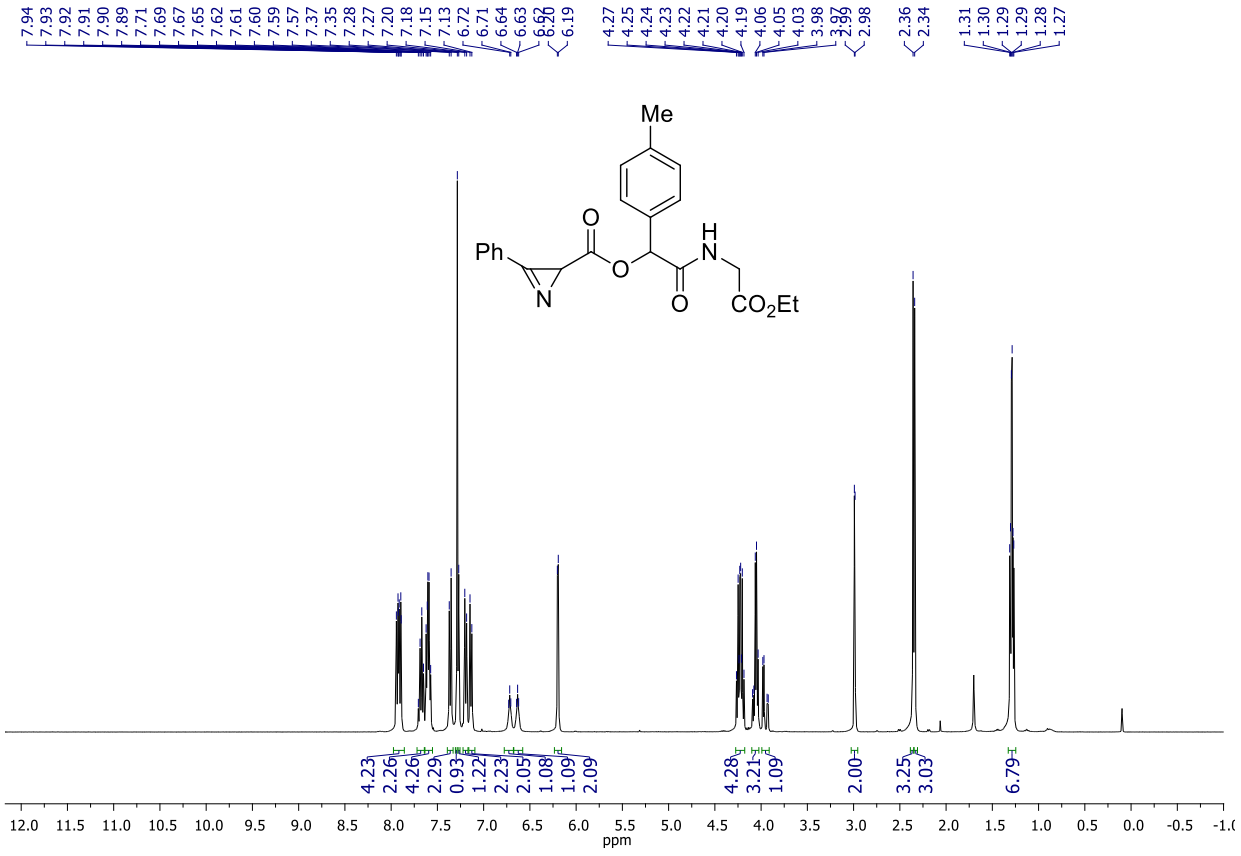


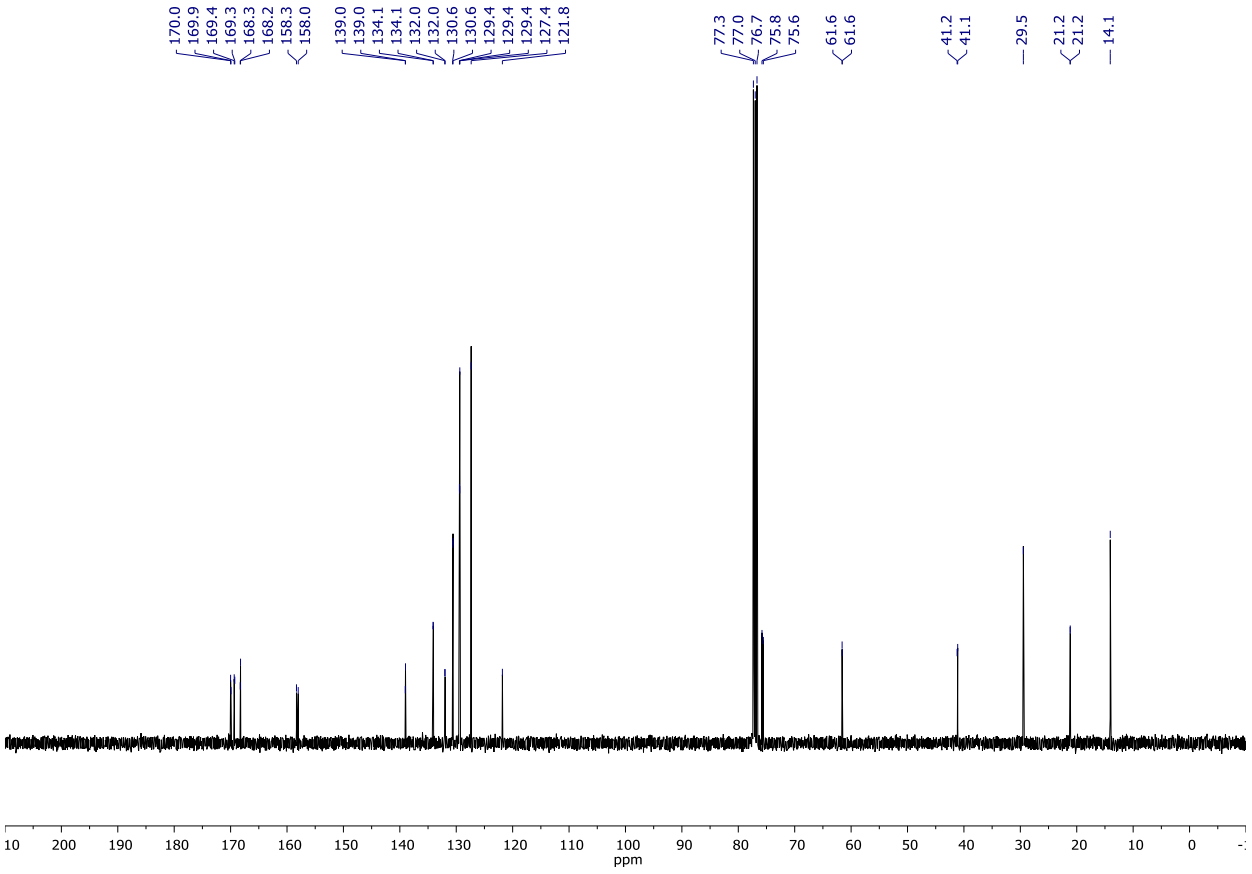
^{1}H and ^{13}C NMR spectra of compound **2v**



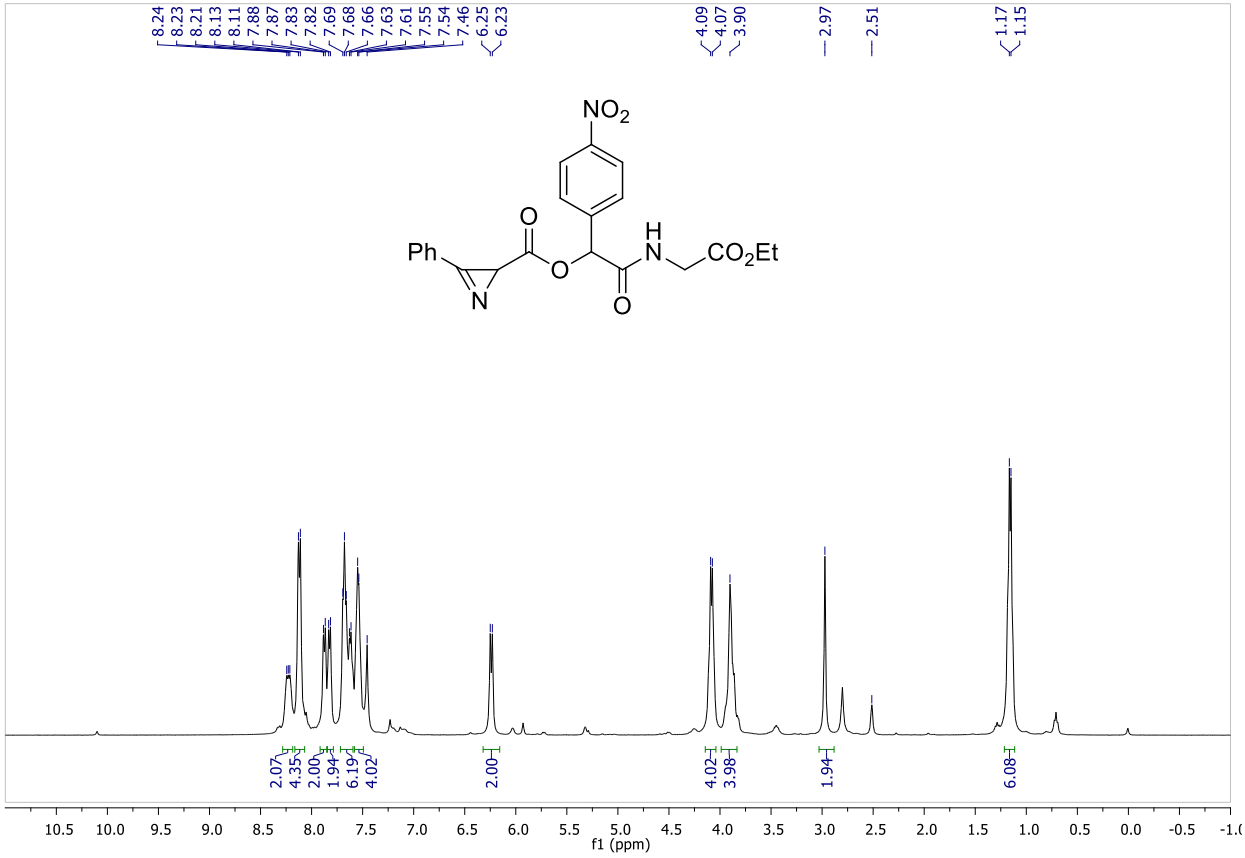


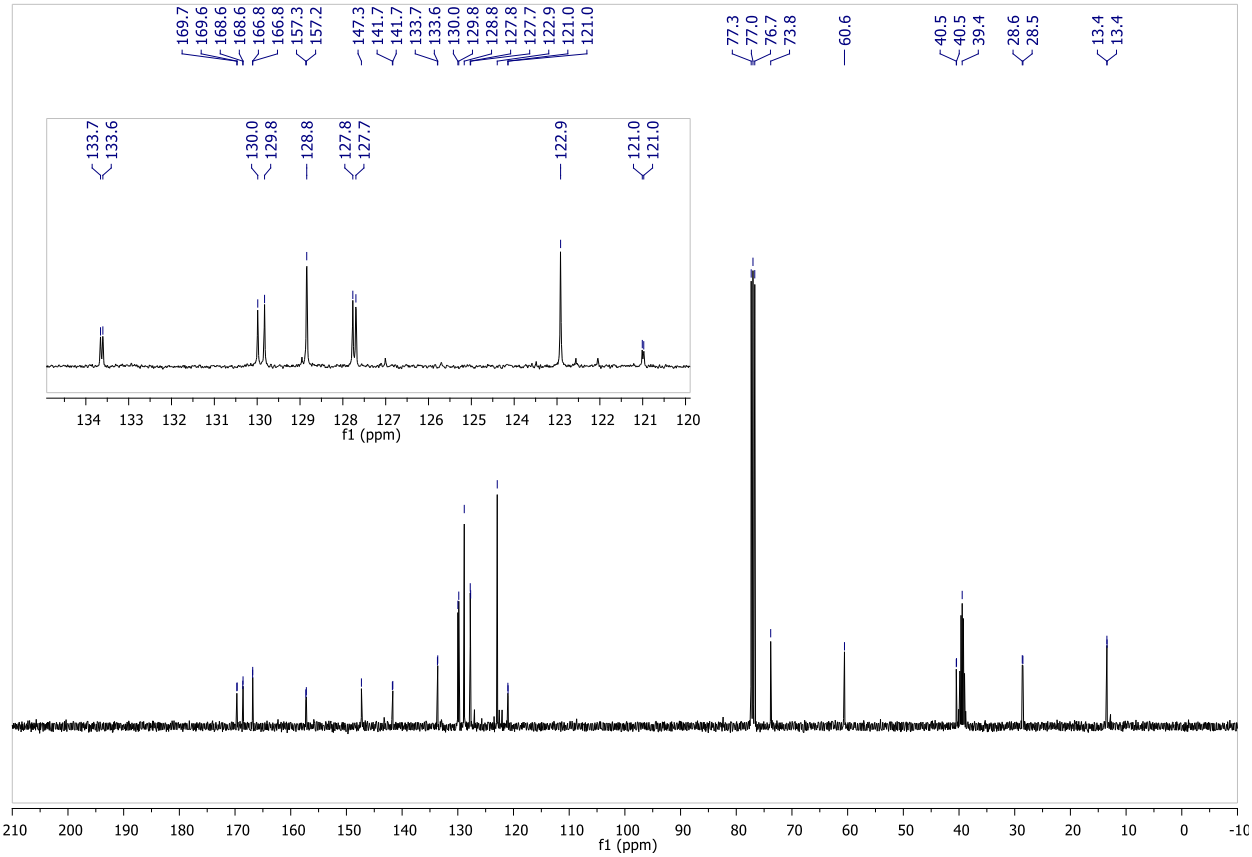
^{1}H and ^{13}C NMR spectra of compound **2w**



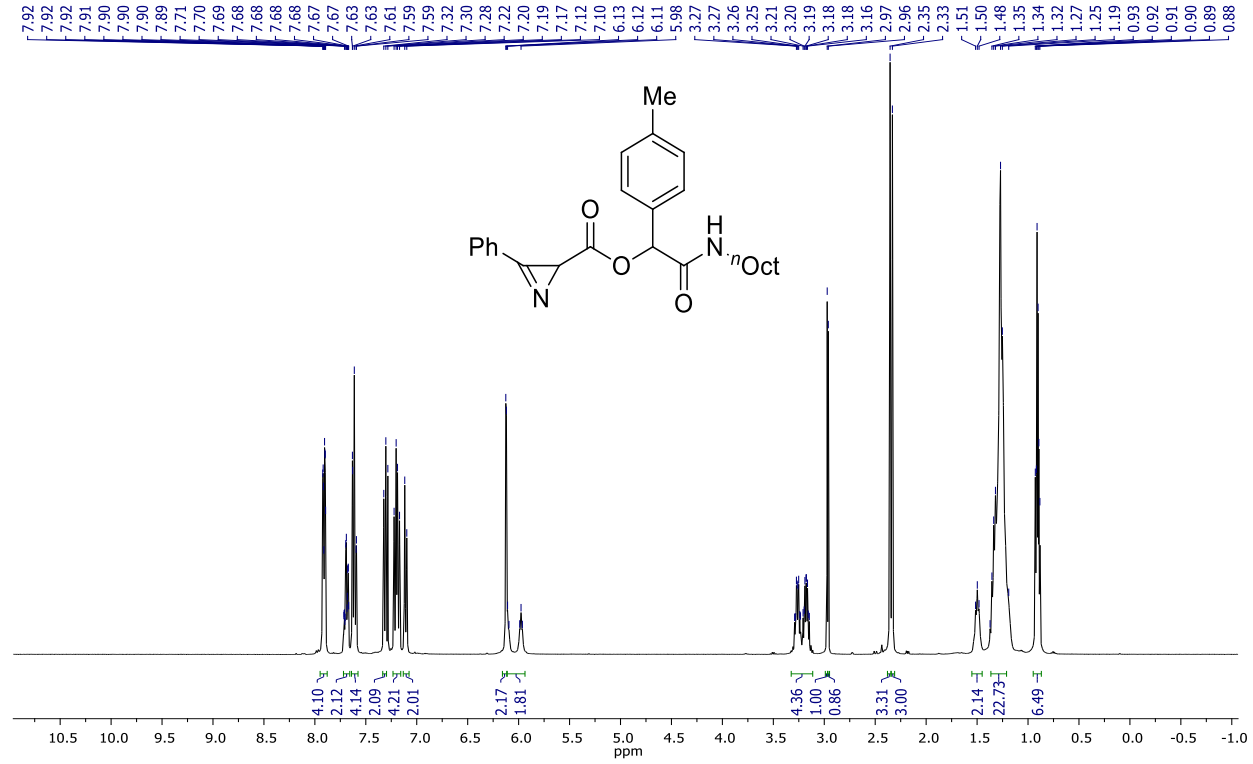


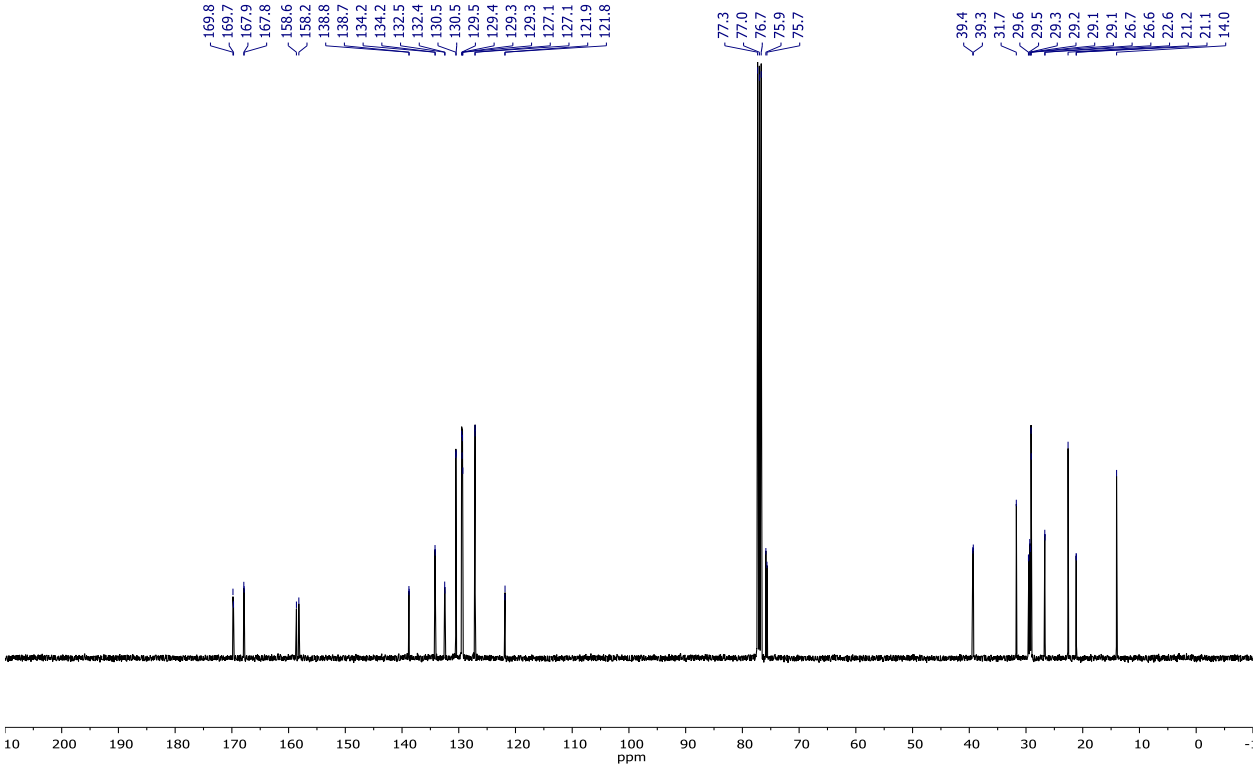
^{1}H and ^{13}C NMR spectra of compound **2x**



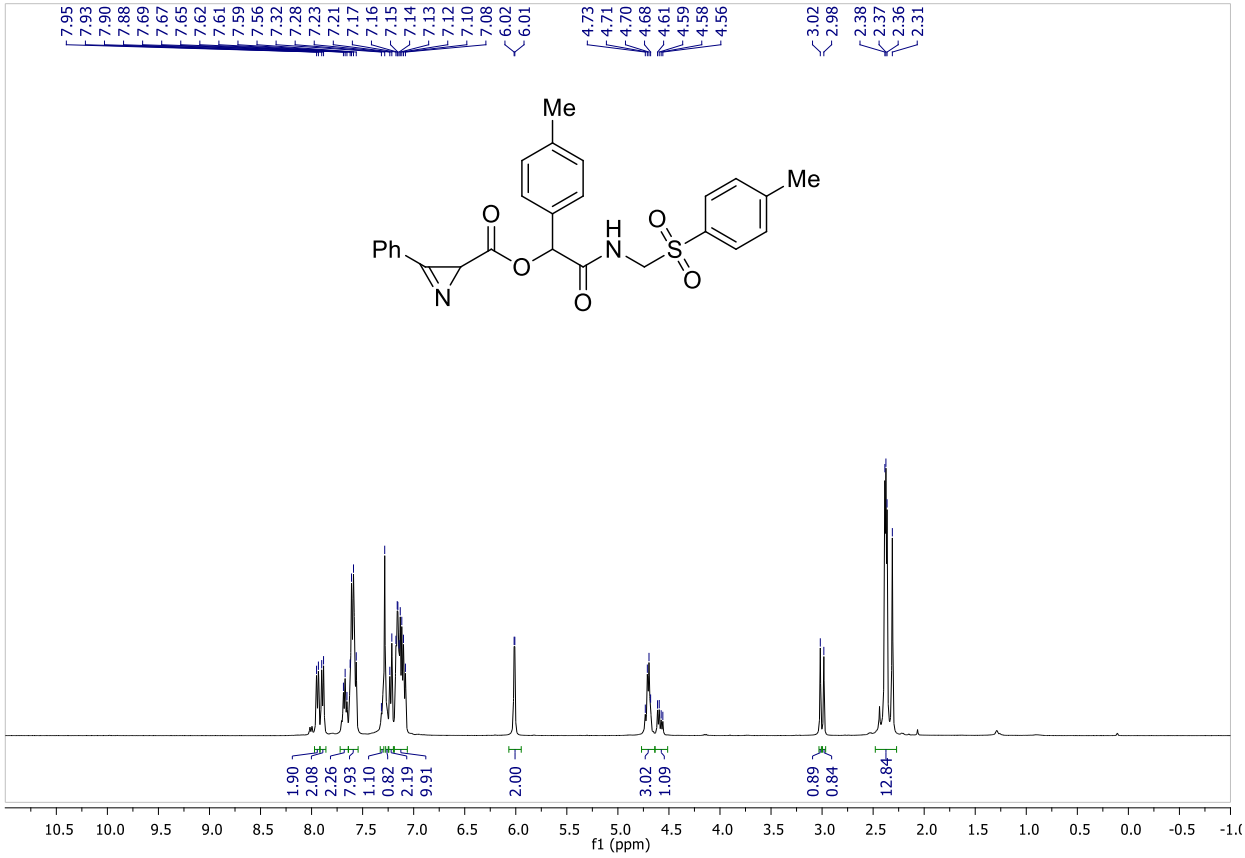


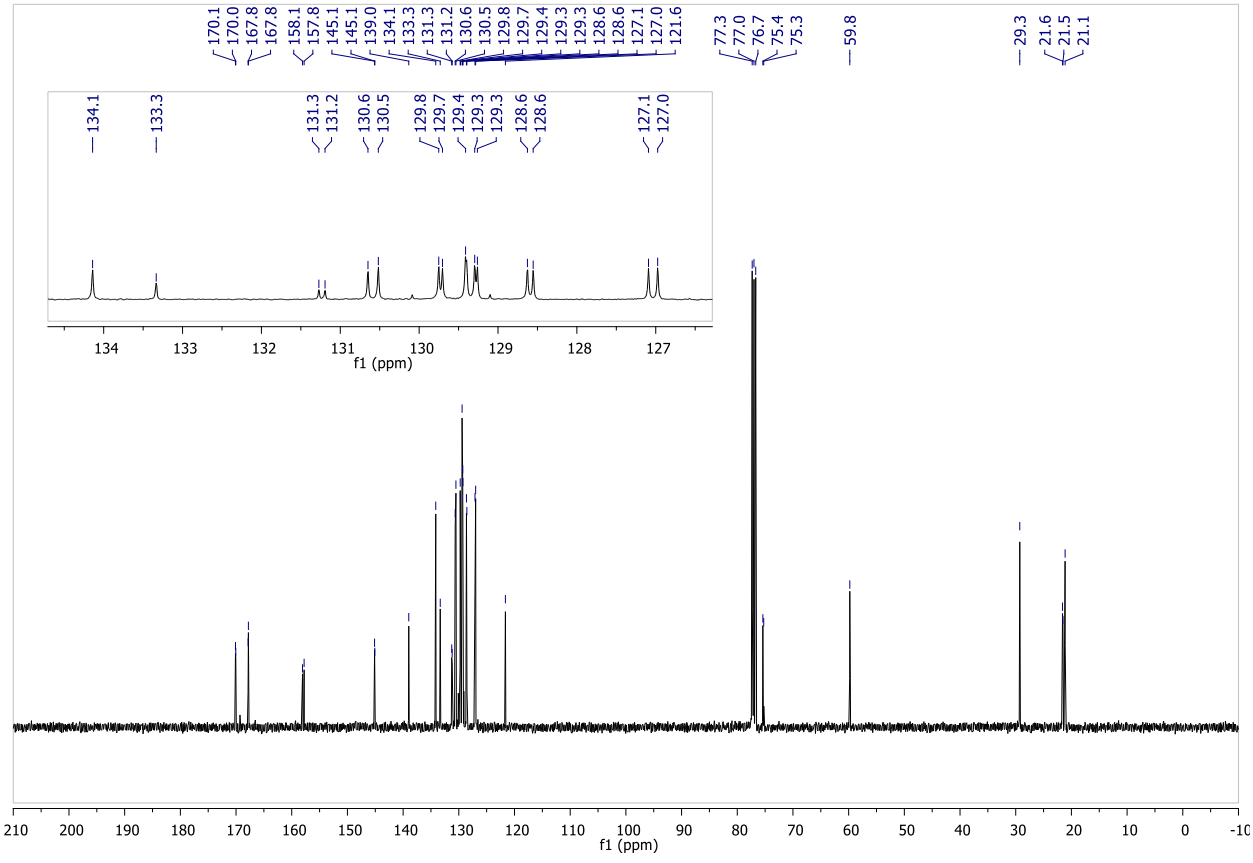
^{1}H and ^{13}C NMR spectra of compound **2y**



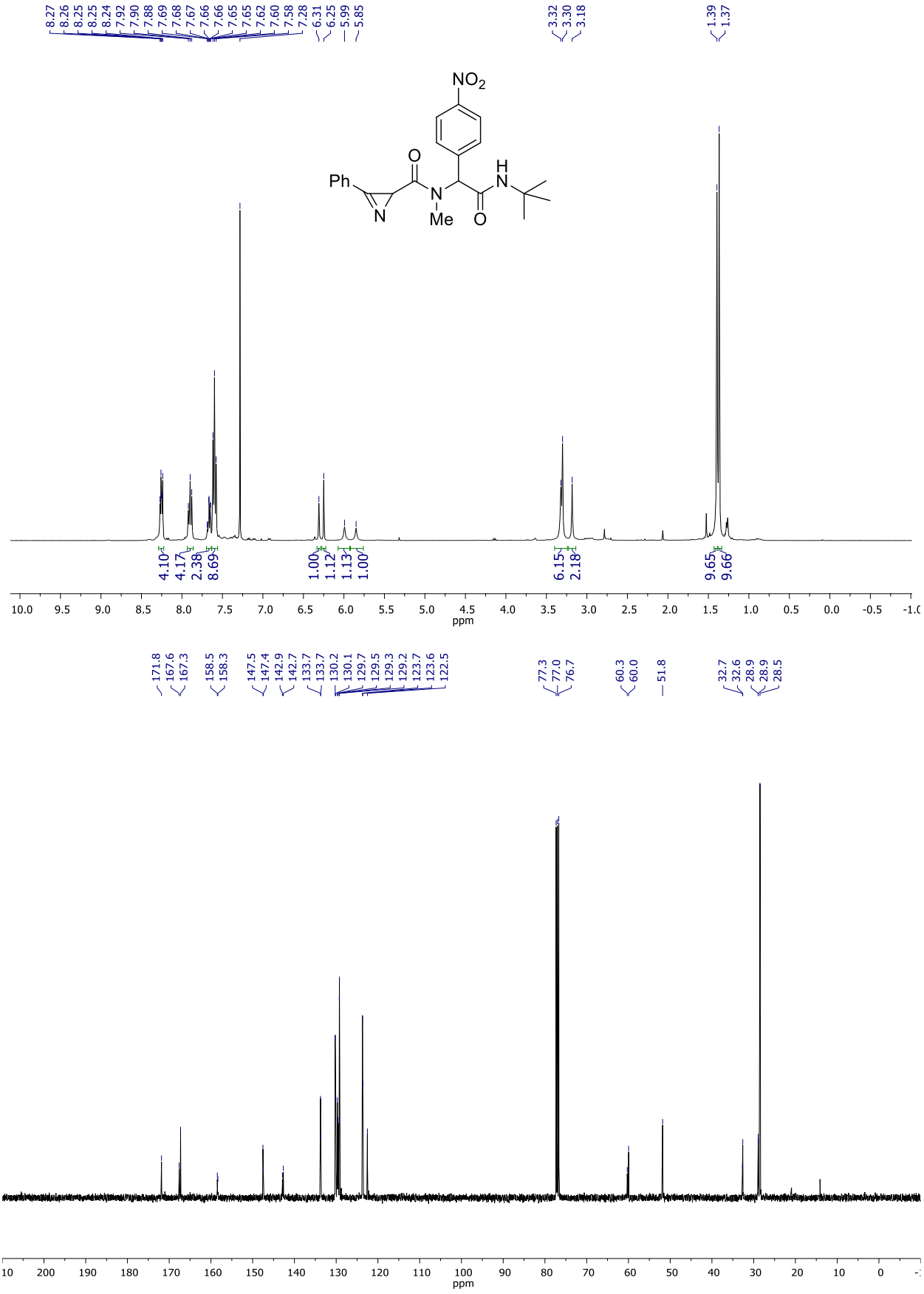


^{1}H and ^{13}C NMR spectra of compound **2z**

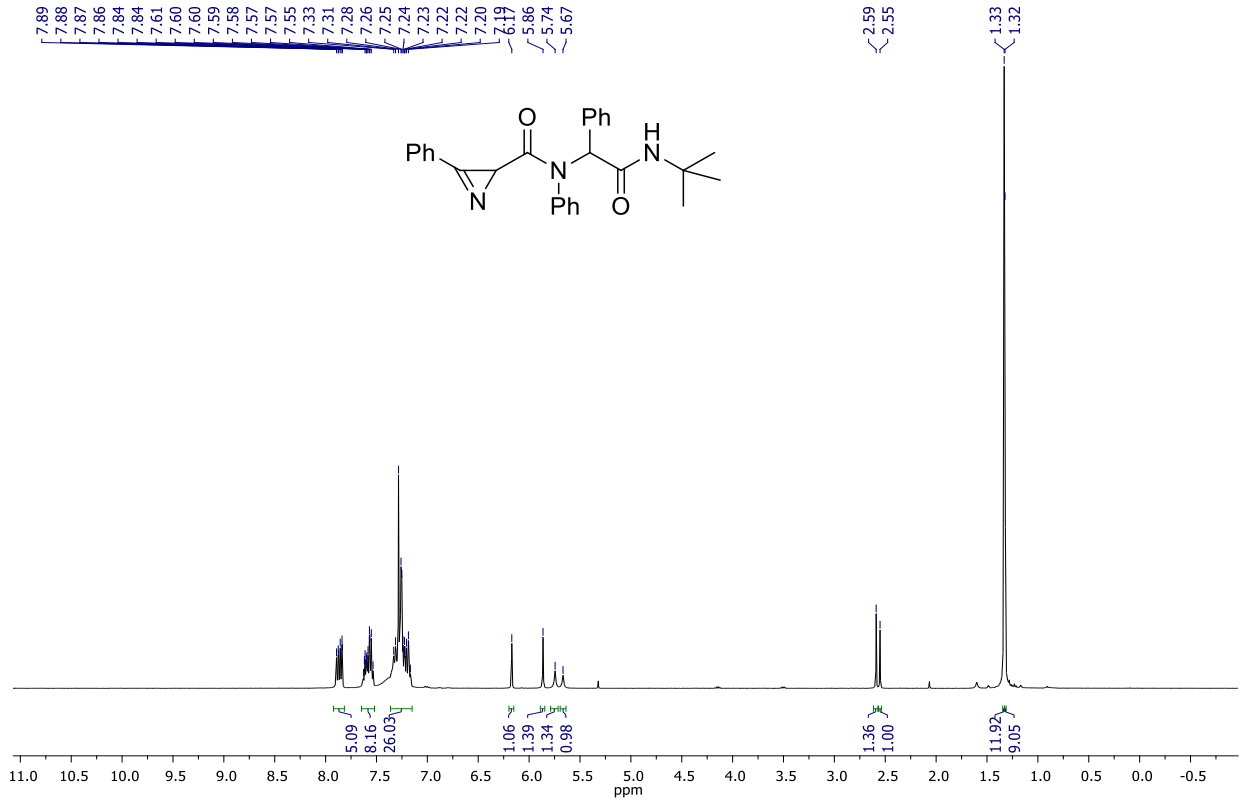


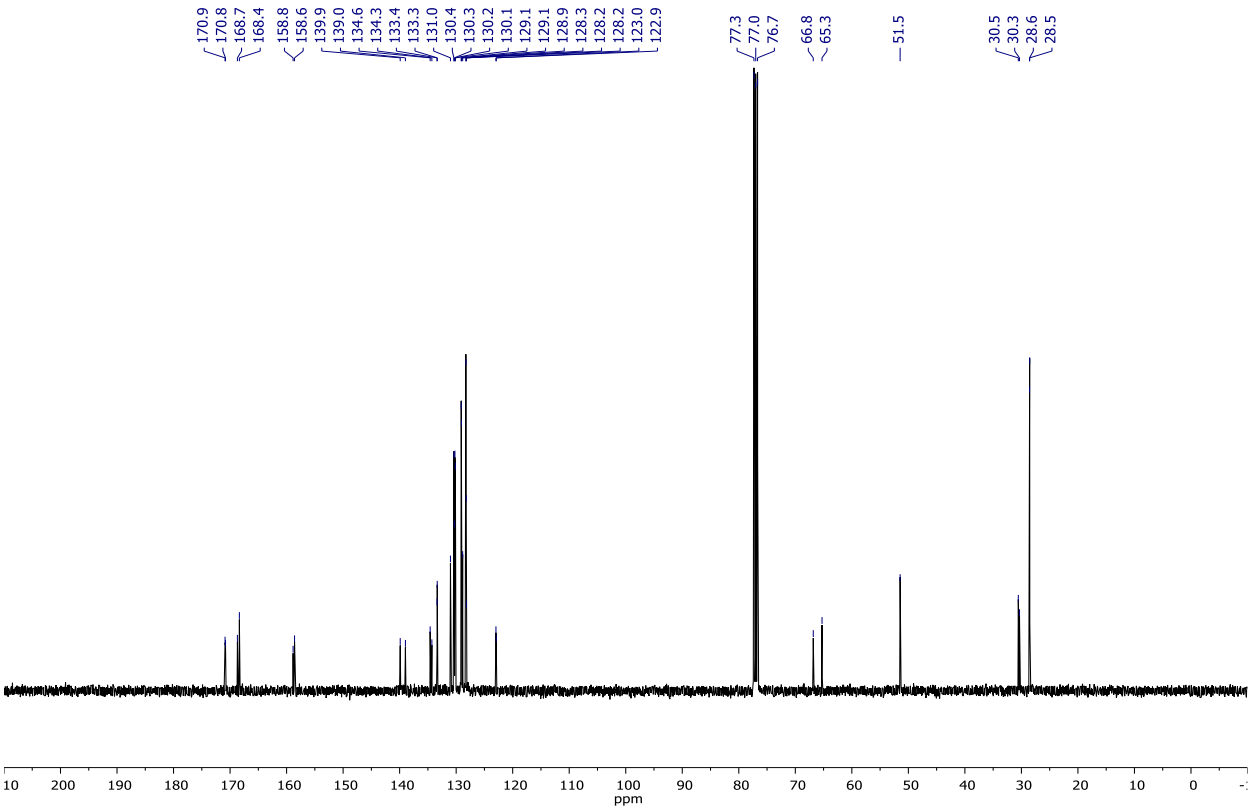


^{1}H and ^{13}C NMR spectra of compound **2za**



^{1}H and ^{13}C NMR spectra of compound **2zb**





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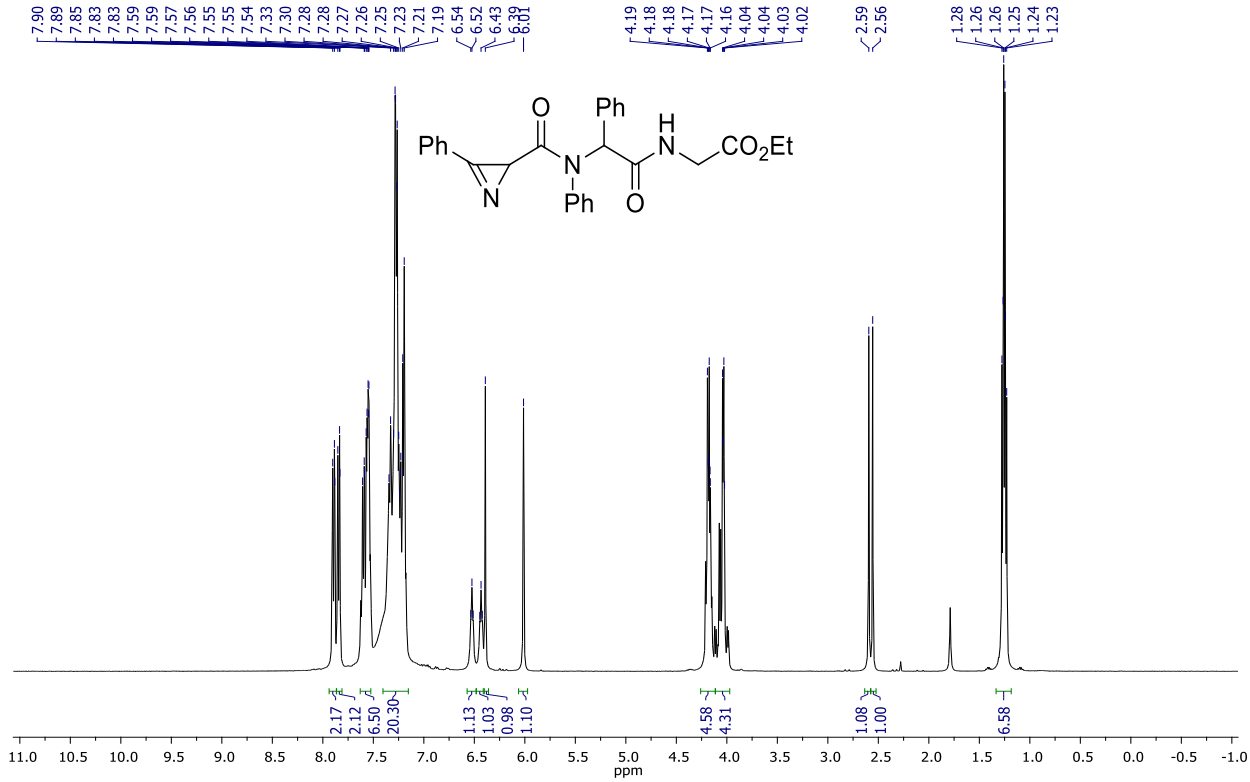
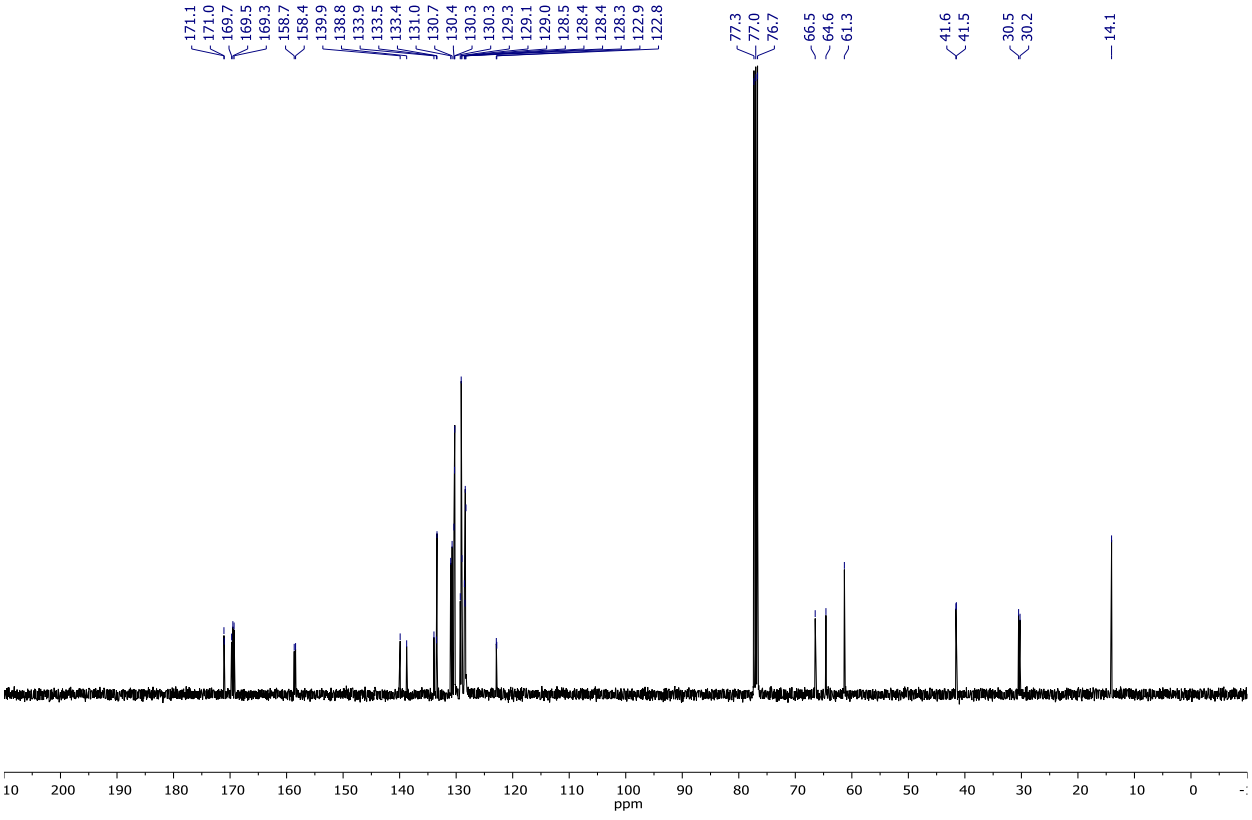
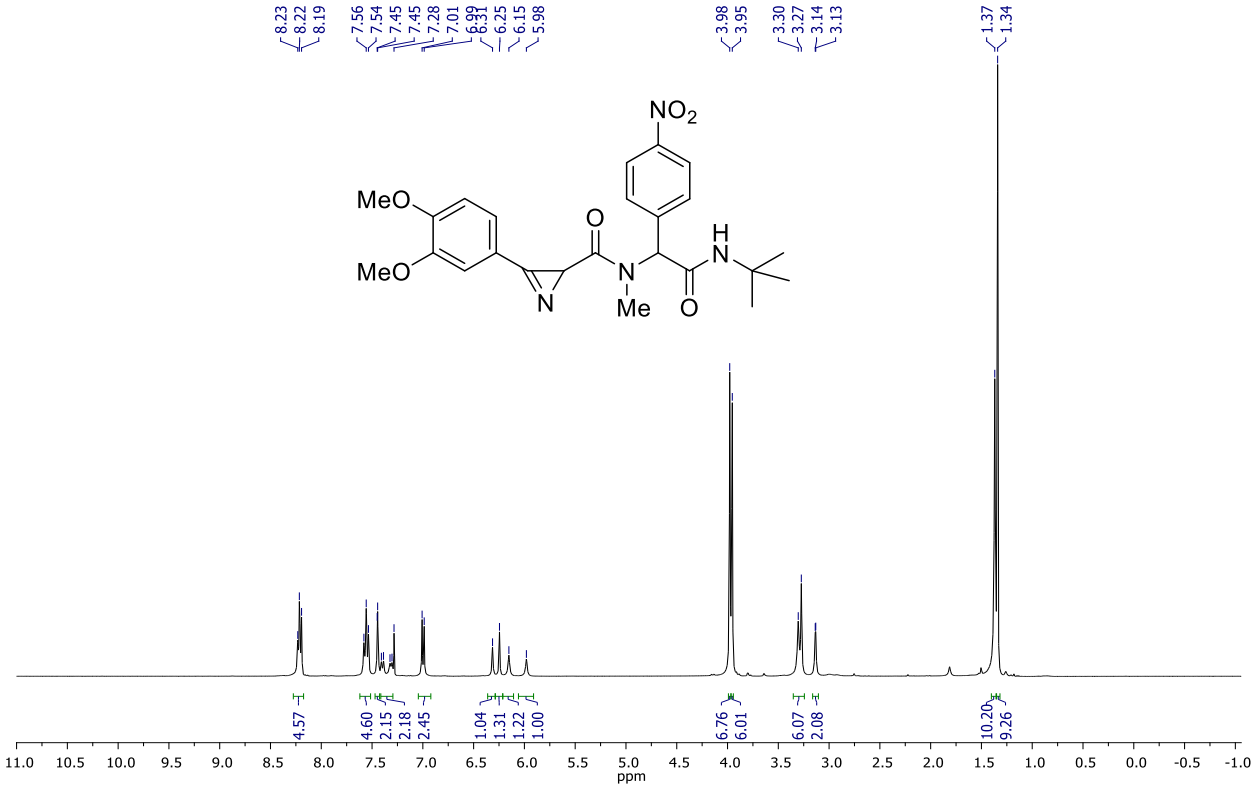
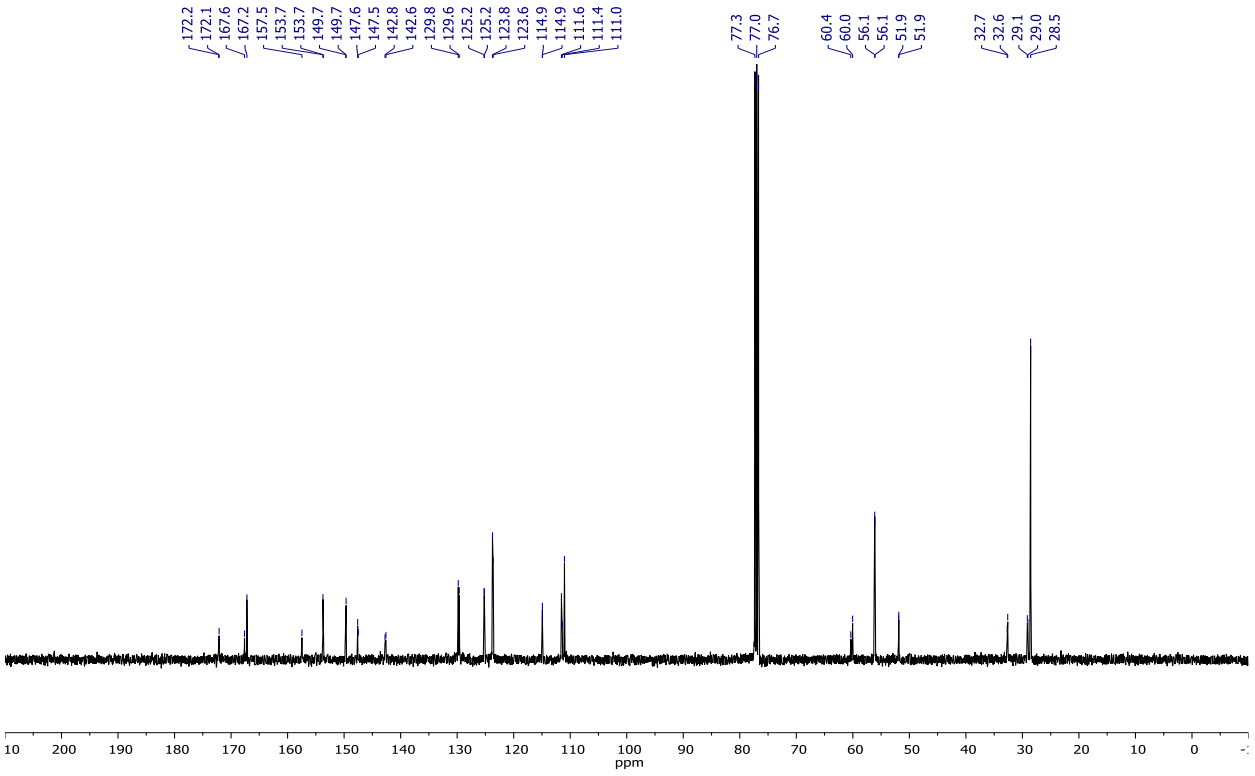


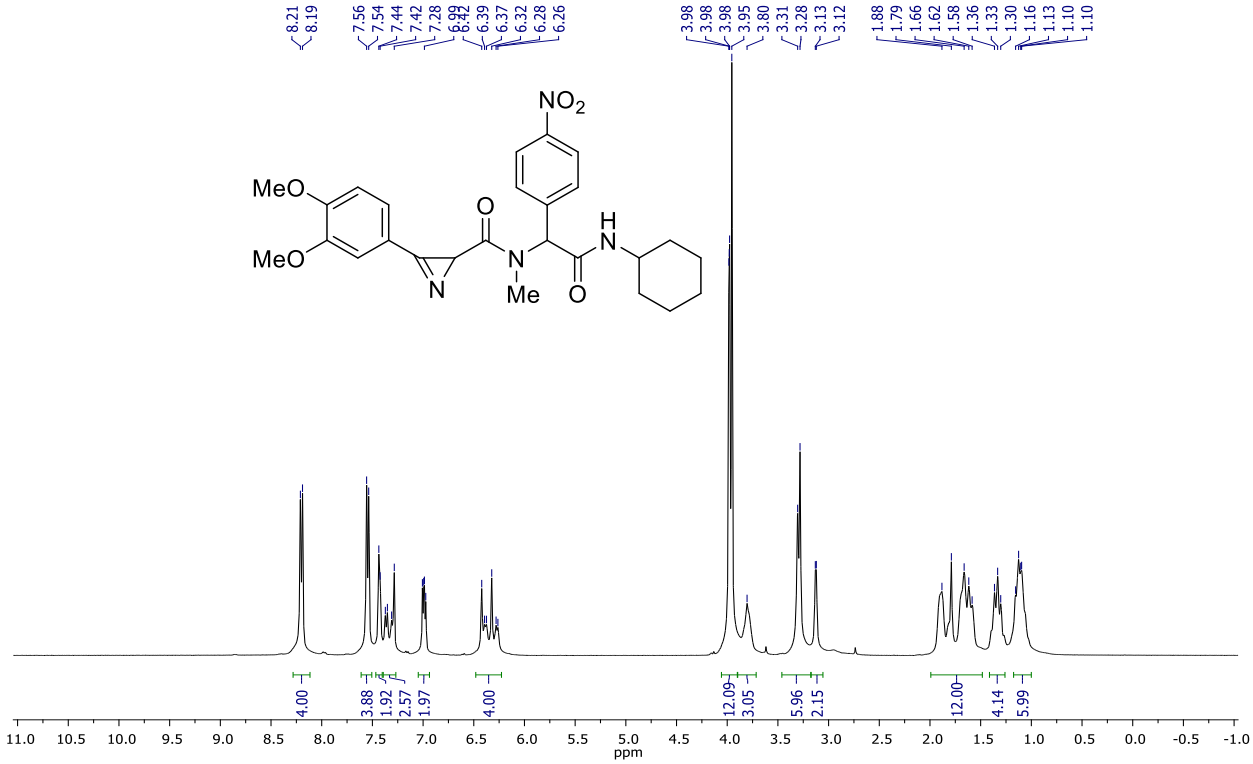


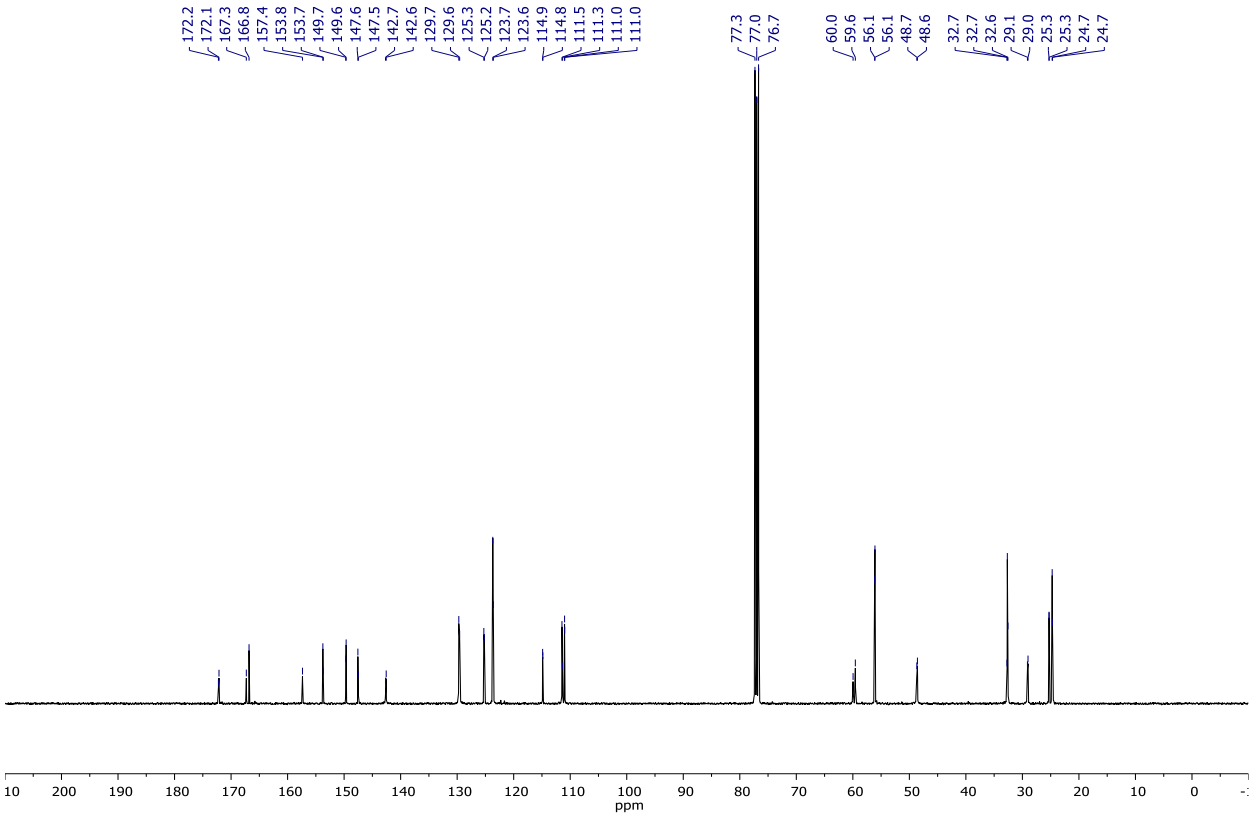
^{1}H and ^{13}C NMR spectra of compound **2zd**



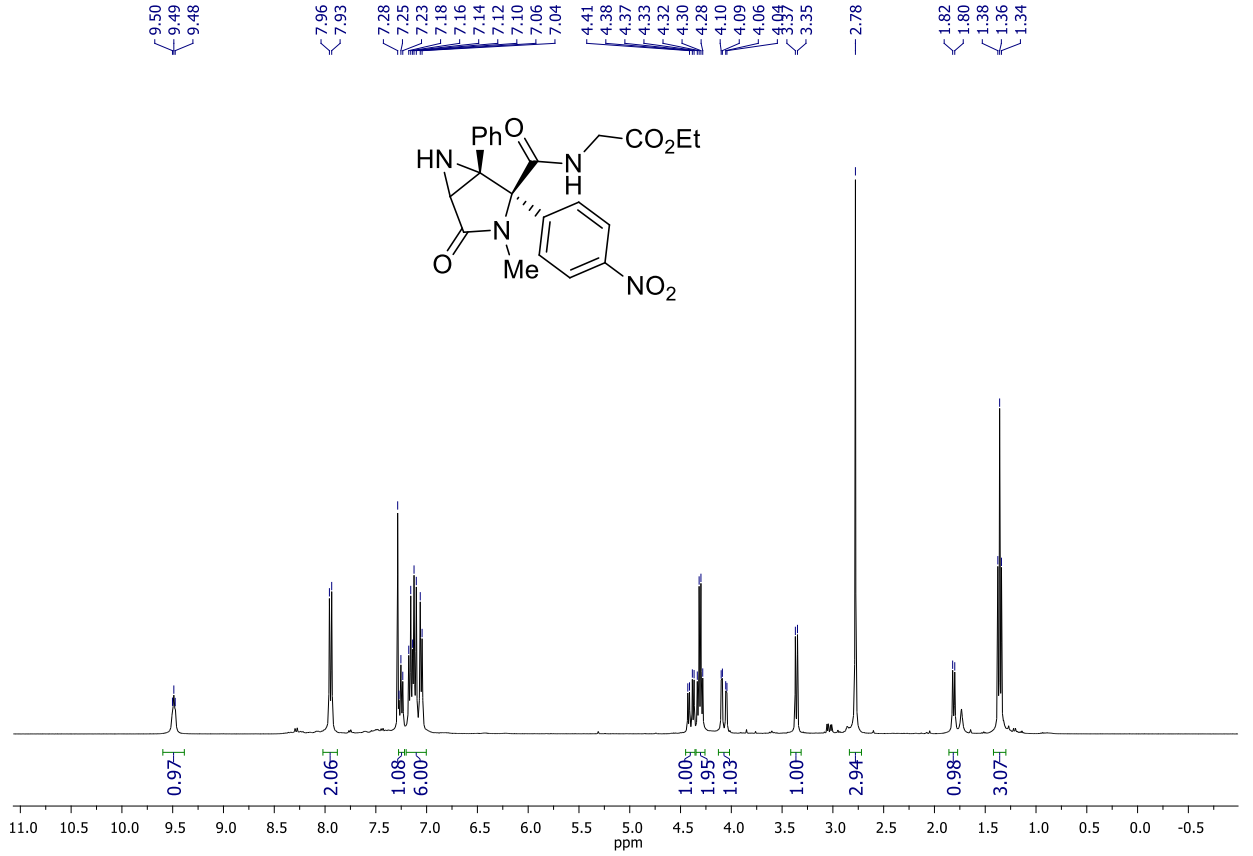


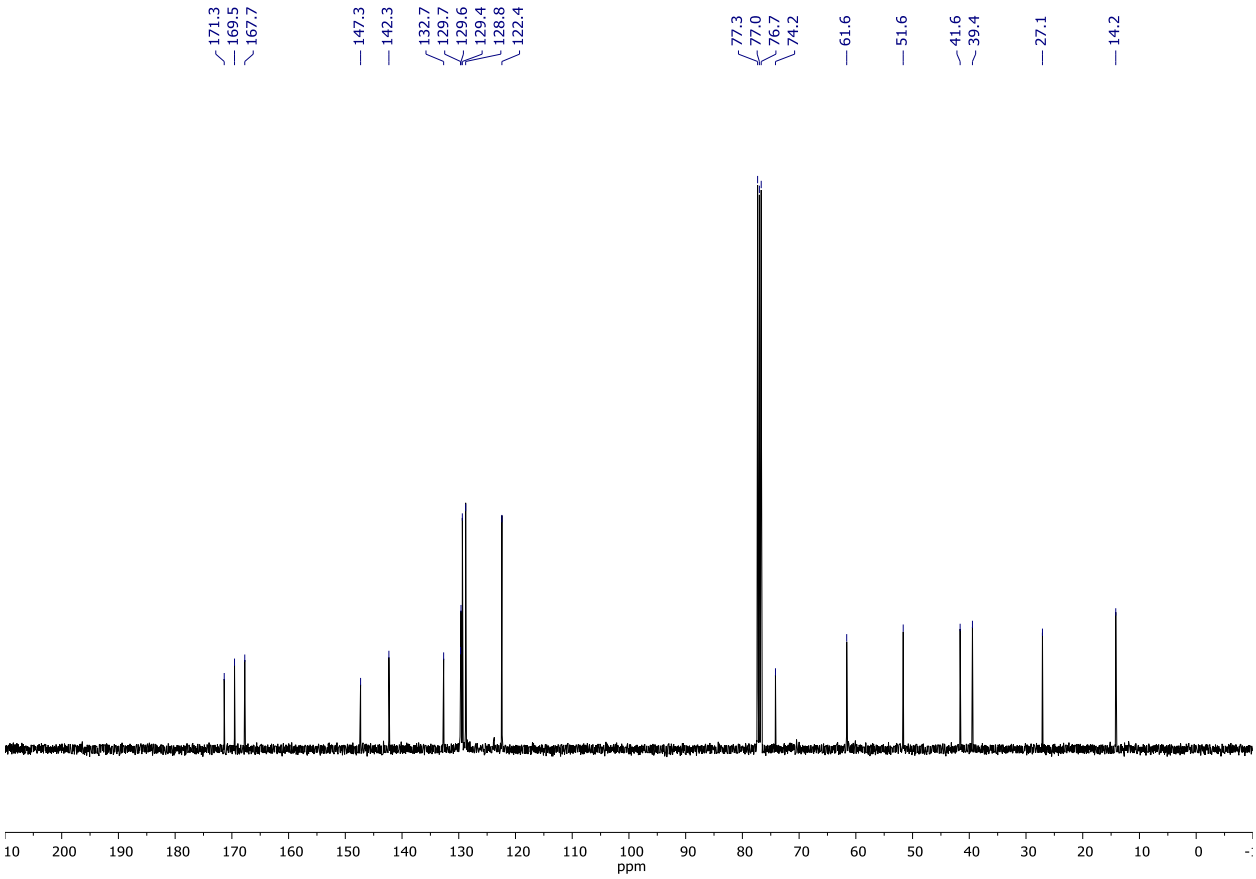
^{1}H and ^{13}C NMR spectra of compound **2ze**



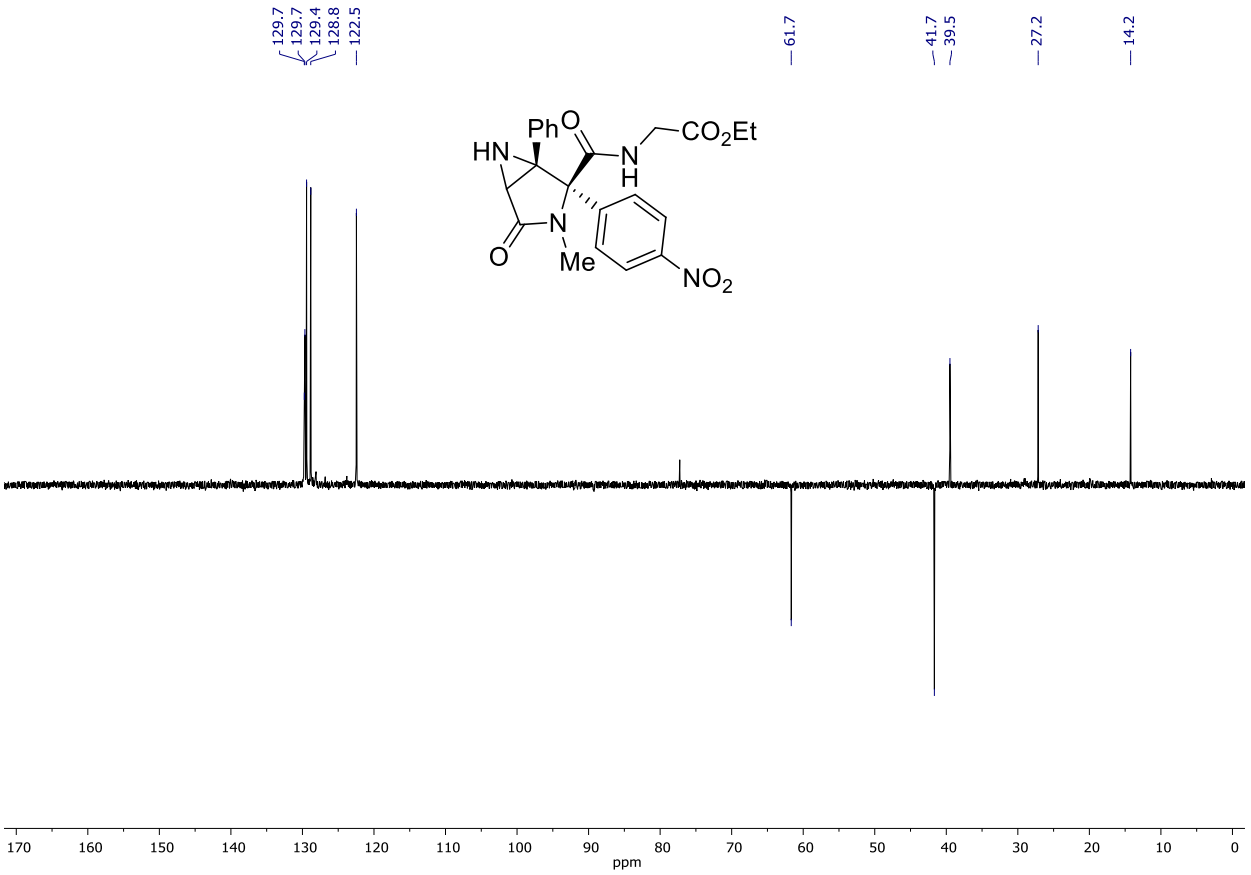


^{1}H and ^{13}C NMR spectra of compound (*RS*,*RS*)-**6a**

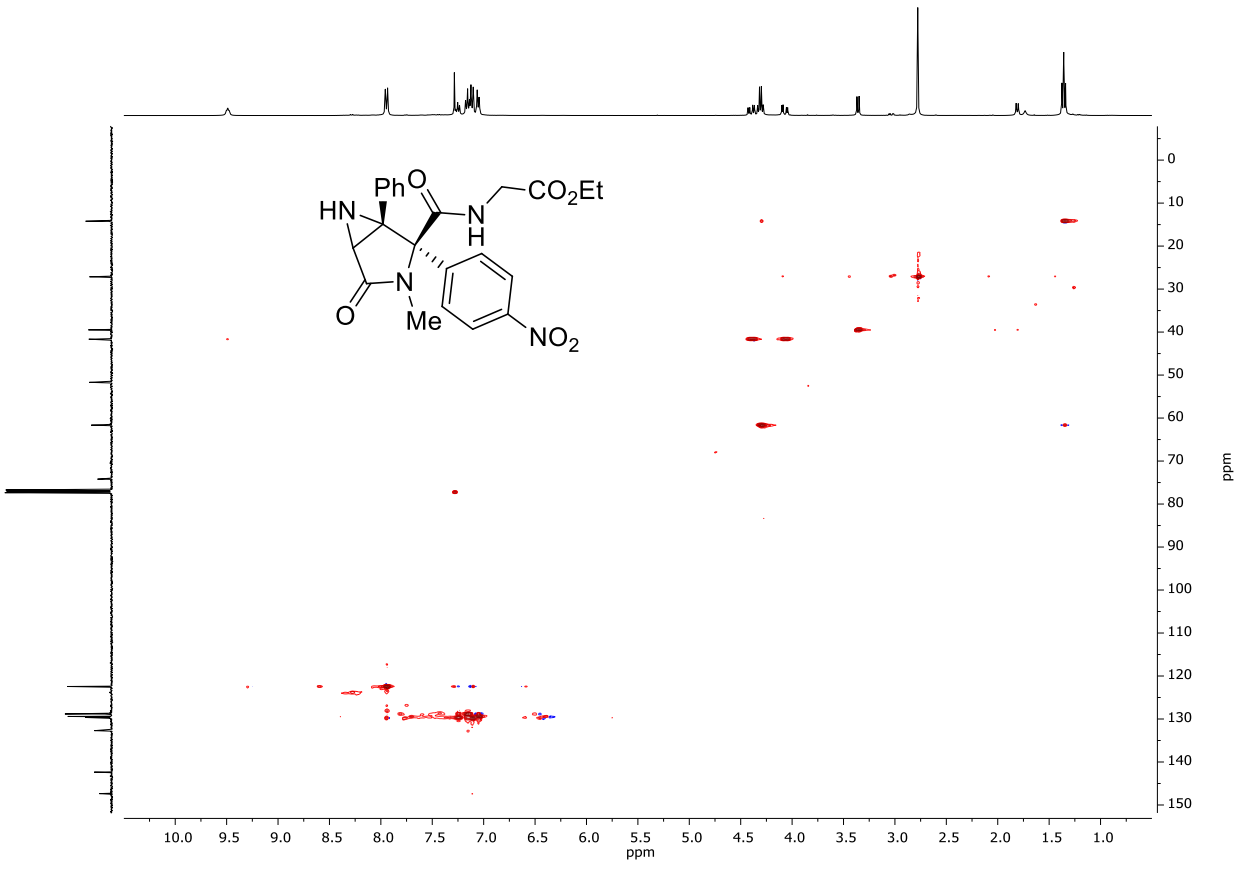




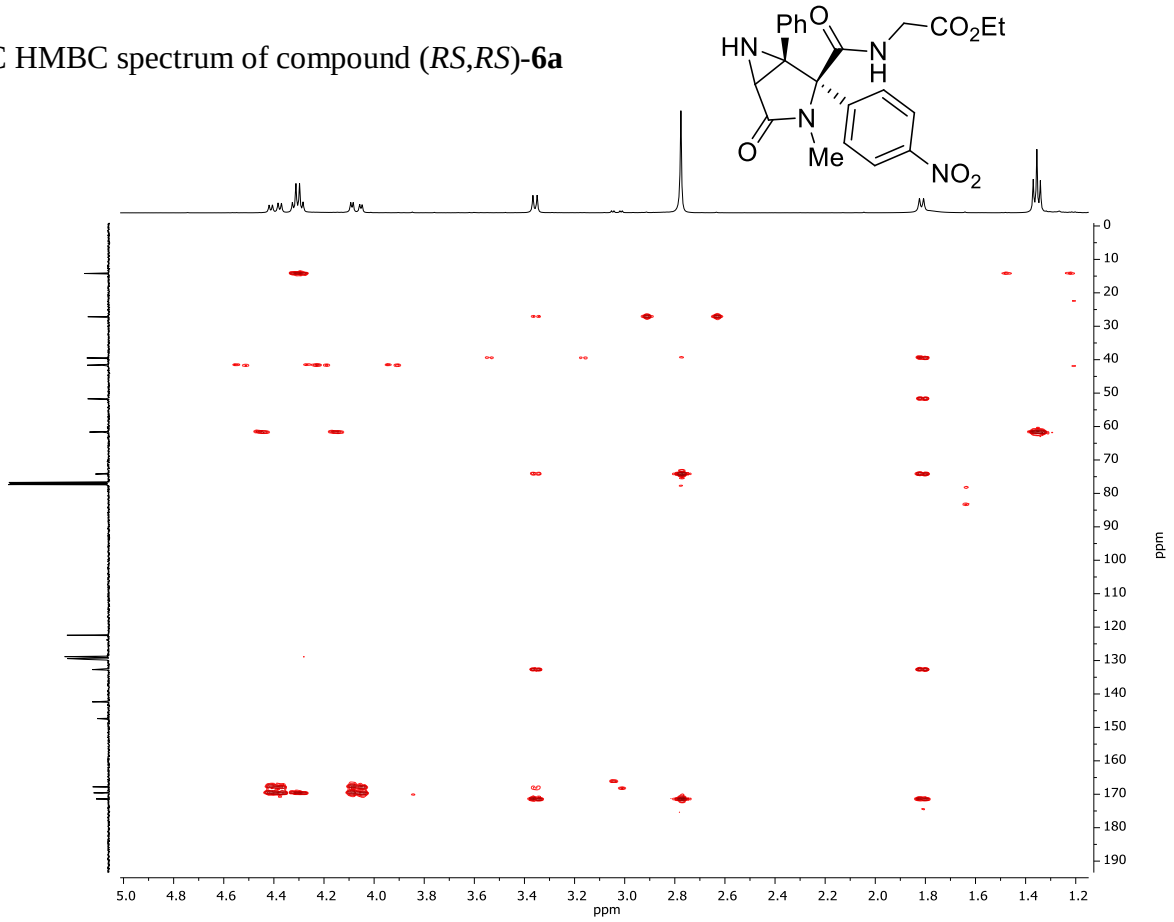
DEPT 135 spectrum of compound (*RS*,*RS*)-**6a**



^{1}H-^{13}C HSQC spectrum of compound (*RS*,*RS*)-**6a**



^{1}H-^{13}C HMBC spectrum of compound (*RS*,*RS*)-**6a**



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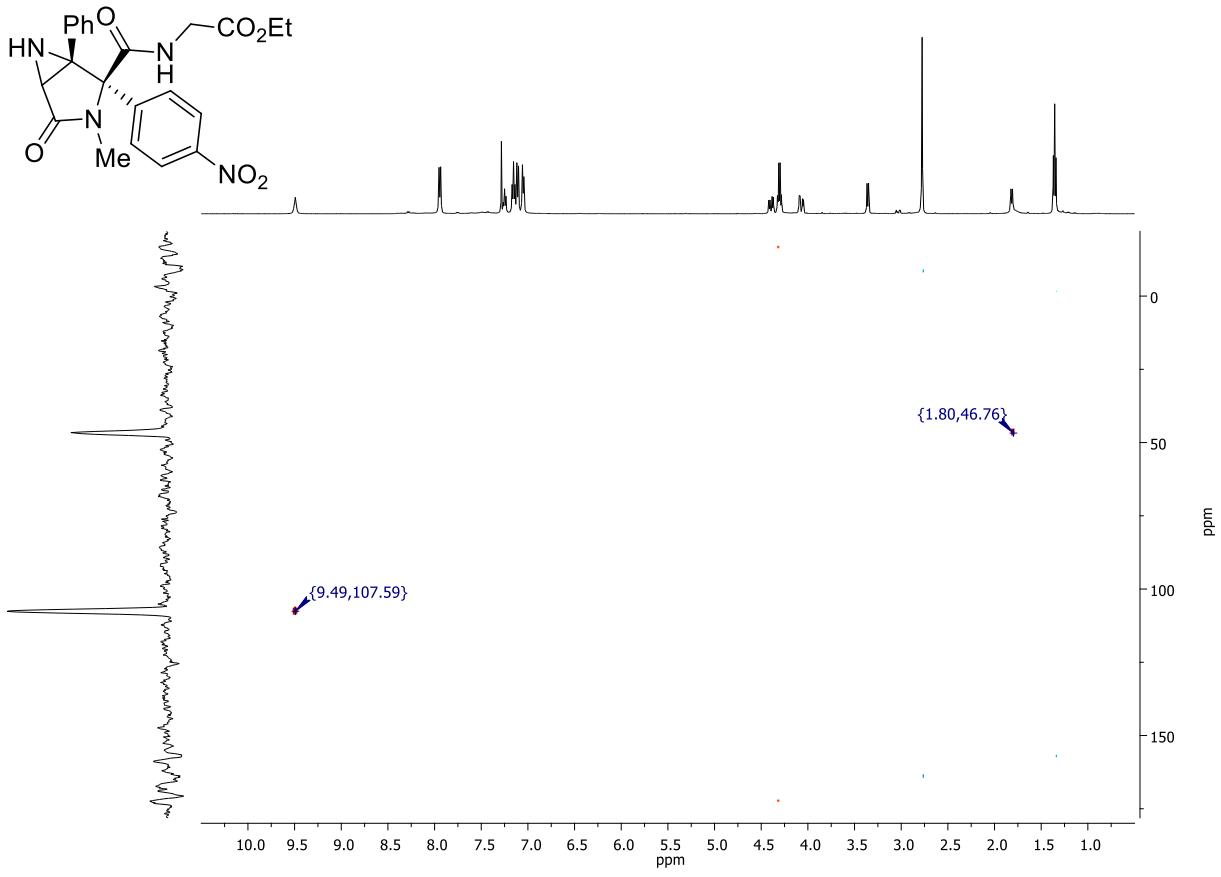
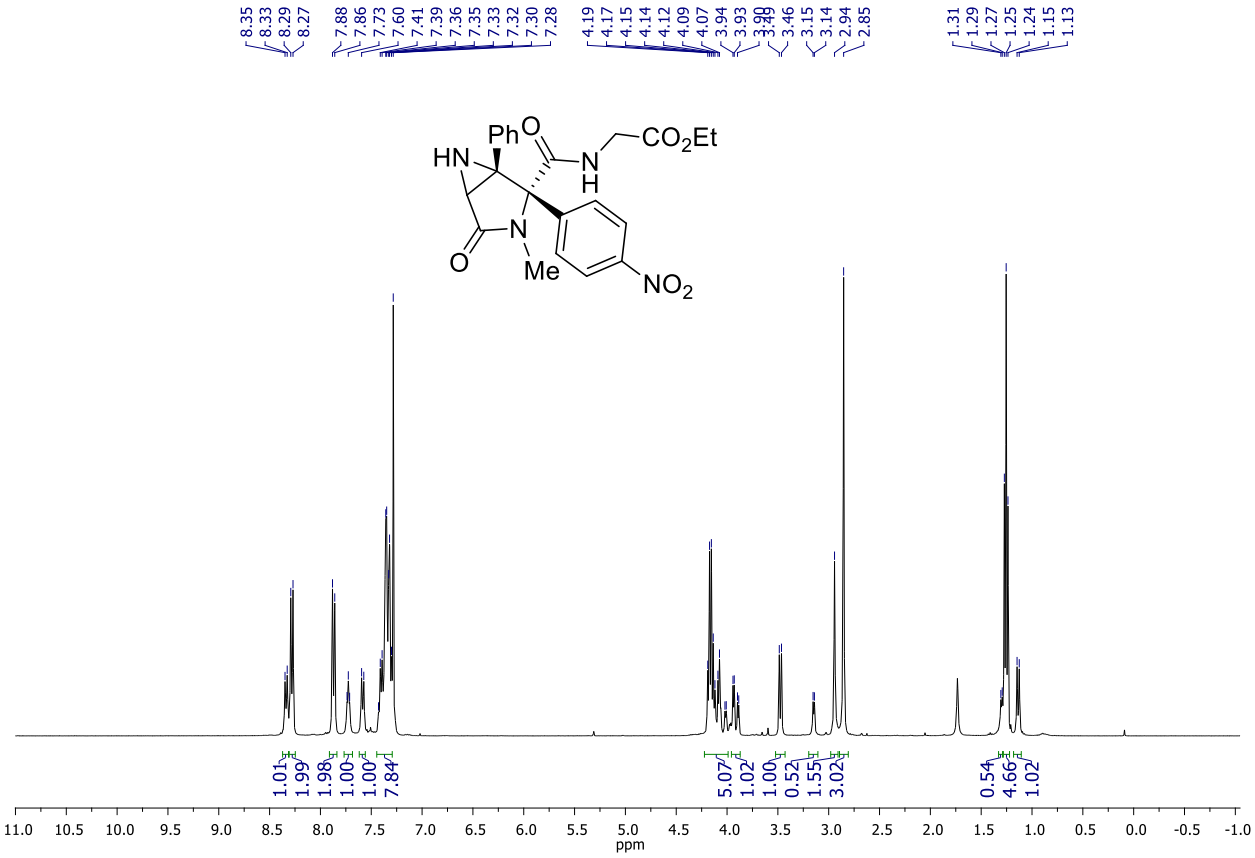
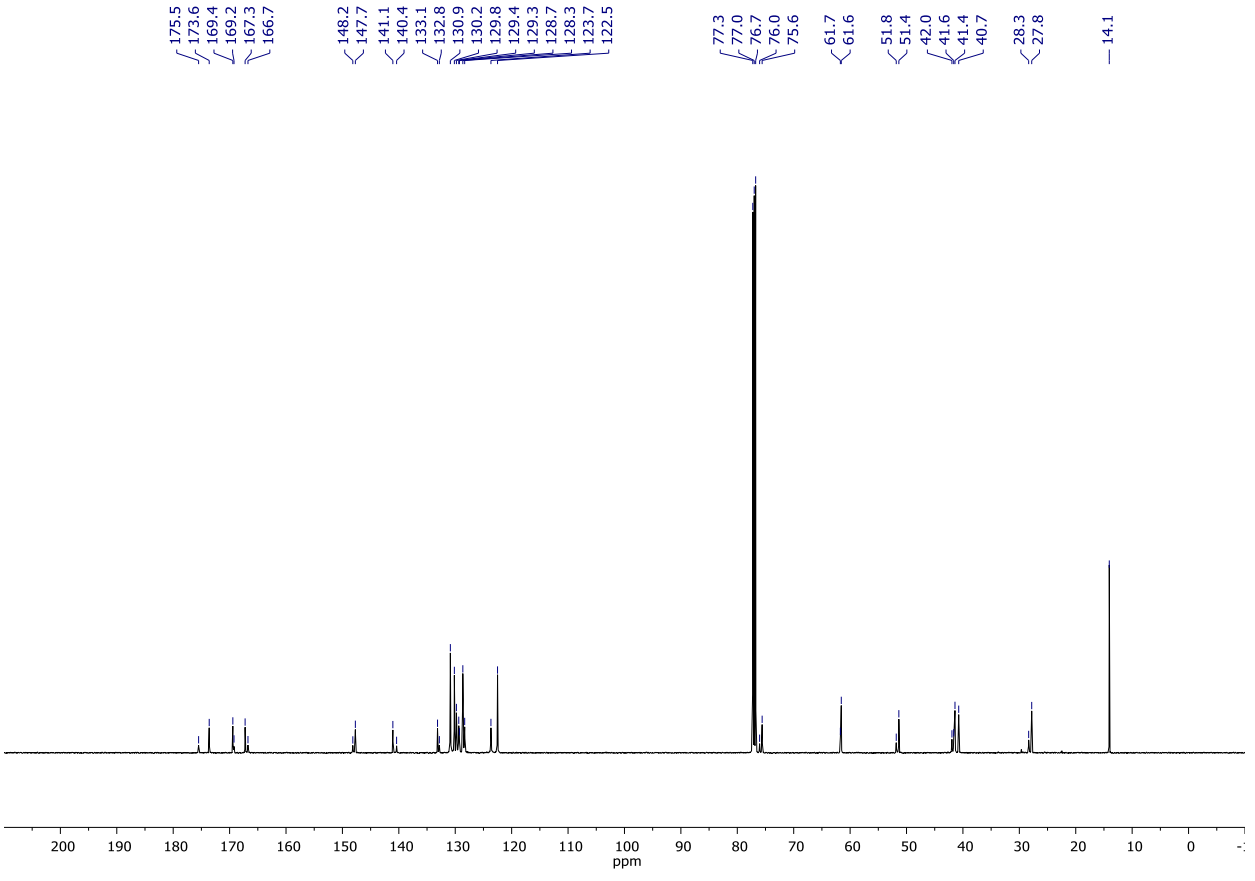
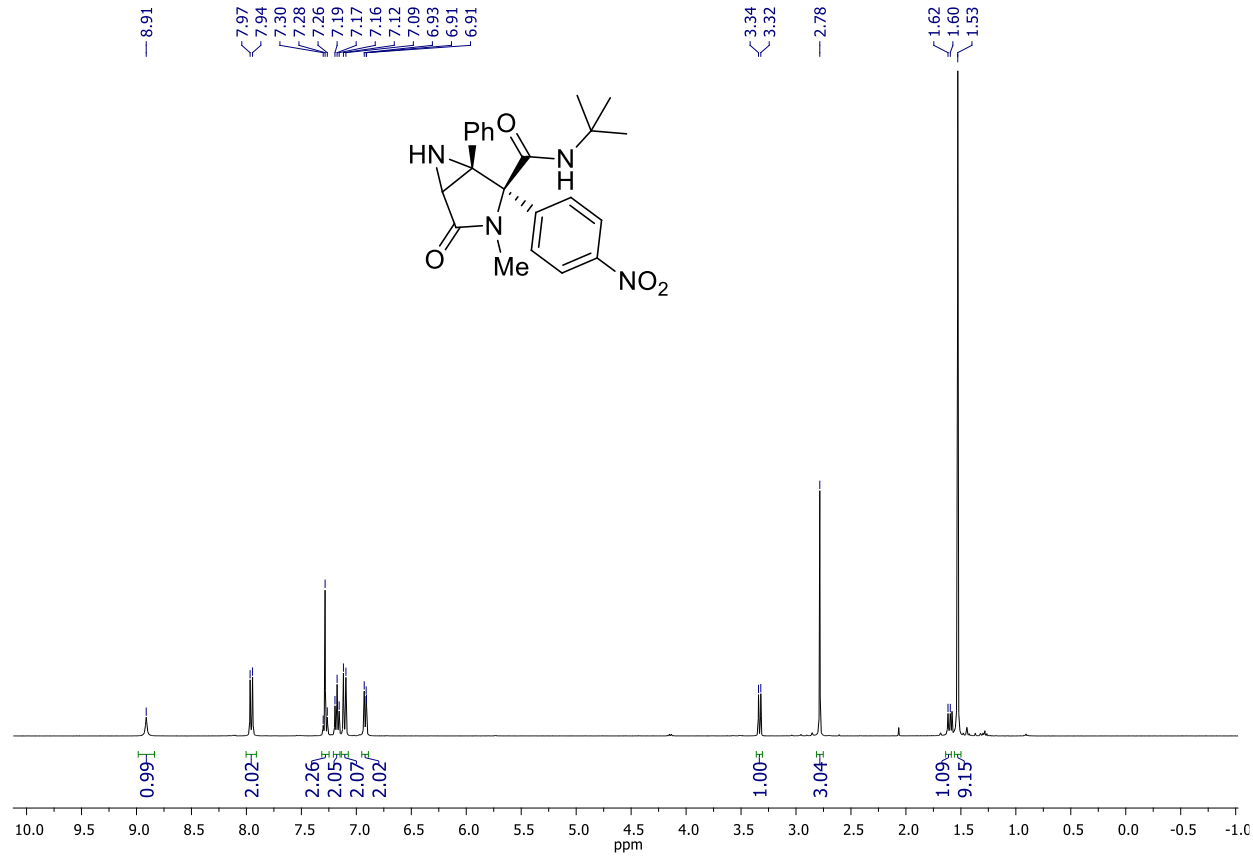


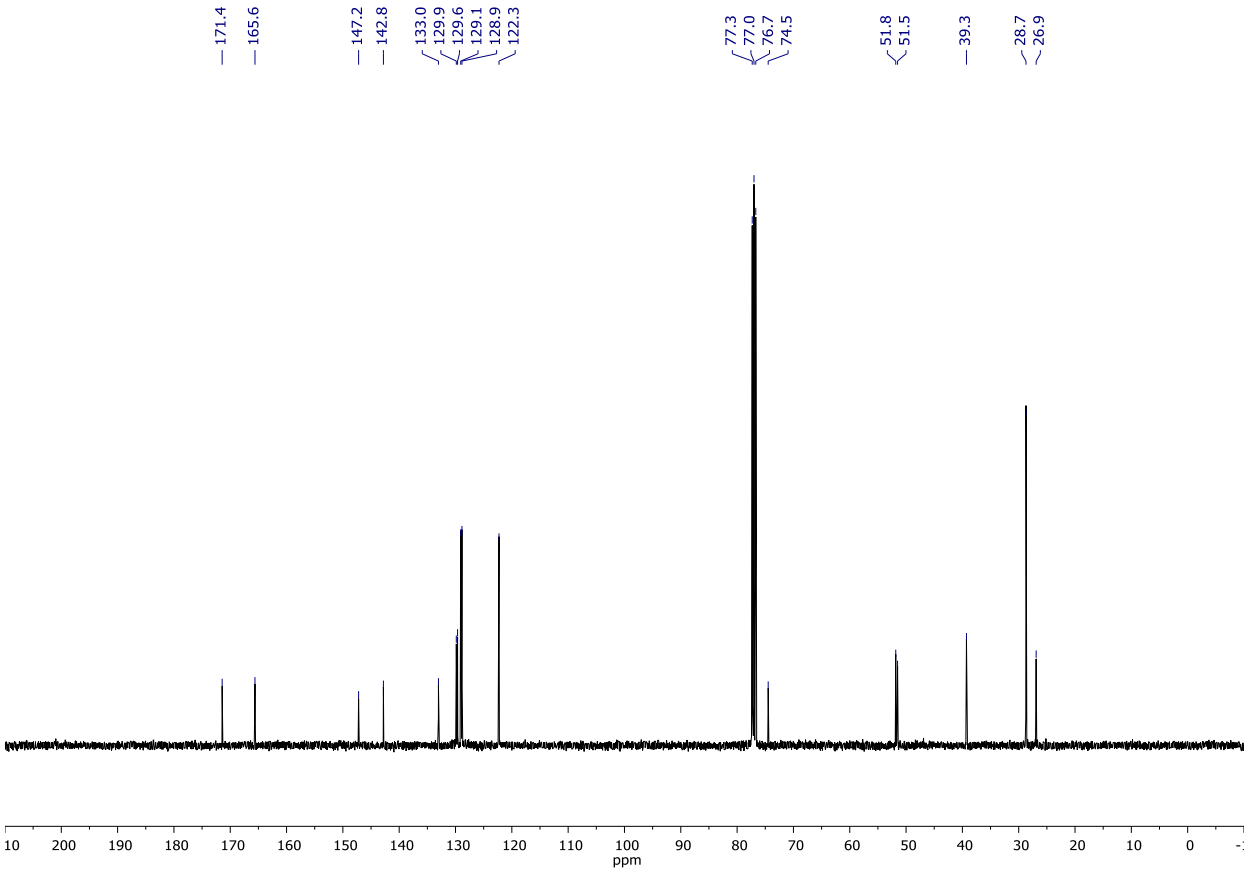
^{1}H and ^{13}C NMR spectra of compound (*RS*,*SR*)-**6a**



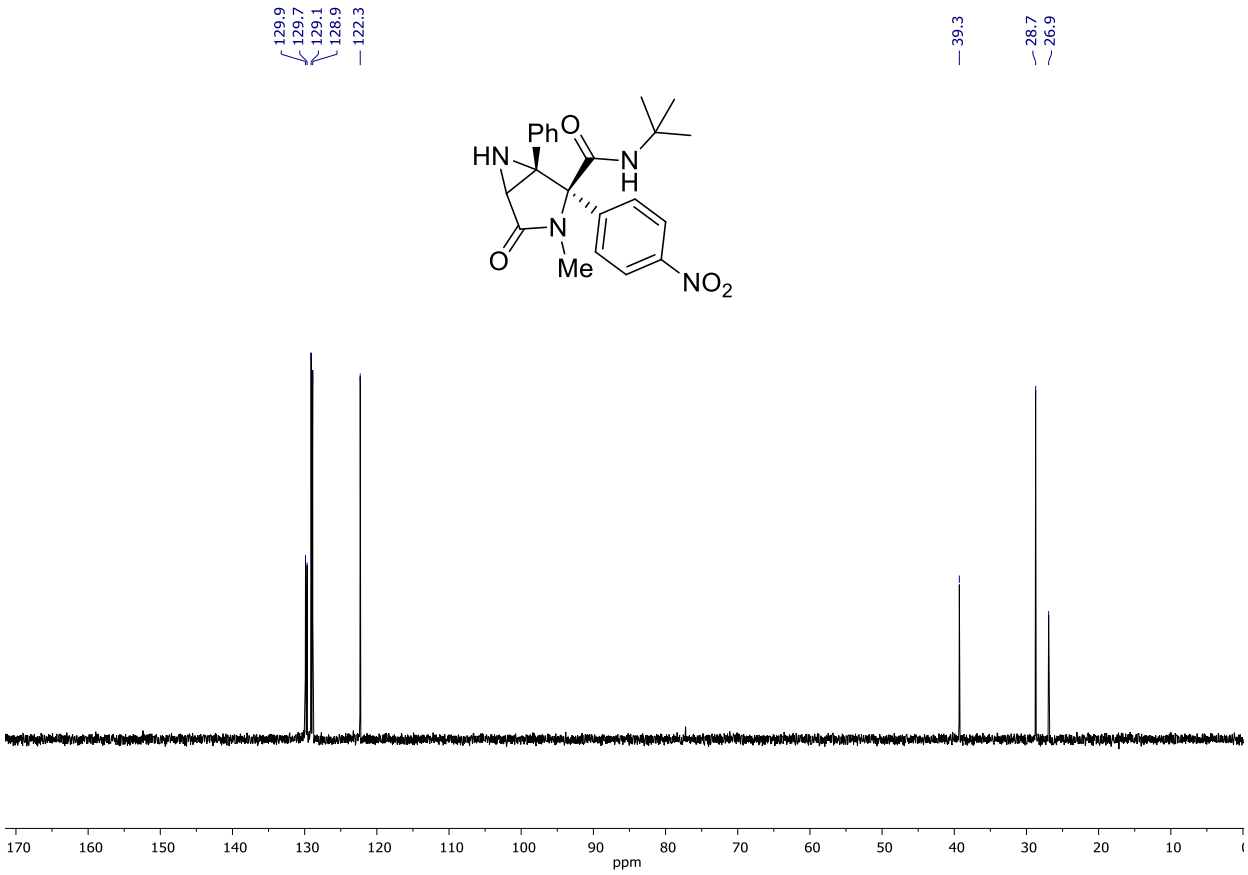


^{1}H and ^{13}C NMR spectra of compound (*RS*,*RS*)-**6b**

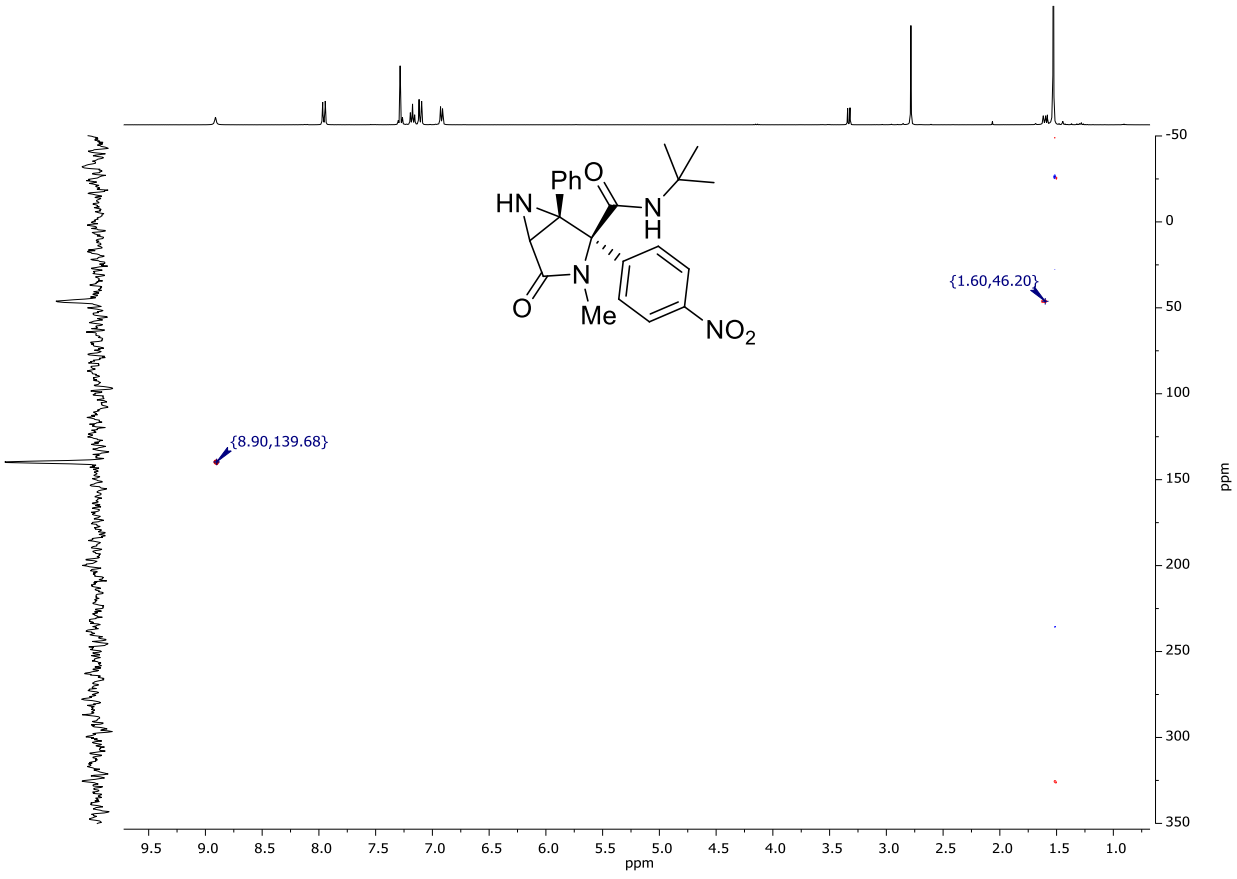




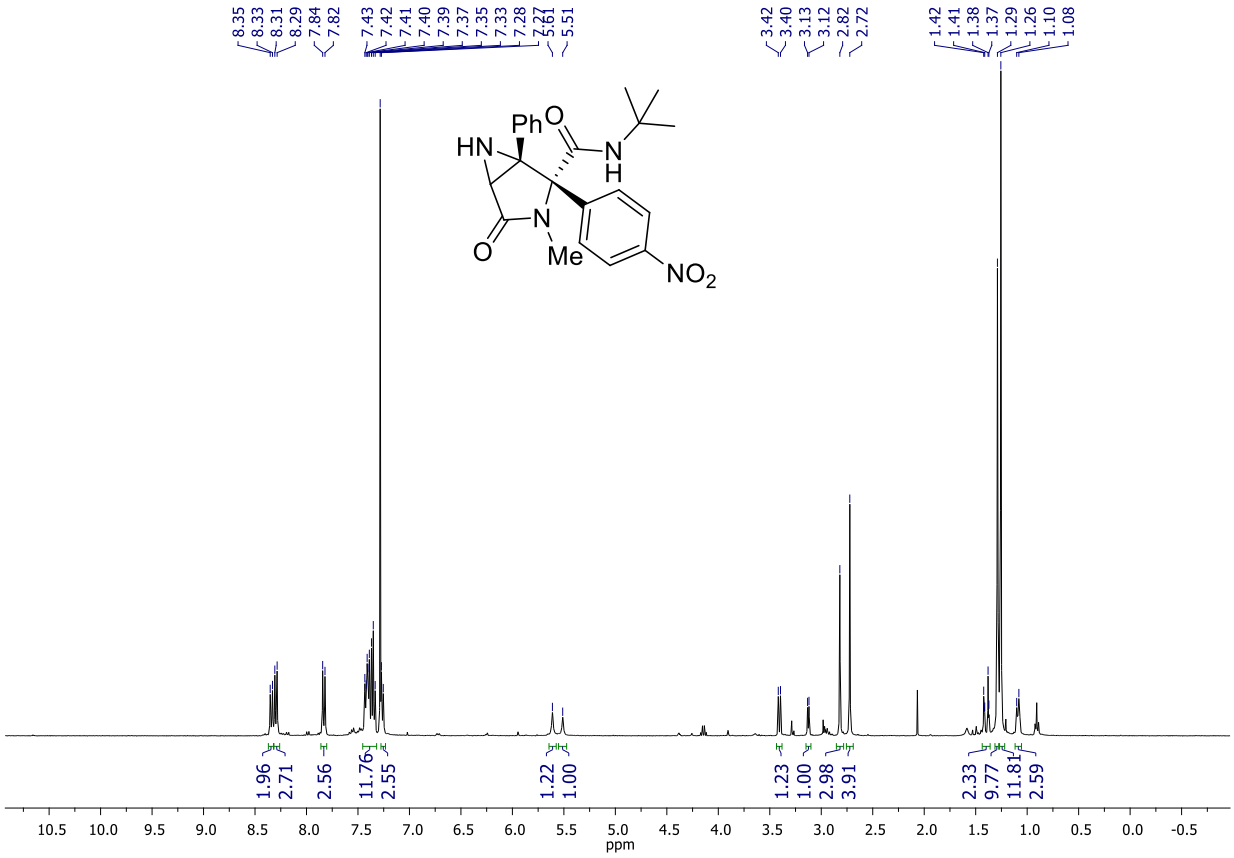
DEPT 135 spectrum of compound (*RS*,*RS*)-**6b**



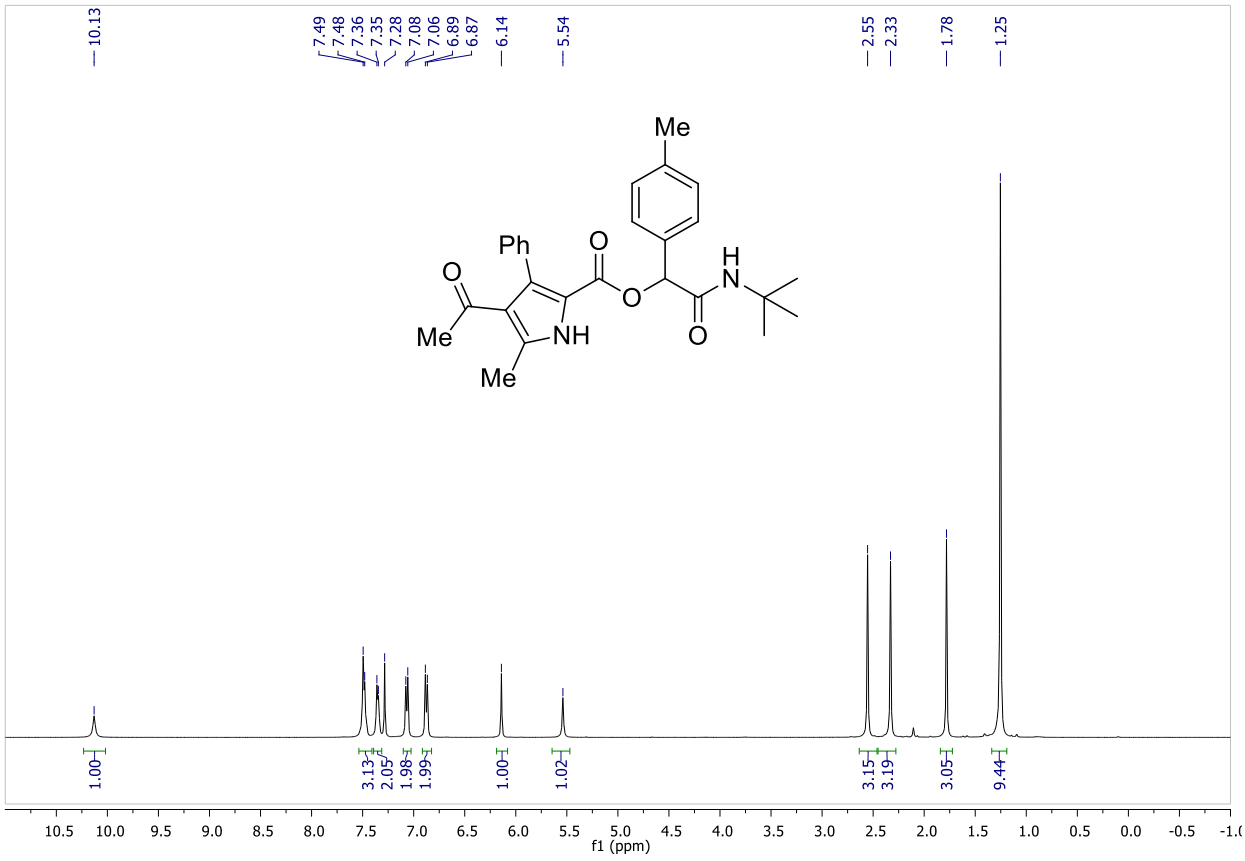
^{1}H-^{15}N HSQC spectrum of compound (*RS*,*RS*)-**6b**

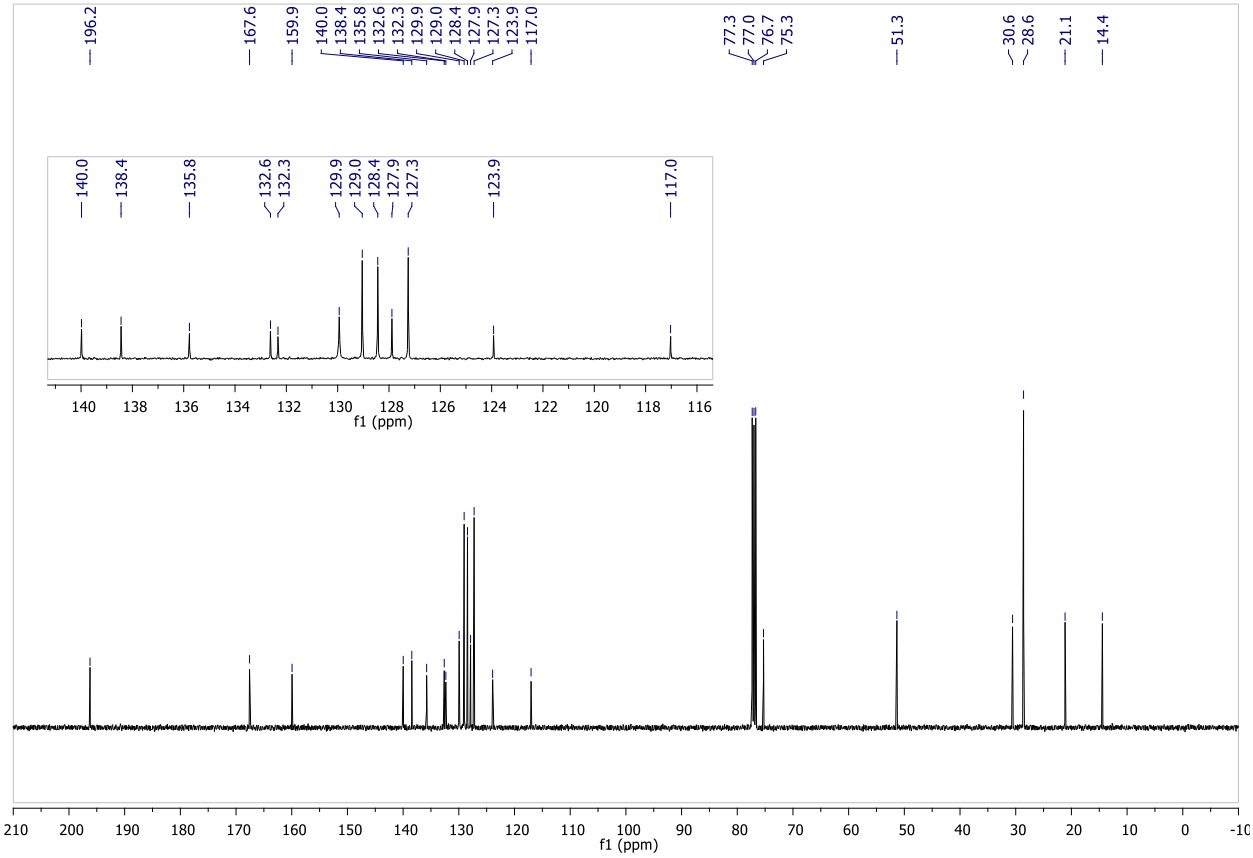


^{1}H NMR spectrum of compound (*RS*,*SR*)-**6b**

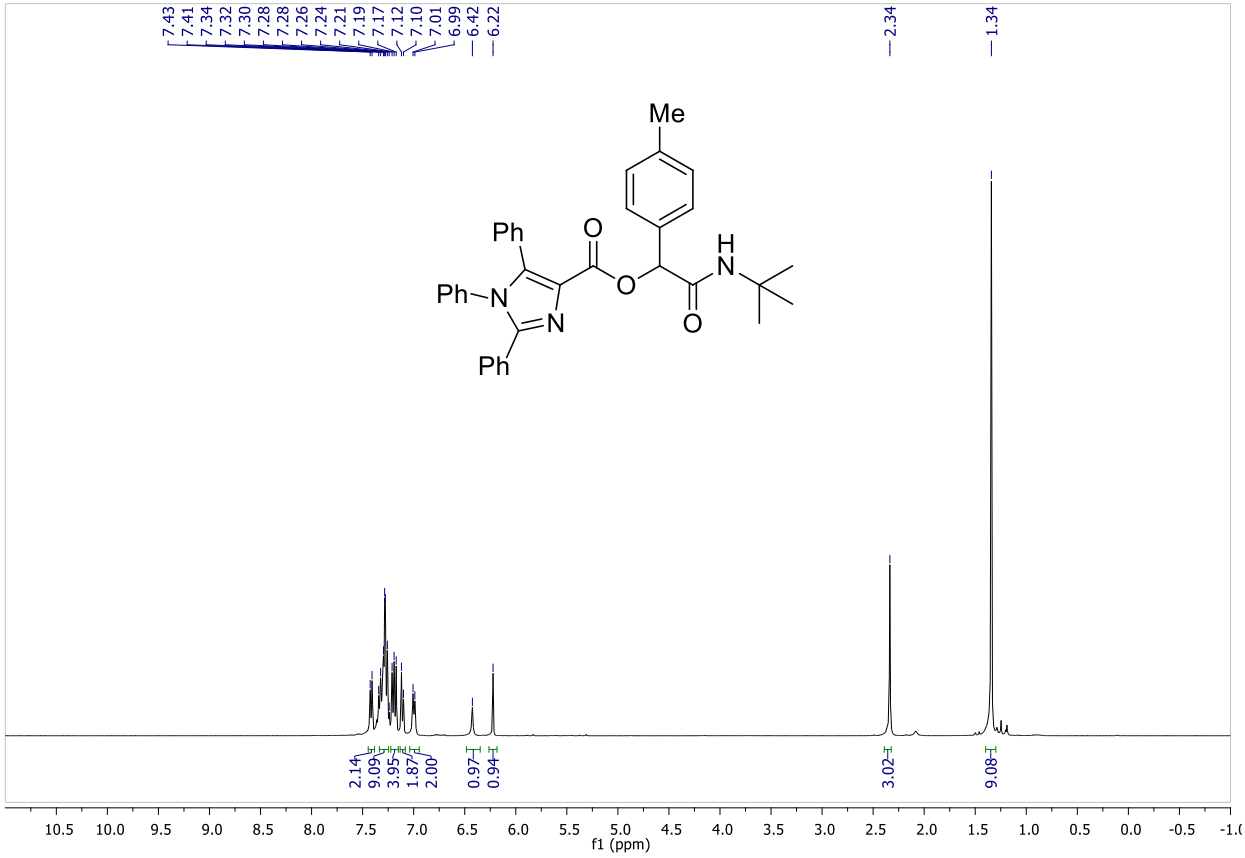


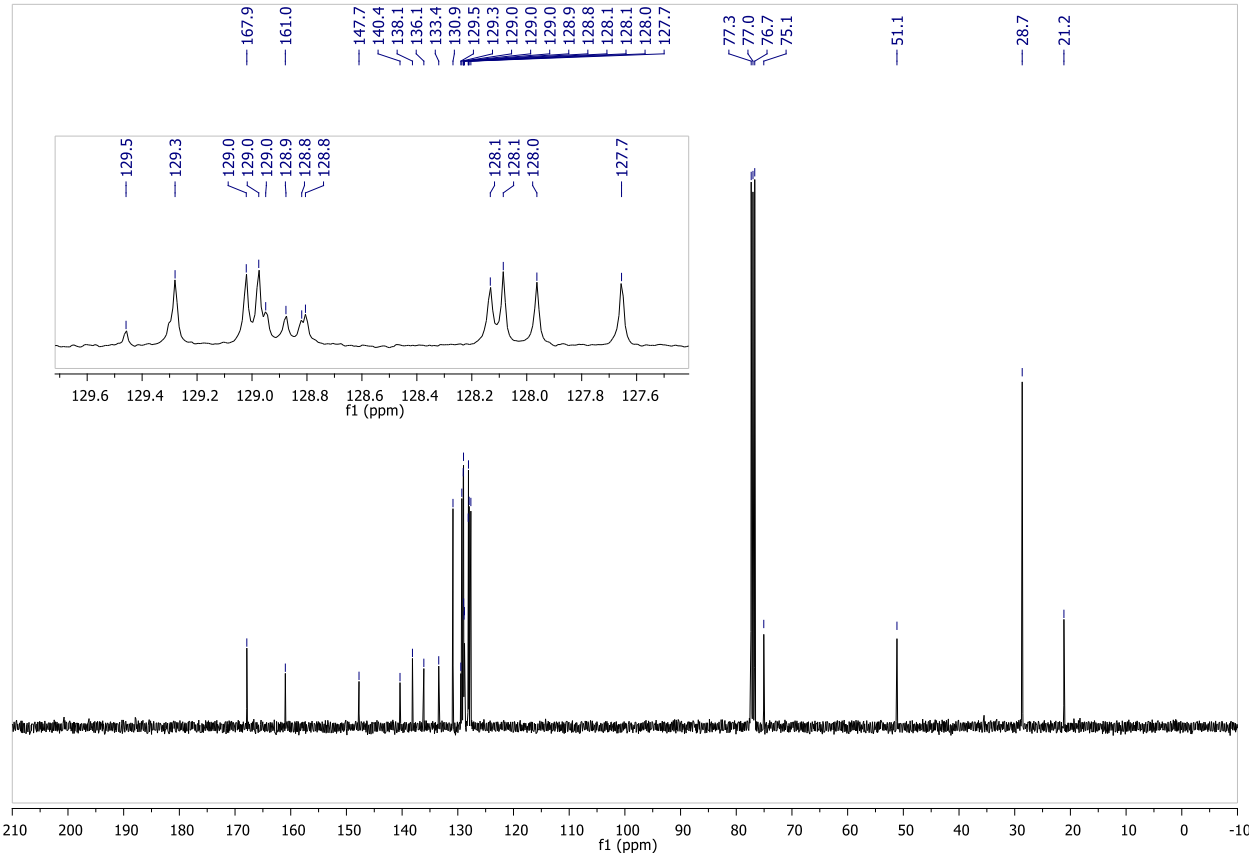
^{1}H and ^{13}C NMR spectra of compound **7**



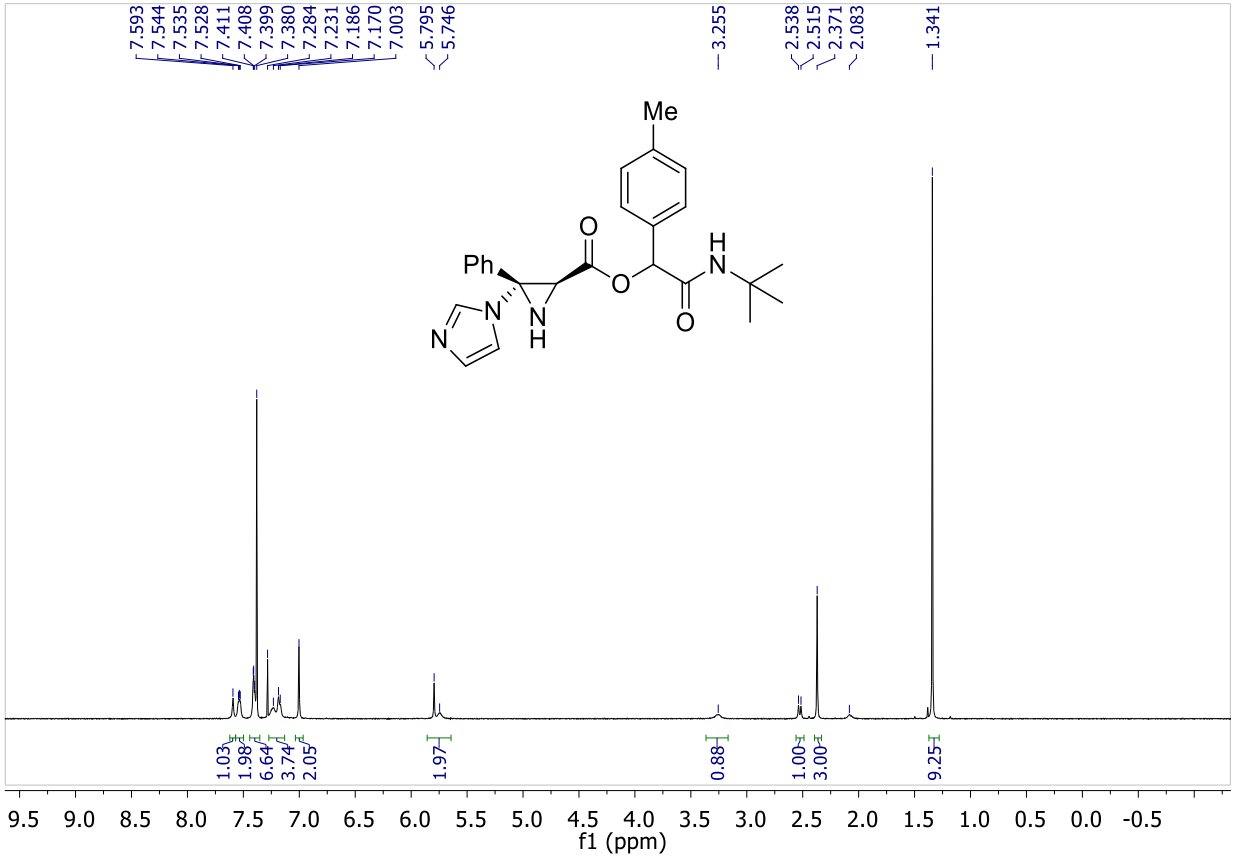


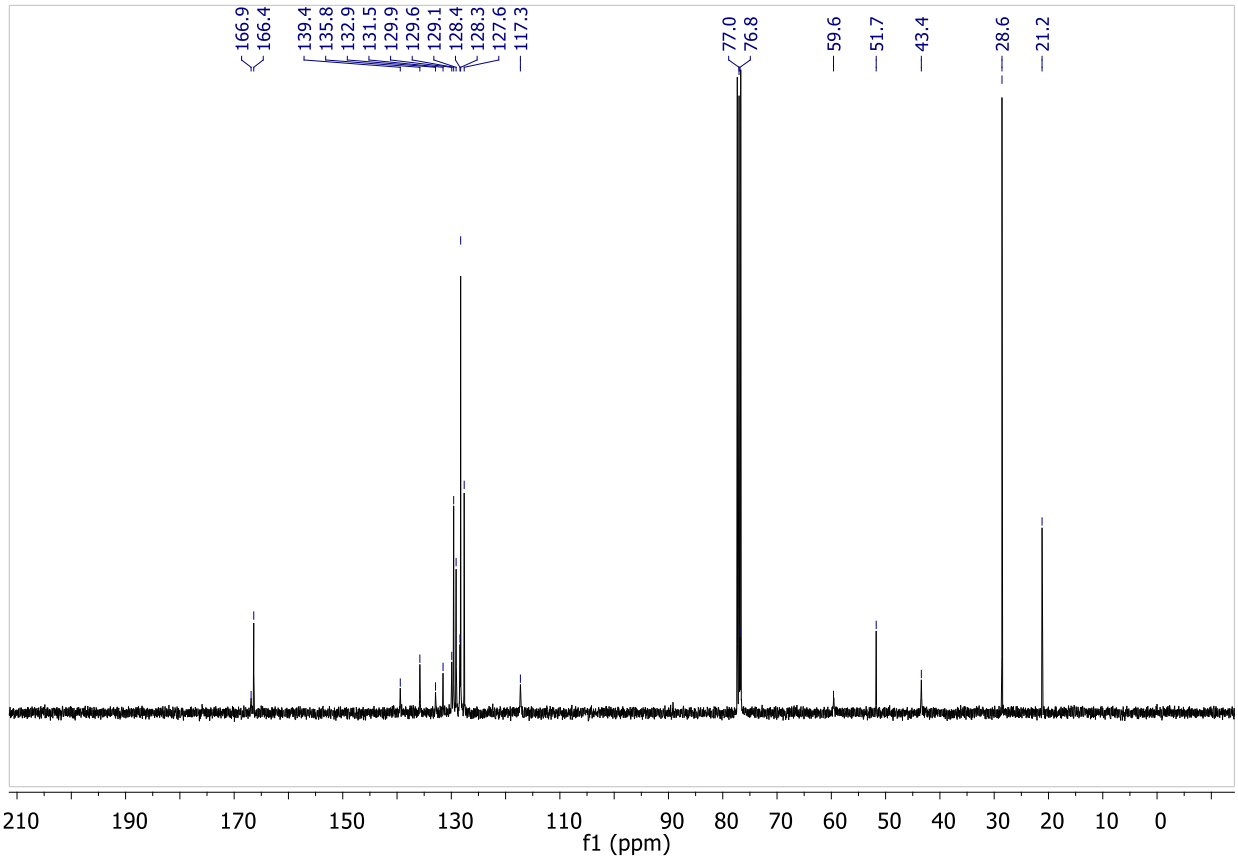
^{1}H and ^{13}C NMR spectra of compound **8**



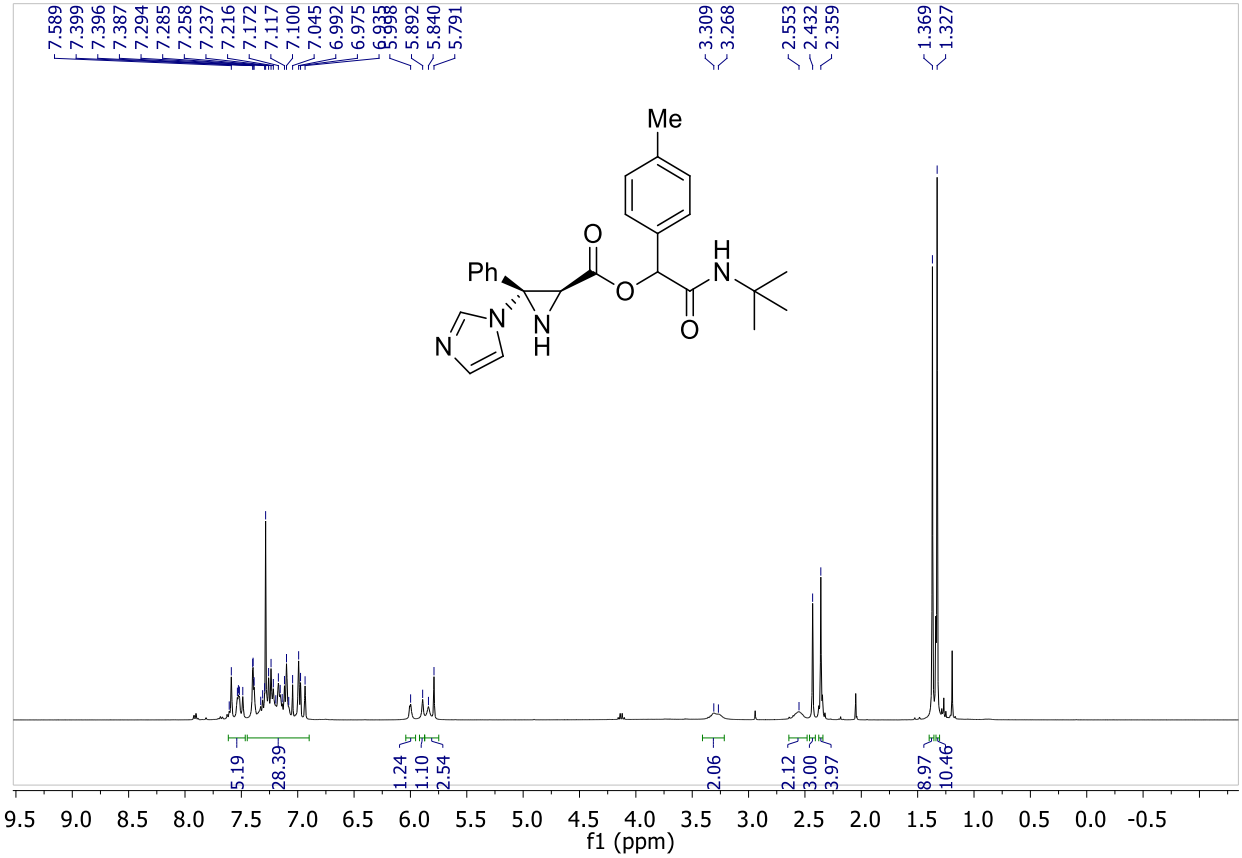


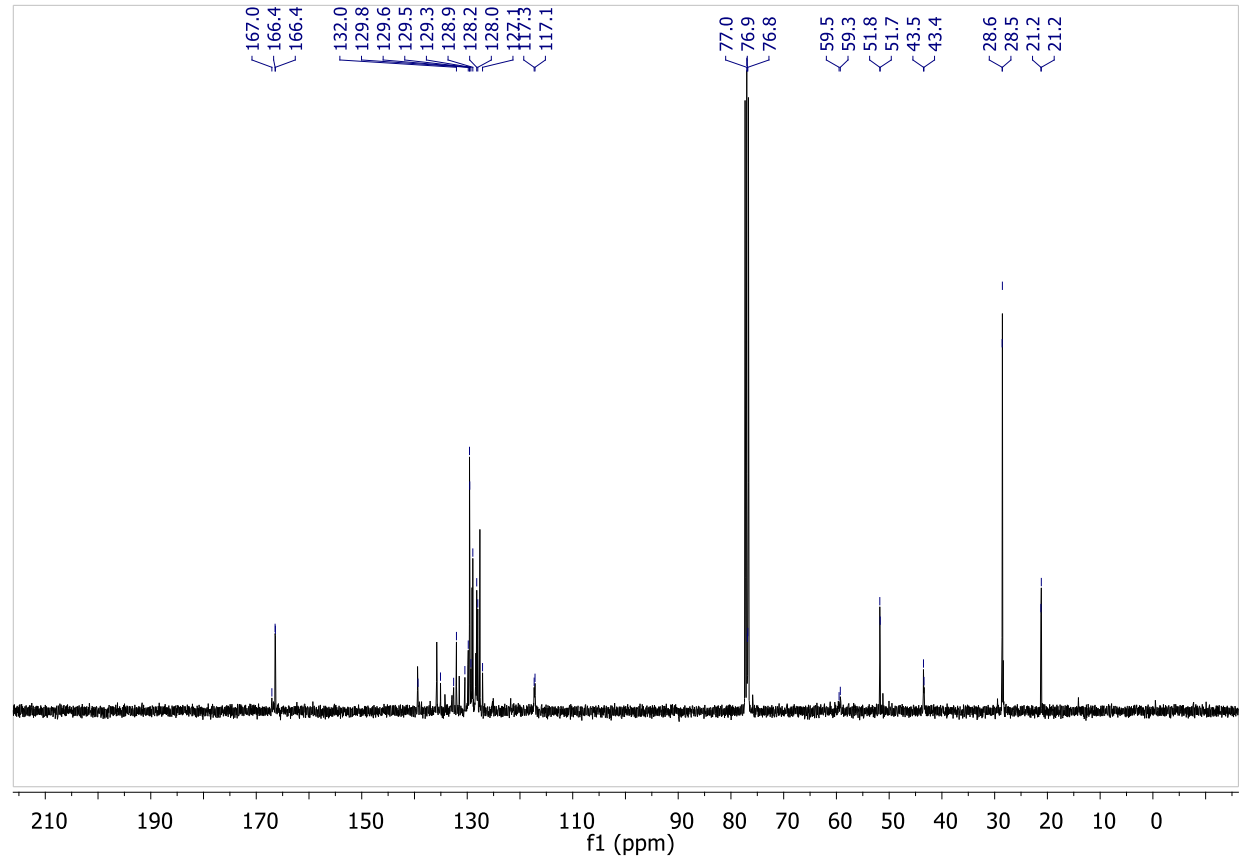
^{1}H and ^{13}C NMR spectra of compound **9** (separated diastereomer)



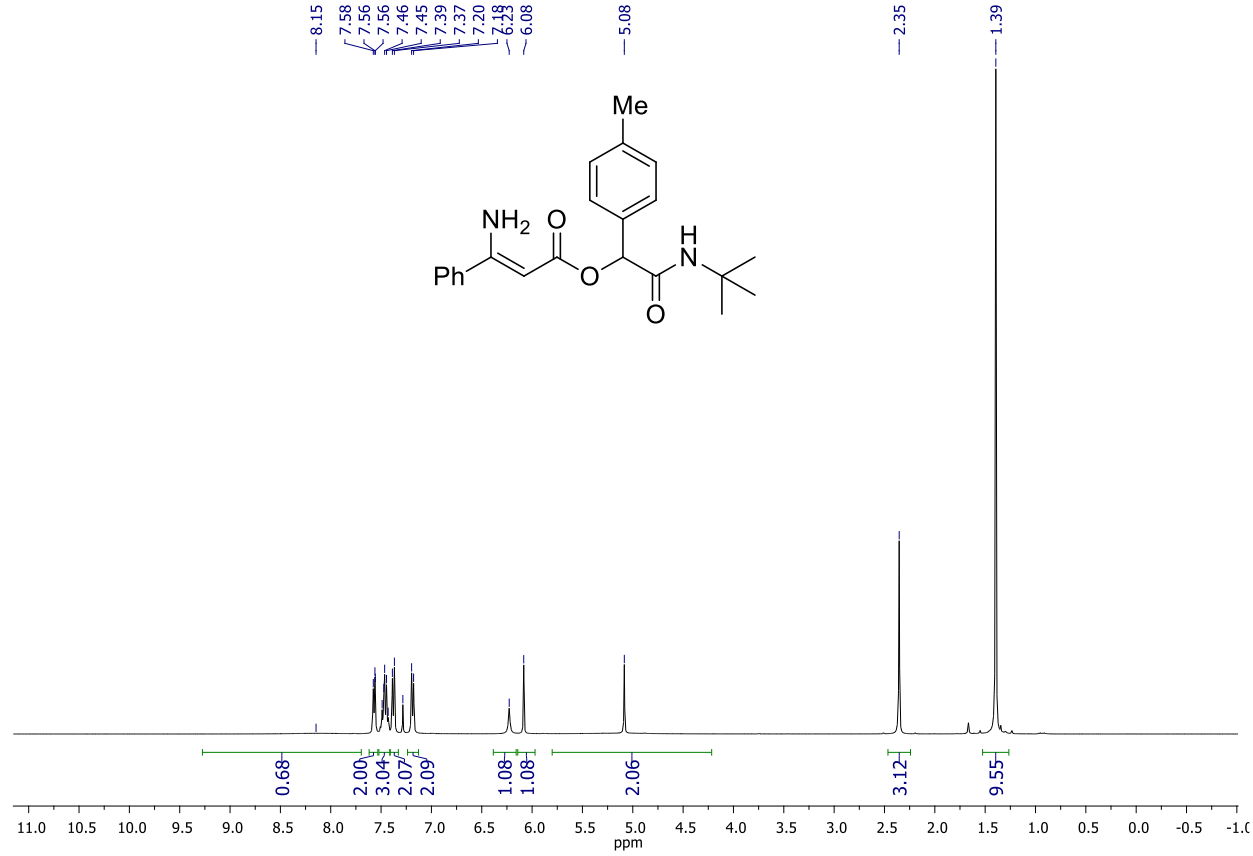


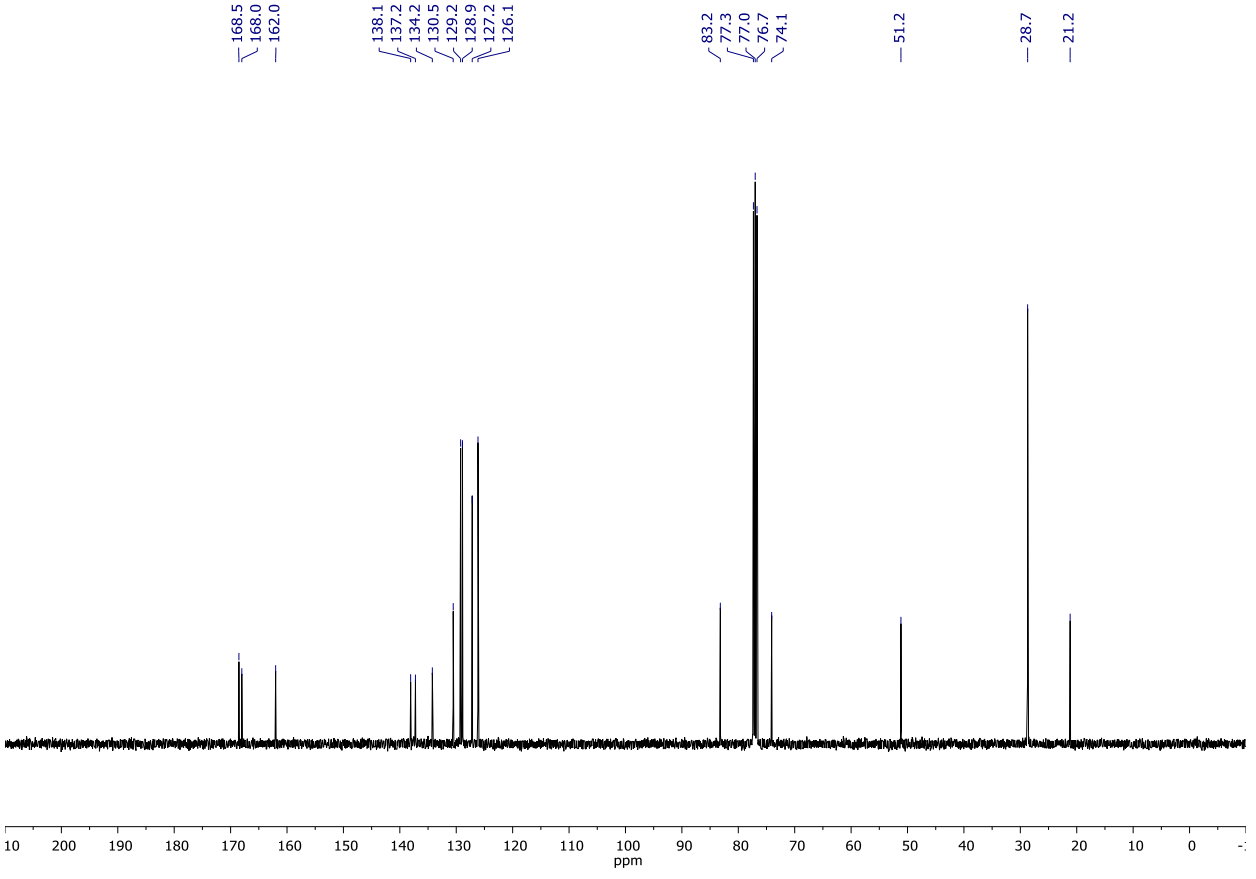
^{1}H and ^{13}C NMR spectra of compound **9** (mixture of diastereomers)



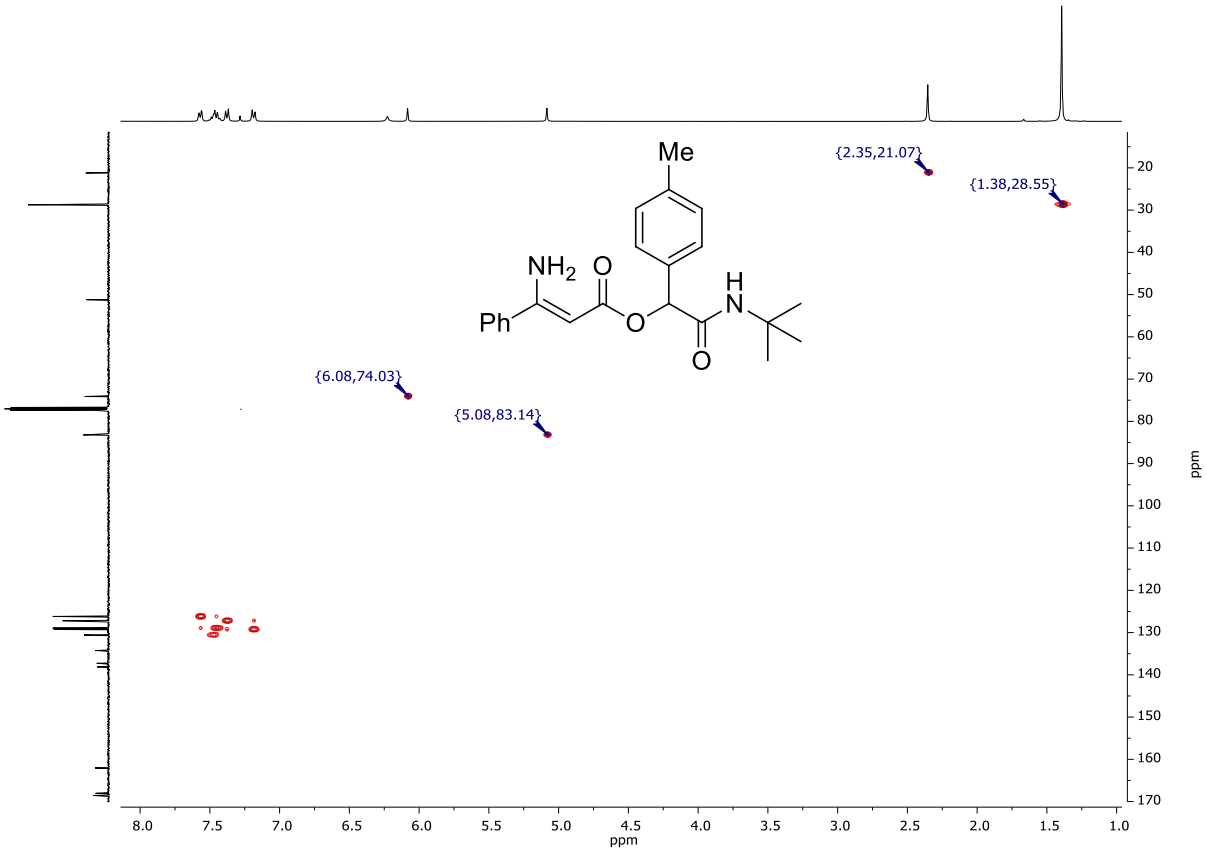


^{1}H and ^{13}C NMR spectra of compound **10**

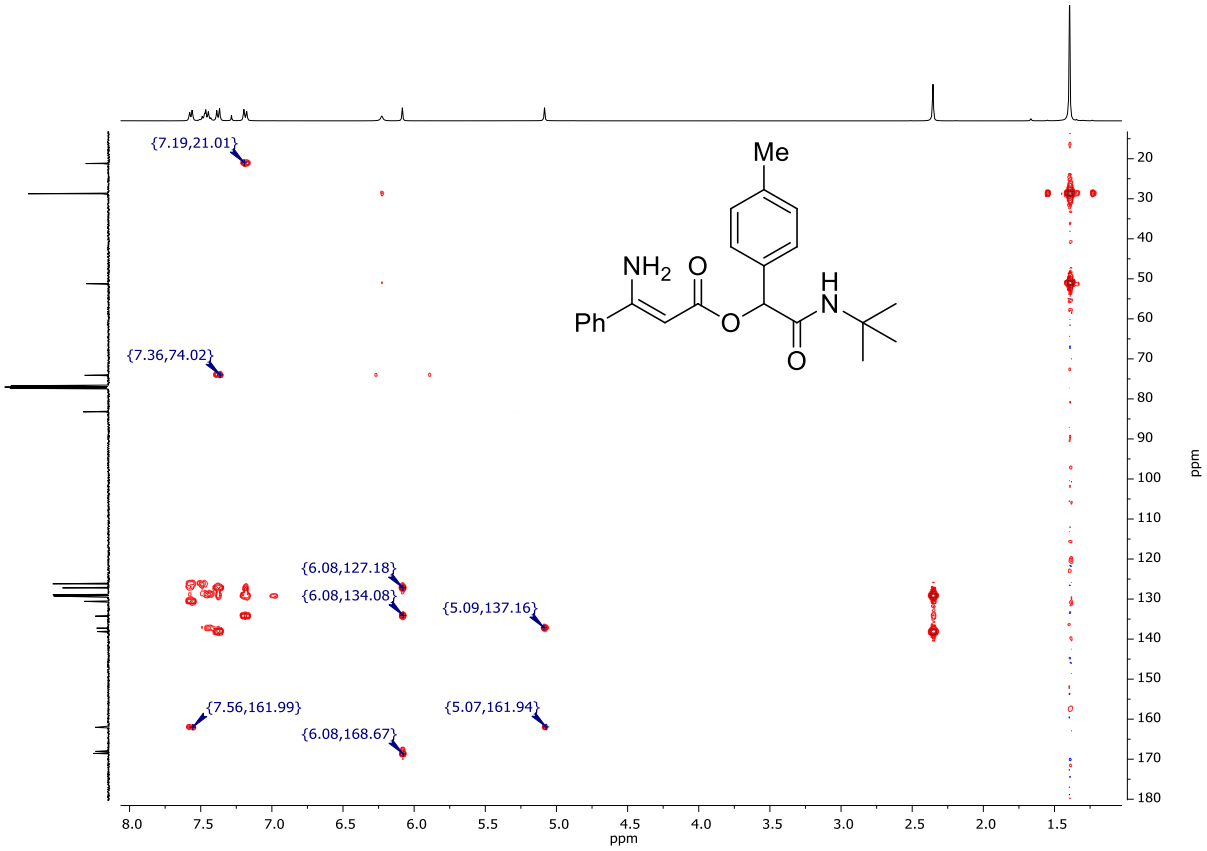




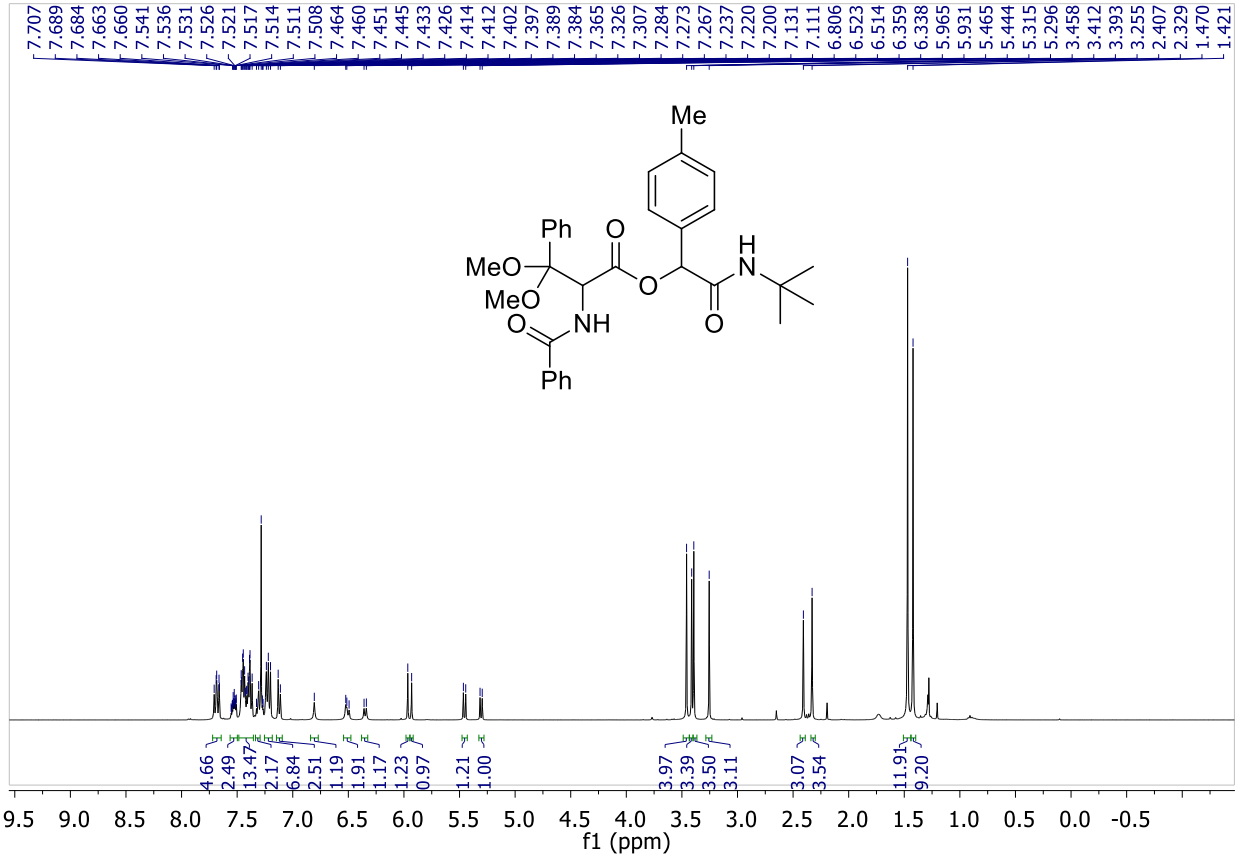
^{1}H-^{13}C HSQC spectrum of compound **10**

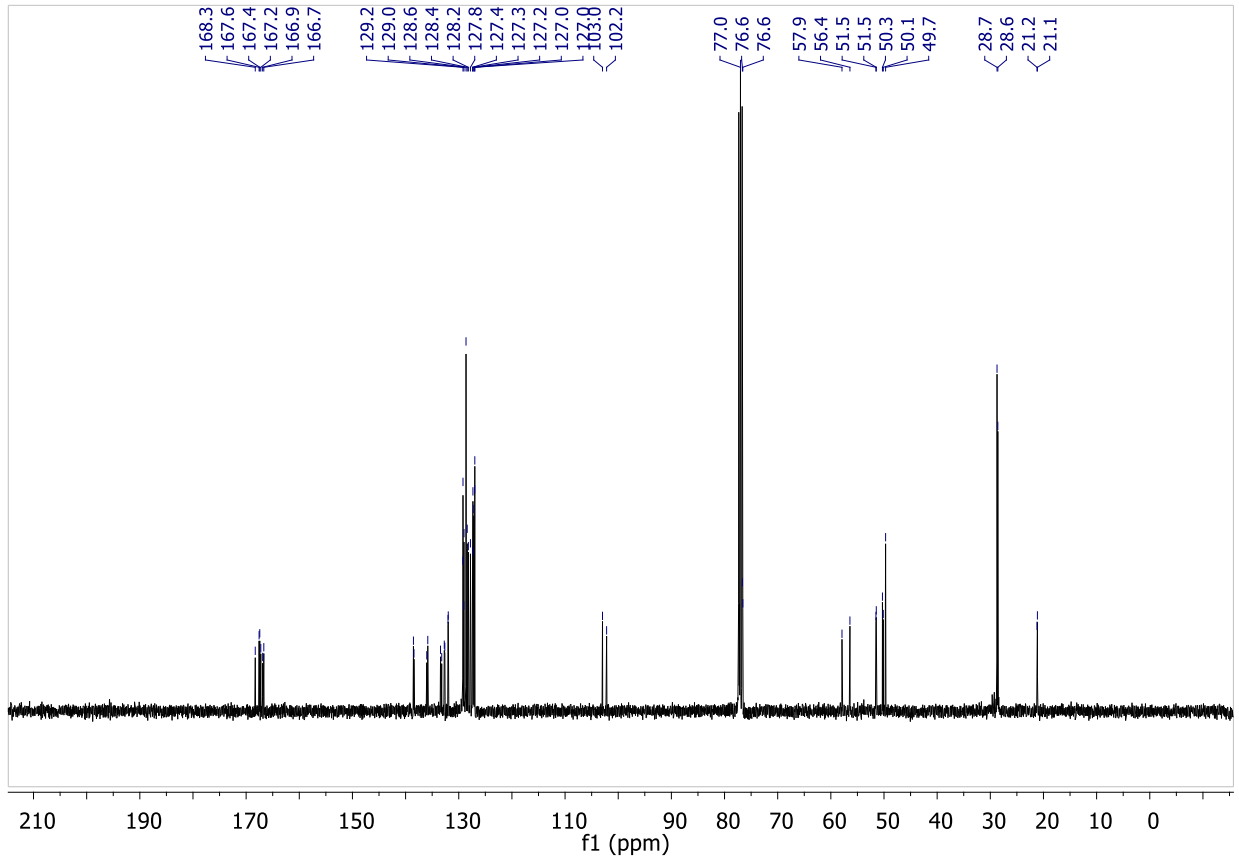


^{1}H-^{13}C HMBC spectrum of compound **10**



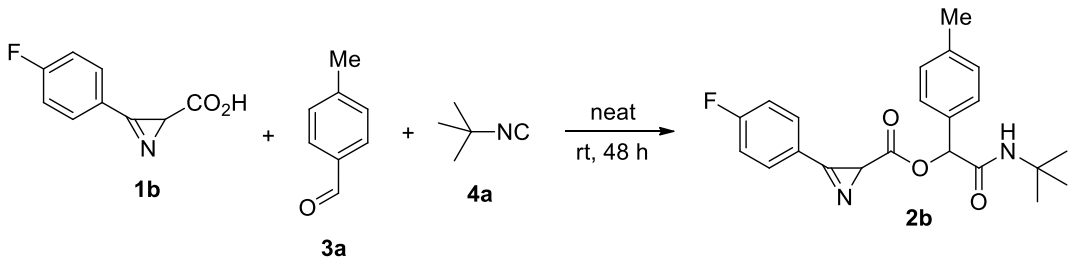
^{1}H and ^{13}C NMR spectra of compound **11**



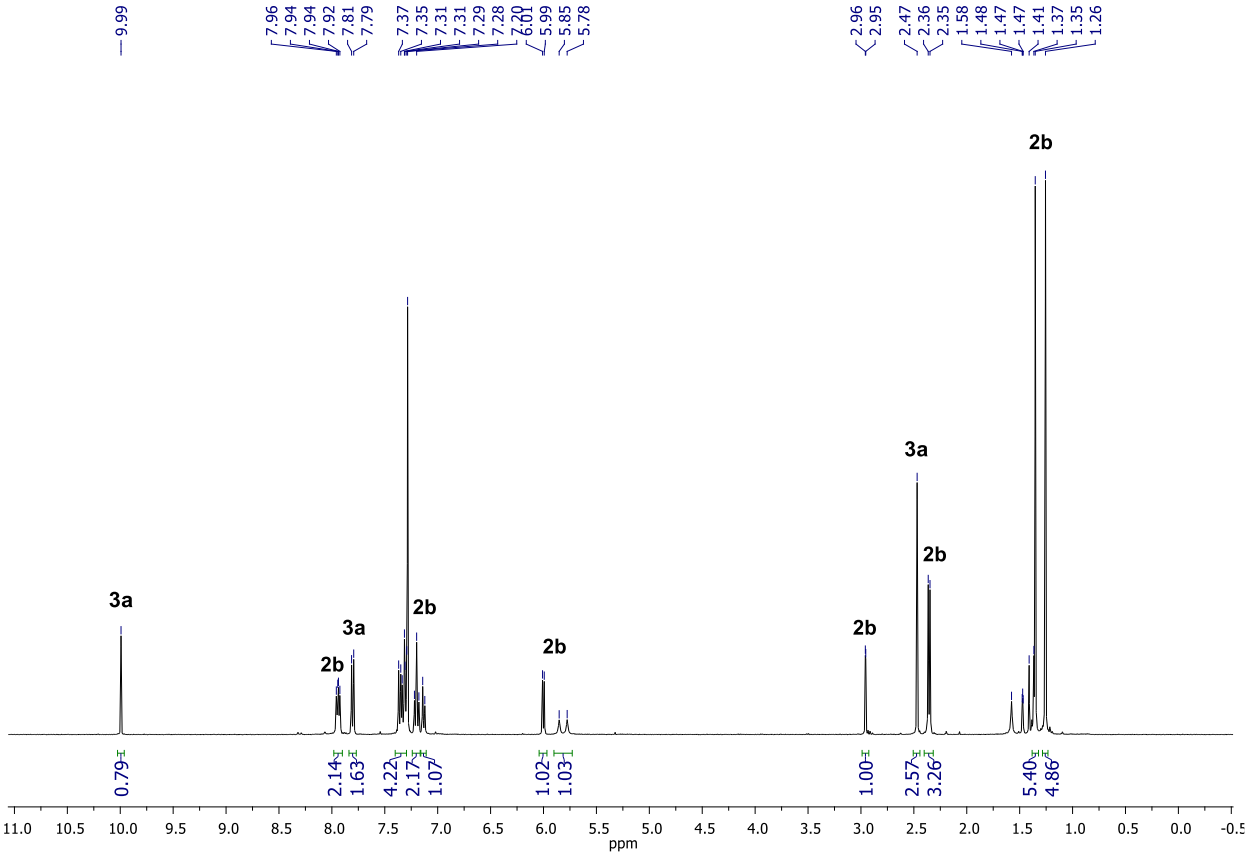


5. ^{1}H NMR spectra and LC-MS data of the reaction mixtures (2b and 2r)

Reaction mixture A:



^{1}H NMR spectrum of the reaction mixture A



LC-MS data of the reaction mixture A

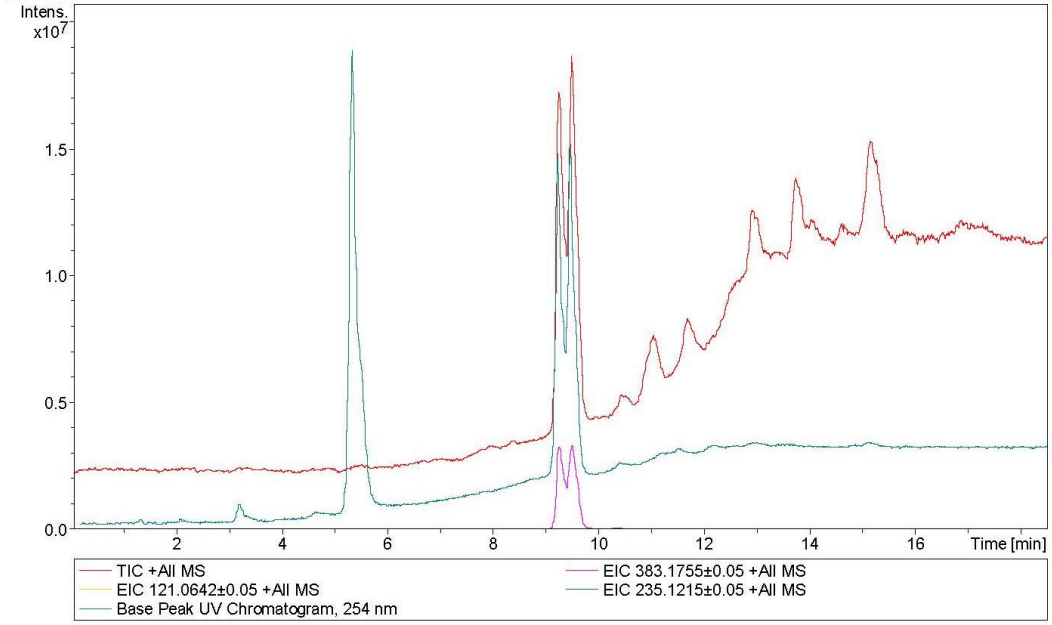
Display Report

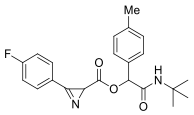
Analysis Info

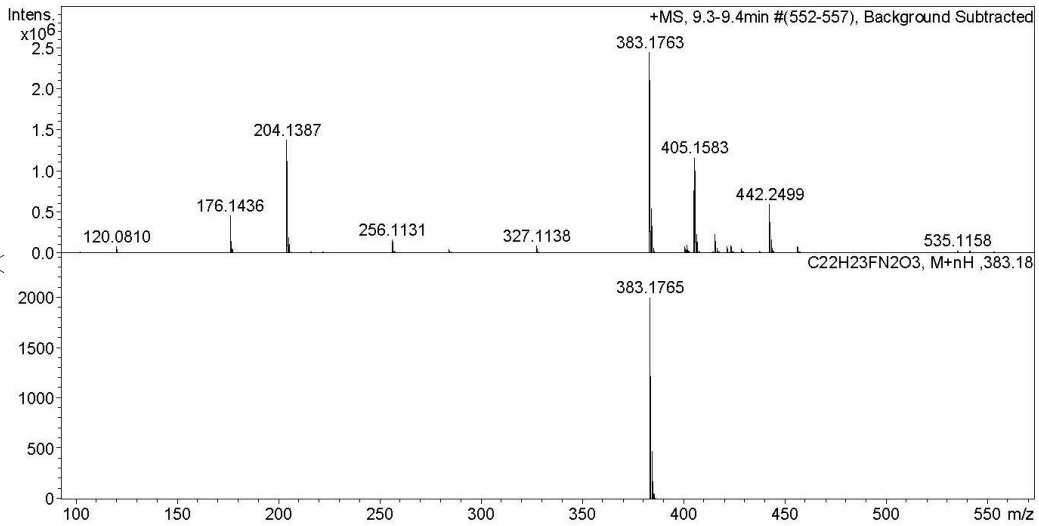
Analysis Name	D:\Data\Work\2020\HPLCMS\Org_Ls-MS\NR_sample1_55-95___P1-F-5_01_2160.d	Acquisition Date	28-Oct-20 20:10:20
Method	tune_low_pos_100_1000_200ulmin.m	Operator	BDAL@DE
Sample Name	NR_sample1_55-95__	Instrument / Ser#	maXis 62
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Active			Set Dry Heater	180 °C
Scan Begin	100 m/z	Set Capillary	4500 V	Set Dry Gas	6.0 l/min
Scan End	1000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source







LC-MS data of aldehyde **3a**

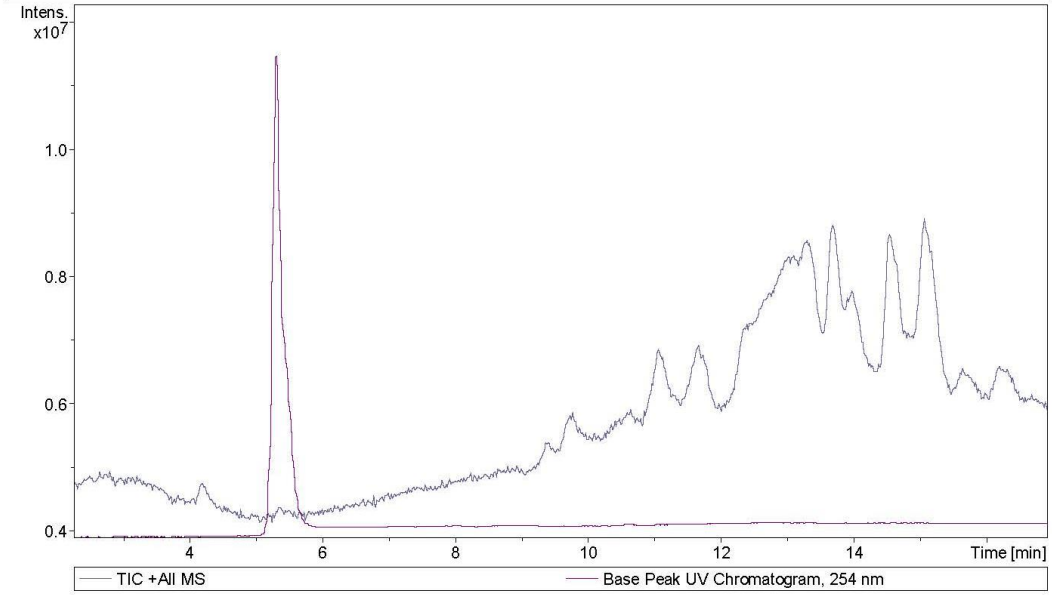
Display Report

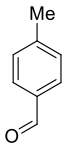
Analysis Info

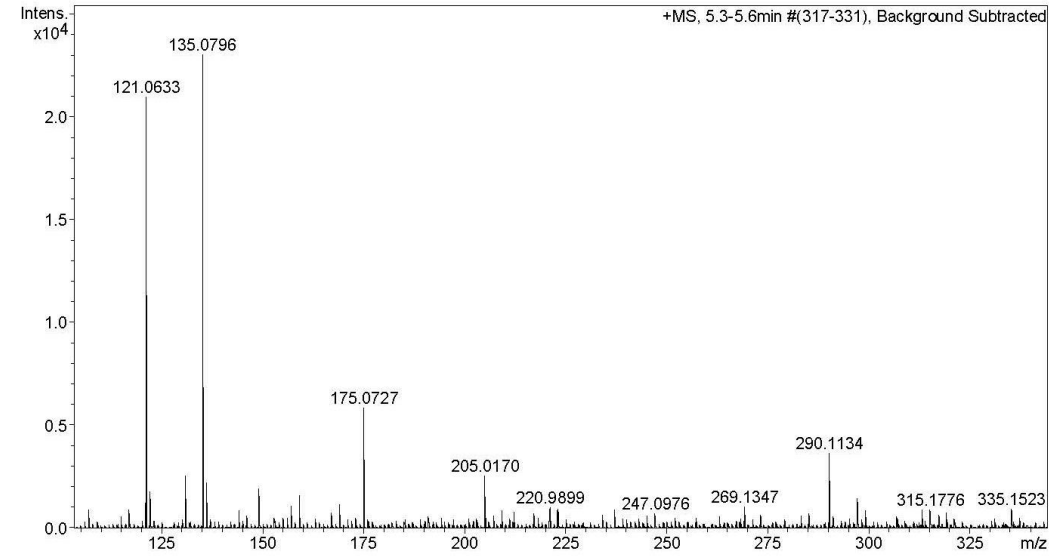
Analysis Name	D:\Data\Work\2020\HPLCMS\Org_Ls-MS\Aldehyde_sample1_55-95_2_P1-F-4_01_2184.d	Acquisition Date	30-Oct-20 19:19:24
Method	tune_low_pos_100_1000_200ulmin.m	Operator	BDAL@DE
Sample Name	Aldehyde_sample1_55-95_2	Instrument / Ser#	maXis 62
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Active			Set Dry Heater	180 °C
Scan Begin	100 m/z	Set Capillary	4500 V	Set Dry Gas	6.0 l/min
Scan End	1000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source

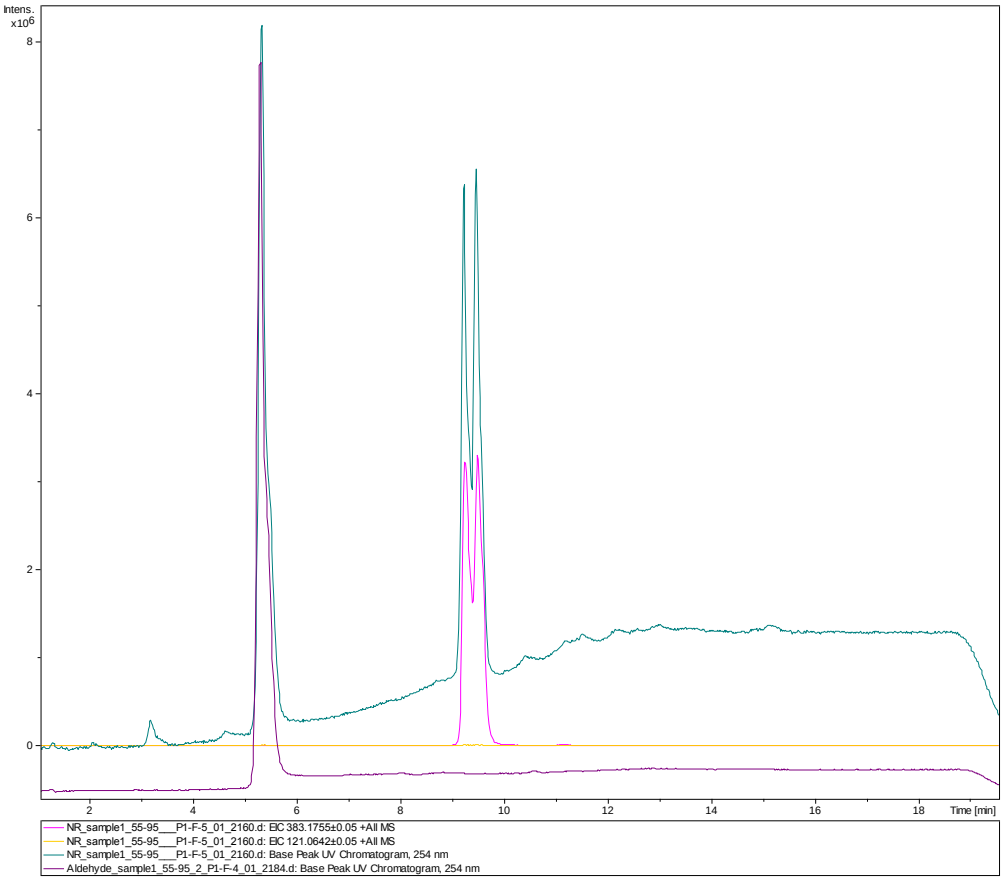


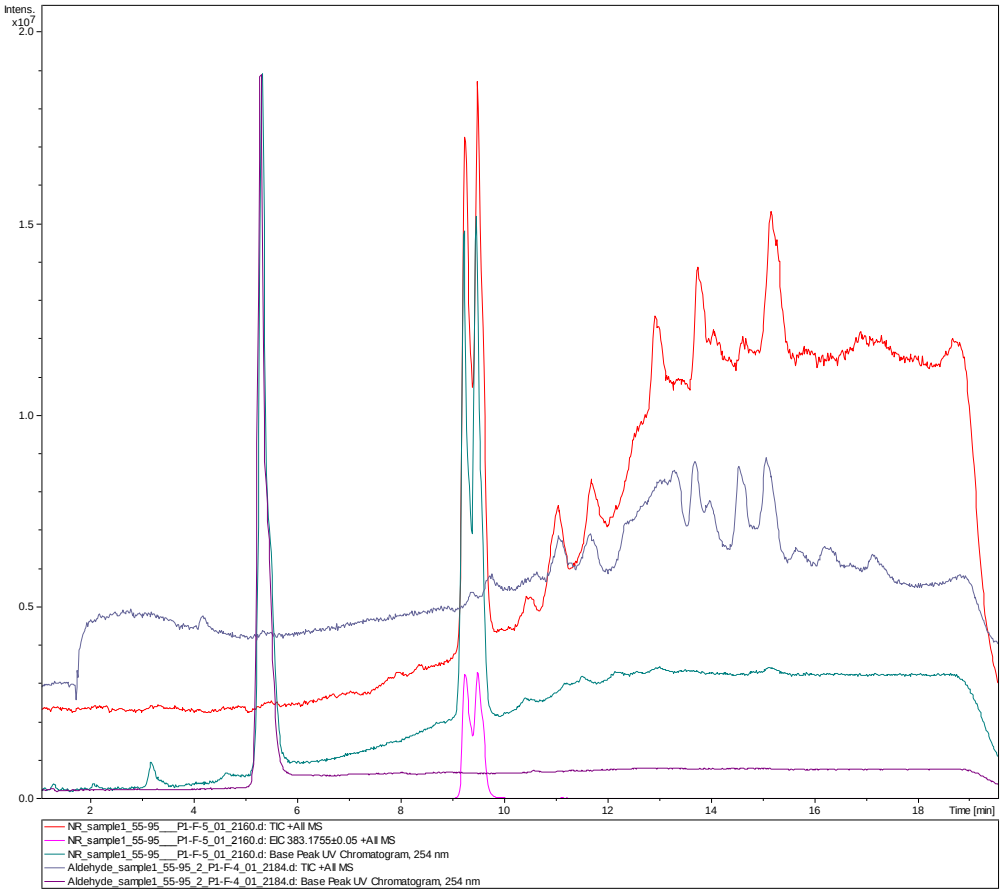




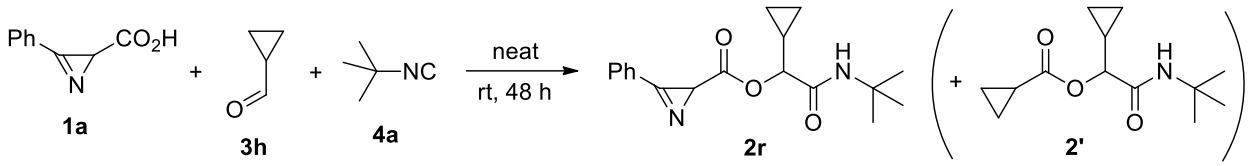
Bruker Compass DataAnalysis 4.0 printed: 30-Oct-20 20:18:18 Page 1 of 1

Superpositions of chromatograms of the reaction mixture A and aldehyde **3a**

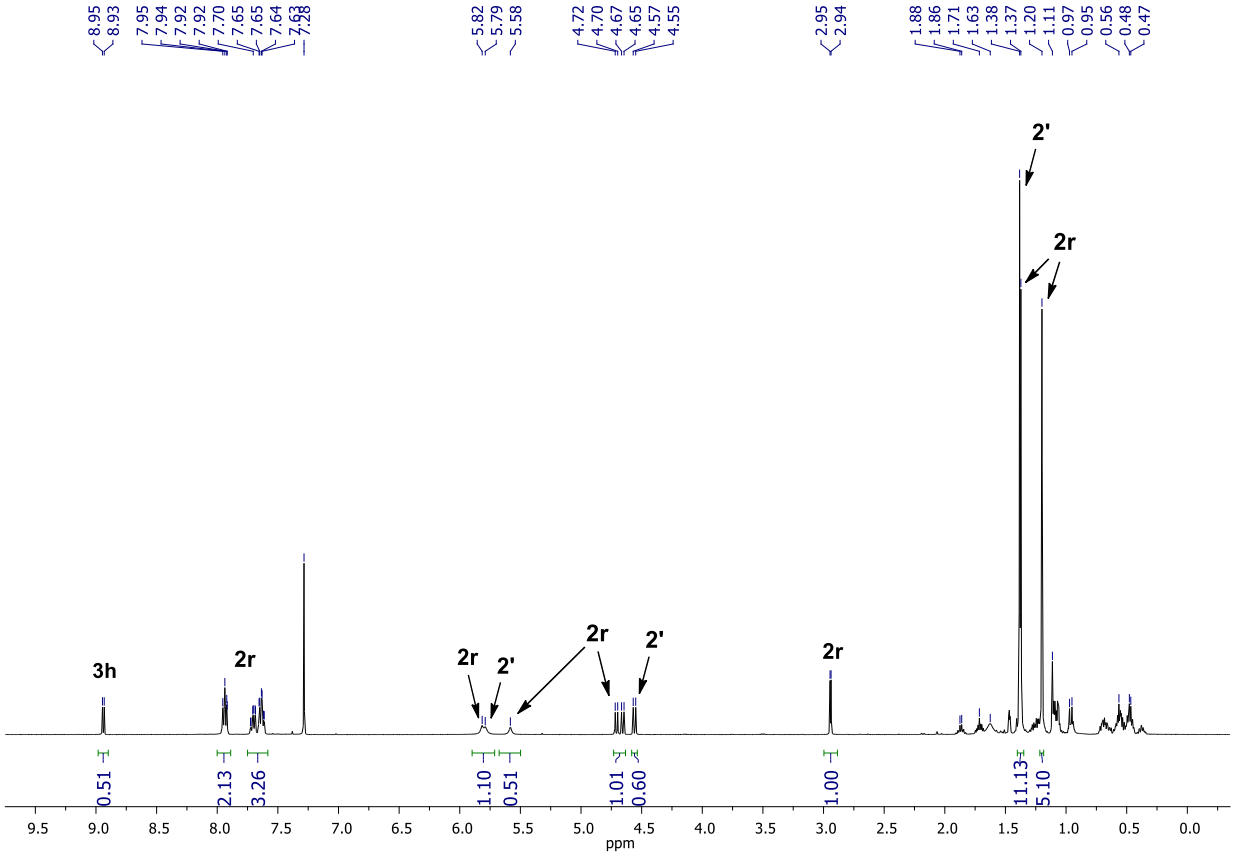




Reaction mixture B:



^{1}H NMR spectrum of the reaction mixture B



LC-MS data of the reaction mixture B

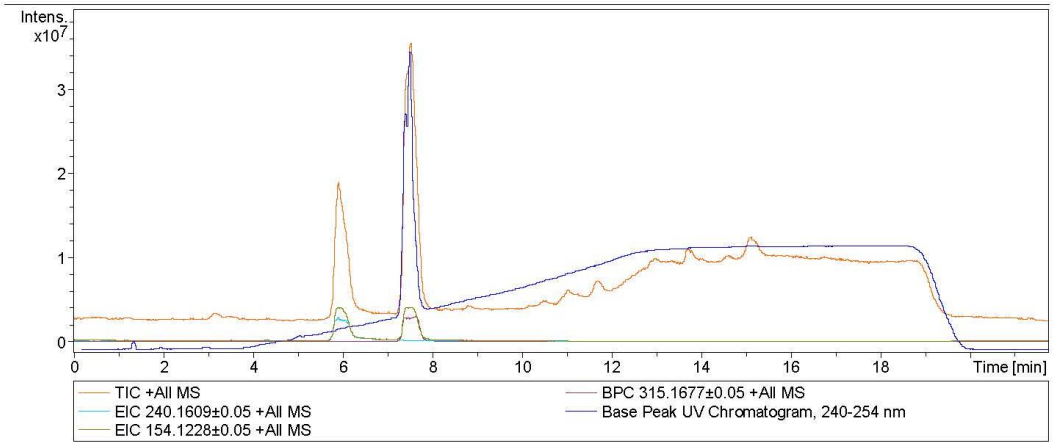
Display Report

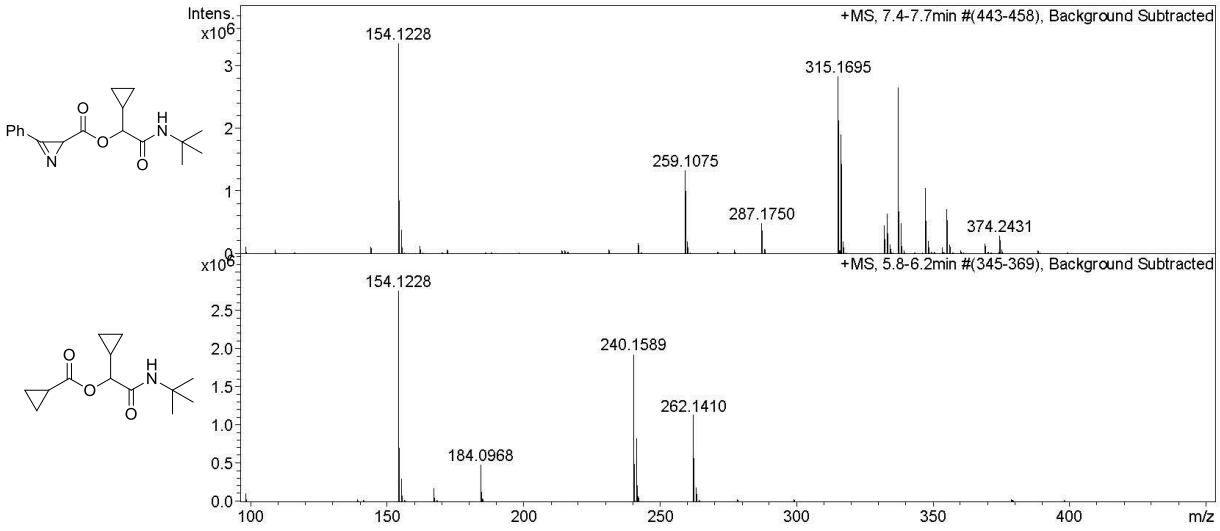
Analysis Info

Analysis Name	D:\Data\Work\2020\HPLCMS\Org_Ls-MS\NR_sample2_50-95___P1-F-6_01_2162.d	Acquisition Date	28-Oct-20 20:57:57
Method	tune_low_pos_100_1000_200ulmin.m	Operator	BDAL@DE
Sample Name	NR_sample2_50-95__	Instrument / Ser#	maXis 62
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Active			Set Dry Heater	180 °C
Scan Begin	100 m/z	Set Capillary	4500 V	Set Dry Gas	6.0 l/min
Scan End	1000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source





Bruker Compass DataAnalysis 4.0 printed: 29-Oct-20 19:03:56 Page 1 of 1