Electronic Supplementary Information

Iron - Catalyzed Domino Reaction of Donor-Acceptor Cyclopropanes: A Diastereoselective Approach towards Diversely Functionalized Pyrrolo - Quinazolines

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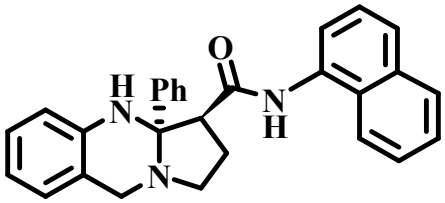
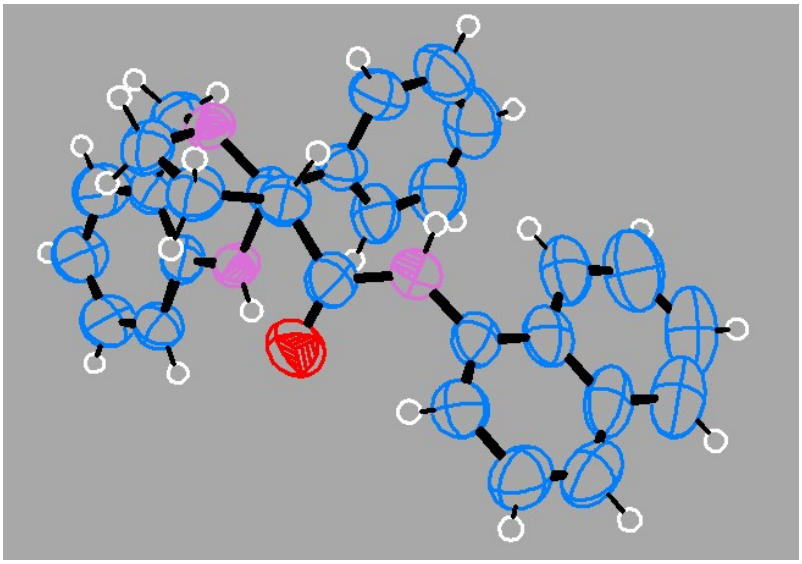
X-ray Crystallography Data of Compound 3n (CCDC 2121353):





The X-ray structure of **3n**. The ellipsoid contour percent probability level is 60%.

Single crystal X-ray data for compound Compound 3n (CCDC 2121353):

Single crystals suitable for X-ray diffraction of **3n** was grown from ethyl acetate. The crystal was carefully chosen using a stereo zoom microscope supported by a rotatable polarizing stage. In all the cases the data were collected at 273(2) K on a CCD diffractometer with graphite monochromated Mo-Kα radiation (0.71073 Å). The data were processed using the package SAINT.[1] Structures were solved by direct and Fourier methods and refined by full-matrix least squares based on F2 using SHELXTL[2] and SHELXL-97[3] packages.

Table 1. Crystallographic data for the compound **3n**

Compound	**3n**
Empirical formula	$C_{28}H_{25}N_3O$
Formula weight	419.51
crystal system	Triclinic
space group	P -1
***a* (Å)**	6.550(17)
***b*(Å)**	12.76(3)
***c* (Å)**	13.50(3)
α (°)	97.07(3)
β (°)	97.80(3)
γ(°)	98.64(3)
***V* (Å^3)**	1094(5)
Z	2
***T*, K**	273(2)
Wavelength (Å)	0.71073
***2θ* (°)**	2.4016- 23.5925
μ (mm^{-1})	0.078
ρ_{calcd} (g cm^{-3})	1.274
***F* (000)**	444.0
absorption correction	multi-Scan
index ranges	-7 ≤*h*≤ 7
	-14 ≤*k*≤ 14
	-15 ≤*l*≤15
reflections collected	13579
independent	3496(0.1396)

reflections (R_{int})	
Goodness-of-fit on F^2	0.875
R_1^a /wR_2^b ($I > 2\sigma(I)$)	0.0878/ 0.2003
R_1^a/wR_2^b (for all data)	0.1615/ 0.2363
Largest diff. peak/hole / e Å^{-3}	0.345/-0.352

$^aR_1 = [\sum||F_o| - |F_c||/\sum|F_o|]$. $^bwR_2 = [\sum w(F_o^2 - F_c^2)^2/\sum wF_o^4]^{1/2}$

References:

1. P. Mukherjee, A. R. Das. *J. Org. Chem.,* 2017, **82**, 2794.

2. *APEX-II, SAINT-Plus,* and *TWINABS;* Bruker-Nonius AXS Inc.: Madison, WI, 2004.

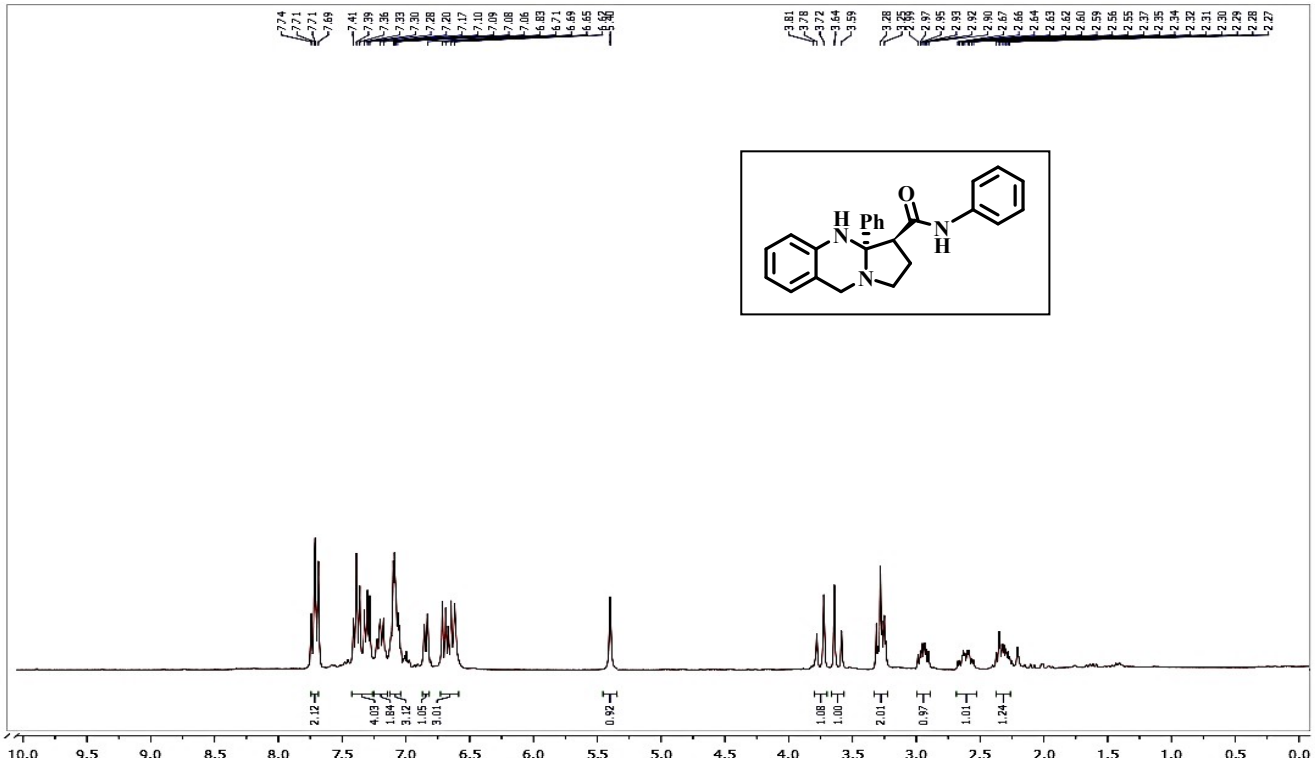
3. *SHELXTL,* version 6.10; Bruker AXS Inc.: Madison, WI, 2002.

4. Sheldrick, G. M. *SHELXL-97, Crystal Structure Refinement Program;* University of Göttingen: Göttingen, Germany, 1997.

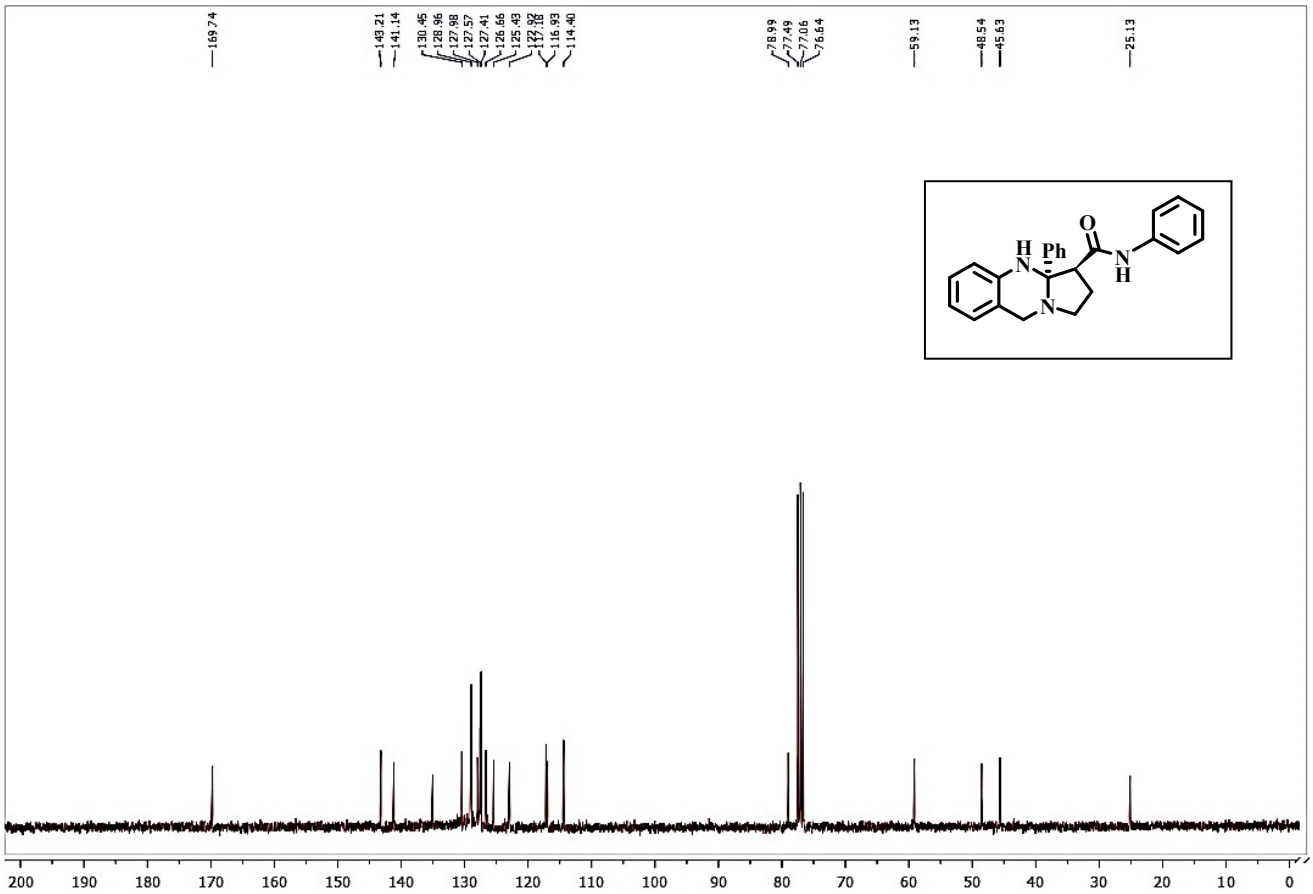
Table S1:

Entry	Catalyst (mol%)	Solvent	Temp (^{0}C)	Yield (%)
1.	$CeCl_3$	DMSO	80	trace
2.	$Zn(OTf)_2$	DMSO	80	-
3.	$Al(OTf)_3$	DMSO	80	-
4.	$CuCl_2$	DMSO	80	20
5.	$Cu(OAc)_2.H_2O$	DMSO	80	-
6.	$Cu(OTf)_2$	DMSO	80	60
7.	$BF_3.OEt_2$	DMSO	80	15-20
8.	TFA	DMSO	80	-
9.	$PTSA.H_2O$	DMSO	80	-

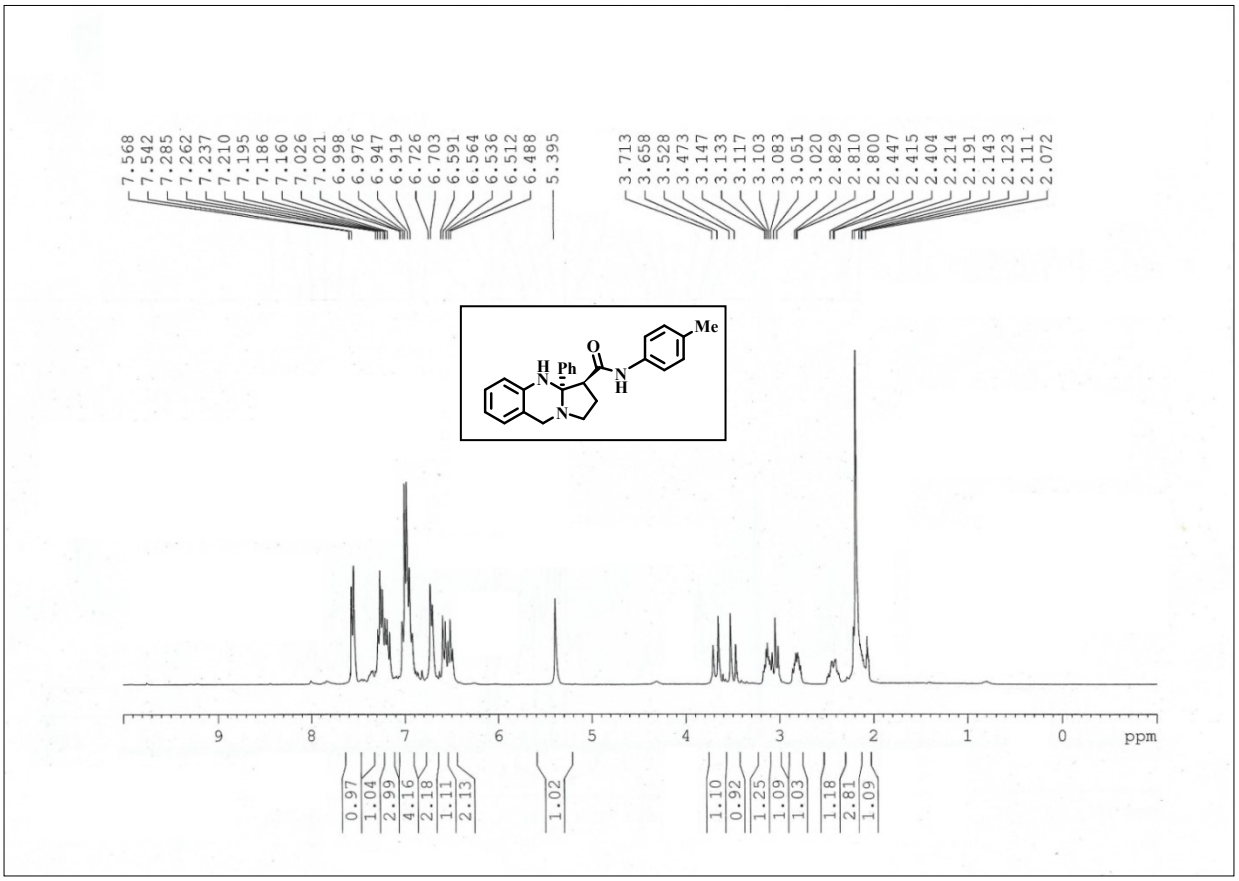
^{1}H NMR of Compound 3a



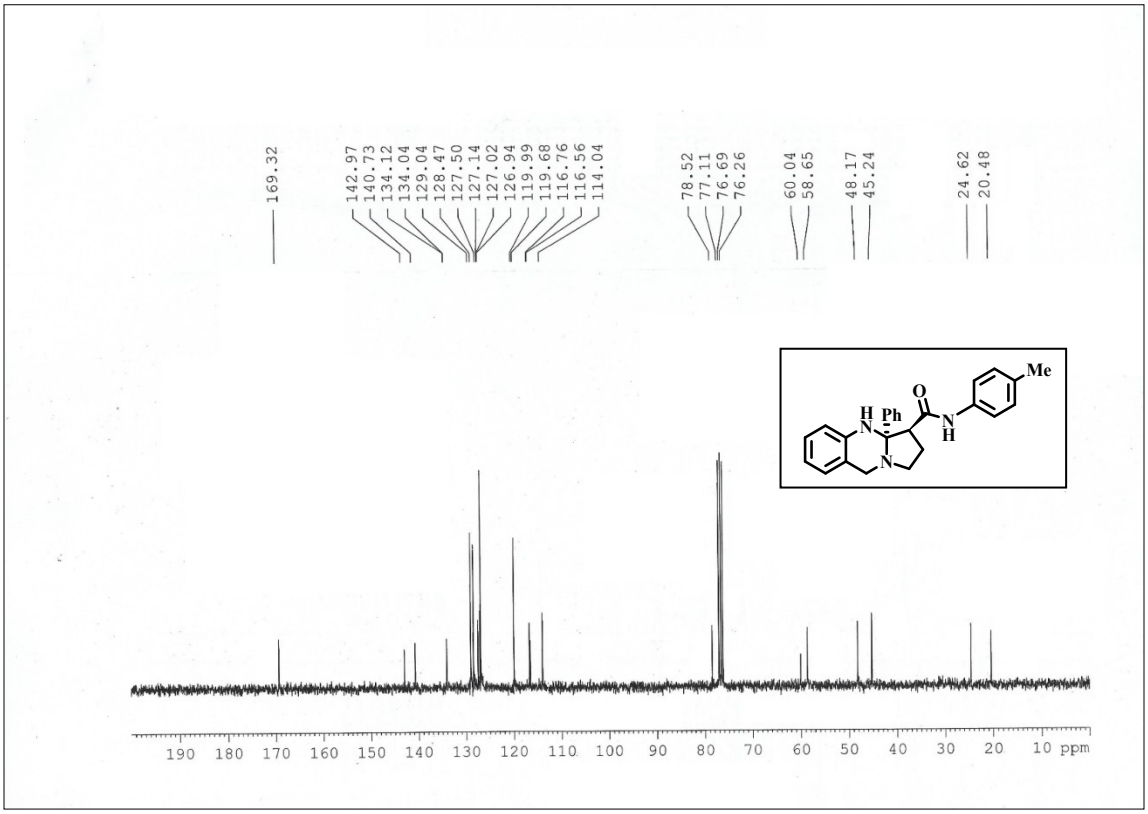
^{13}C NMR of Compound 3a



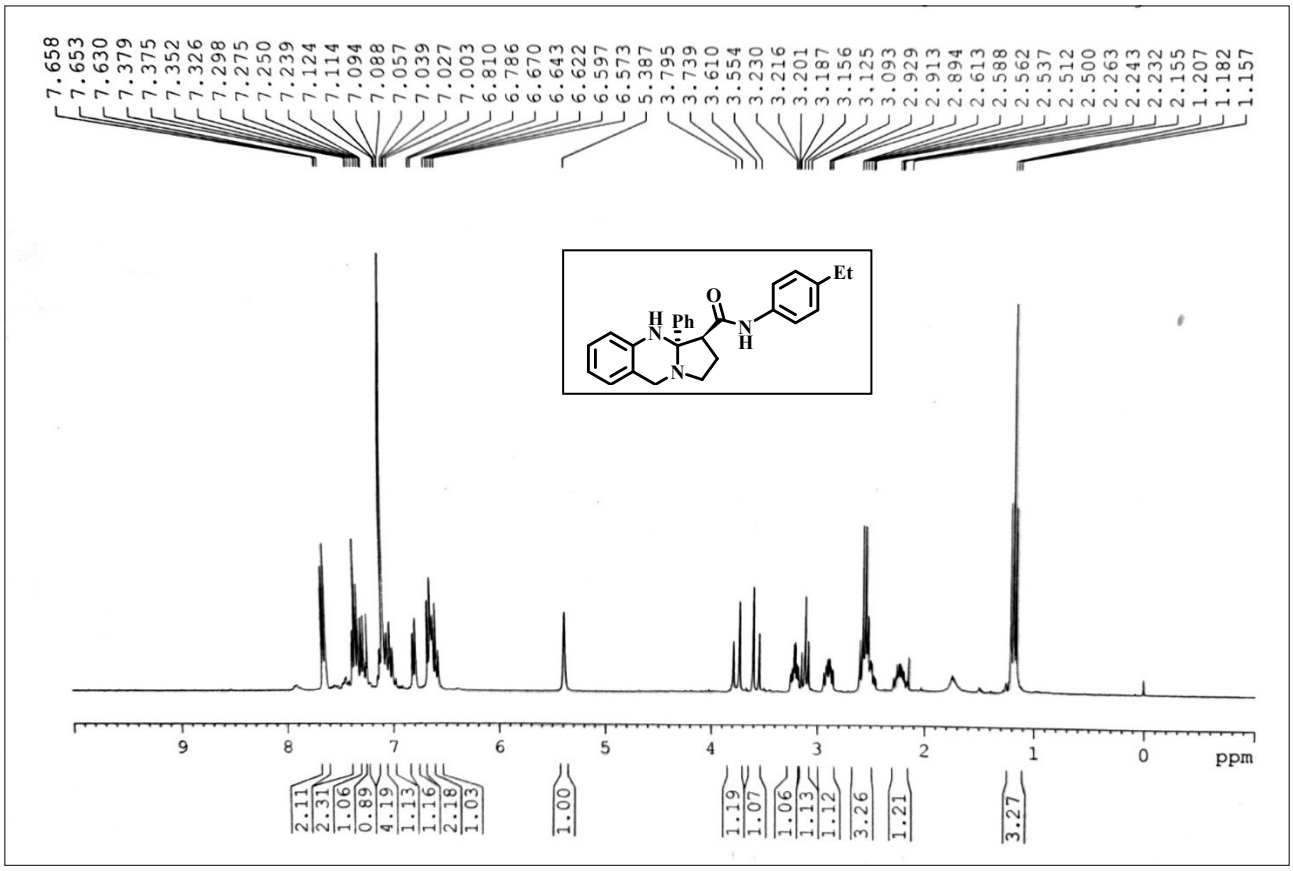
[1]H NMR of Compound 3b



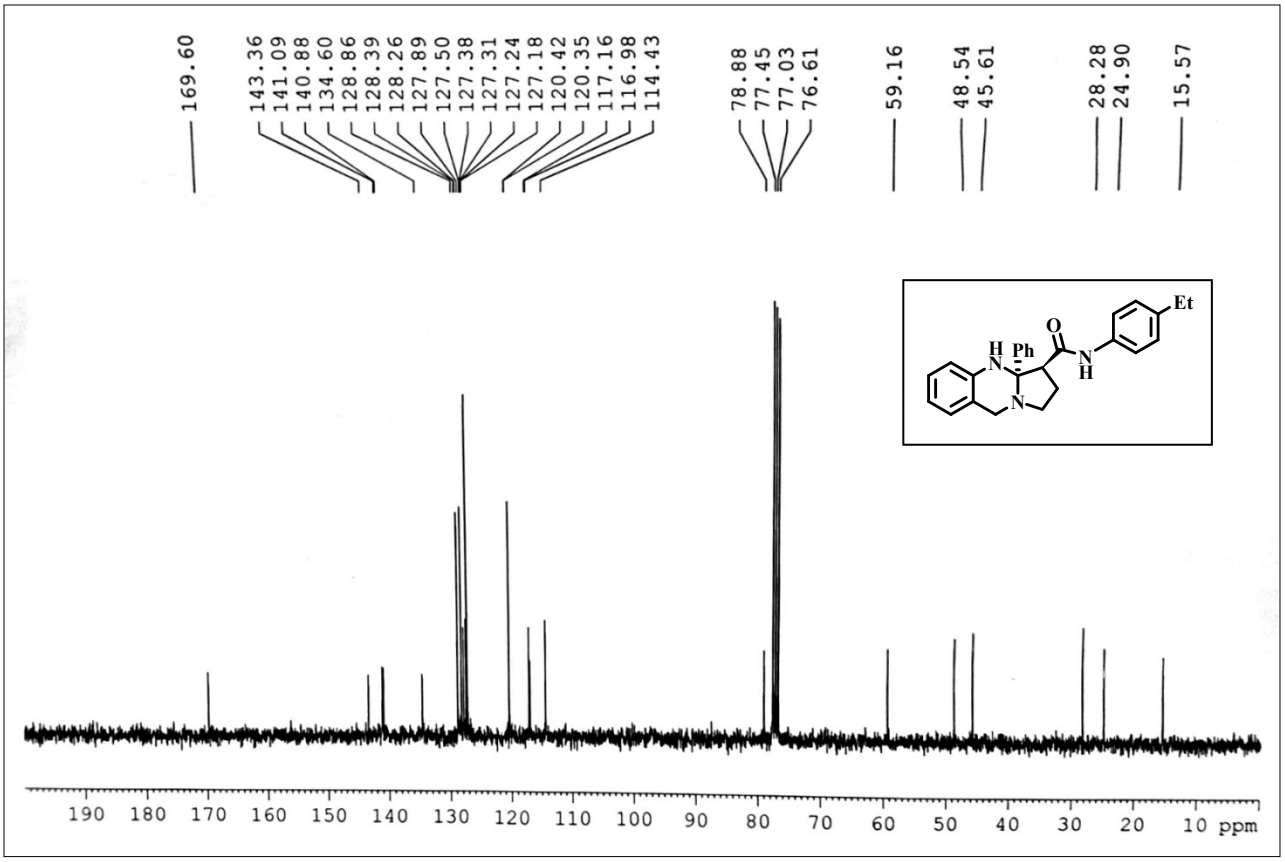
[13]C NMR of Compound 3b



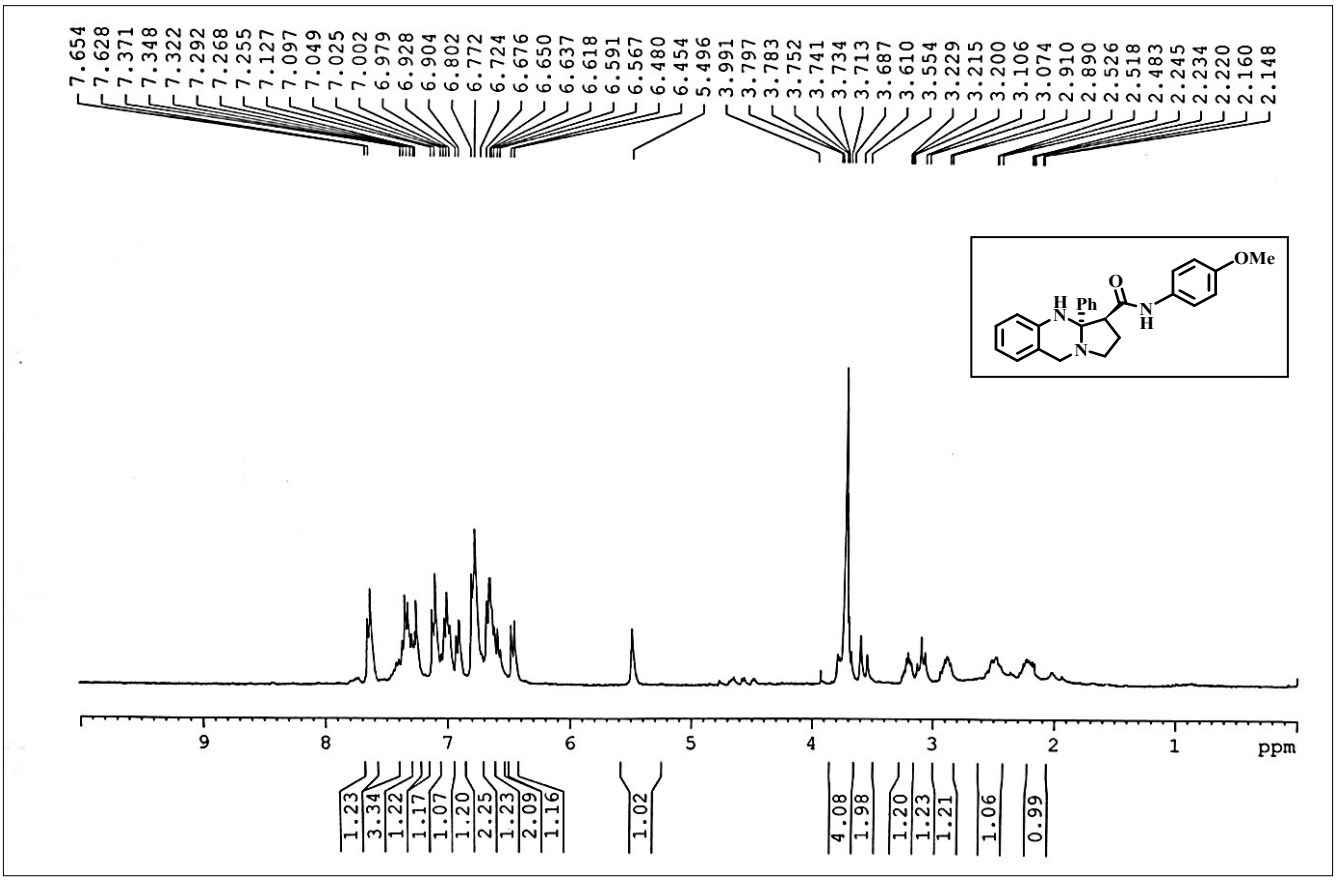
^{1}H NMR of Compound 3c



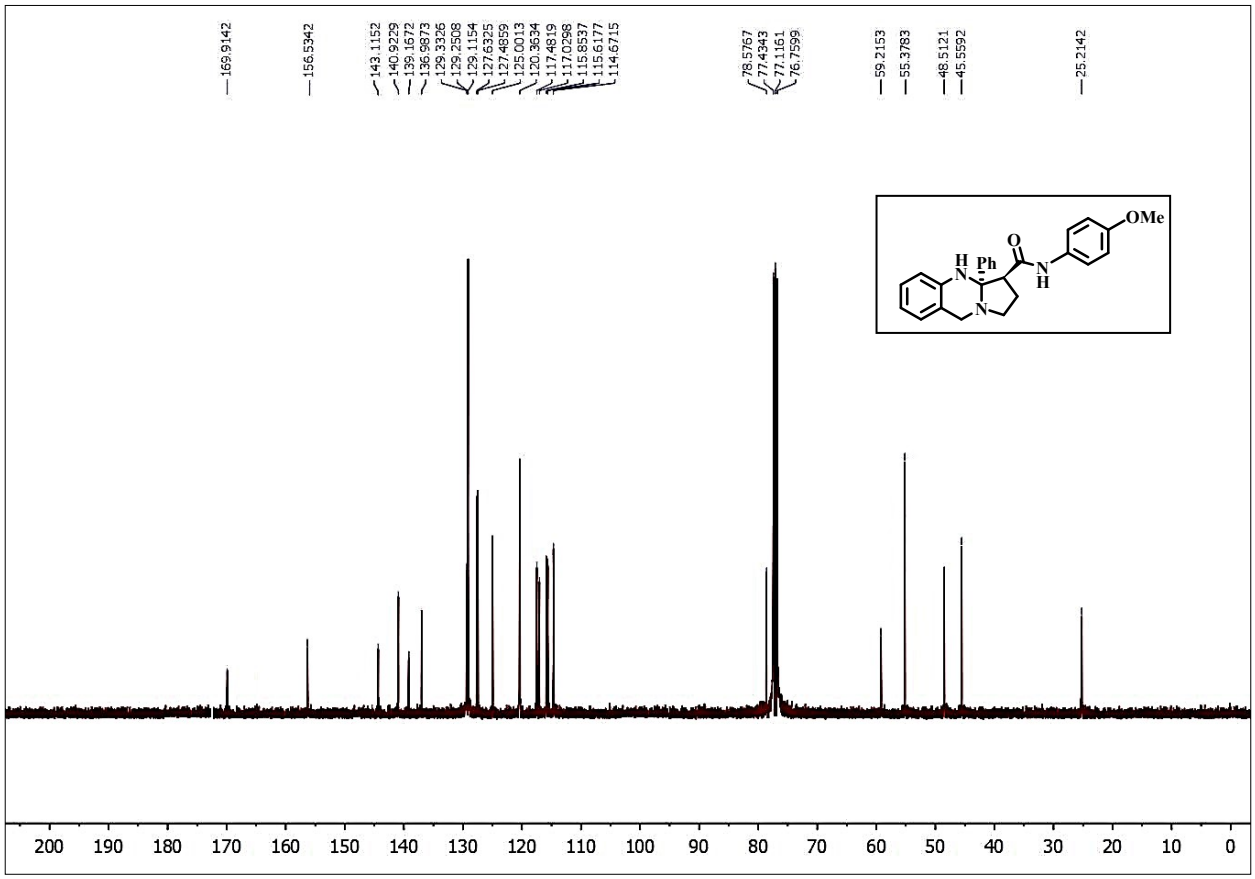
^{13}C NMR of Compound 3c



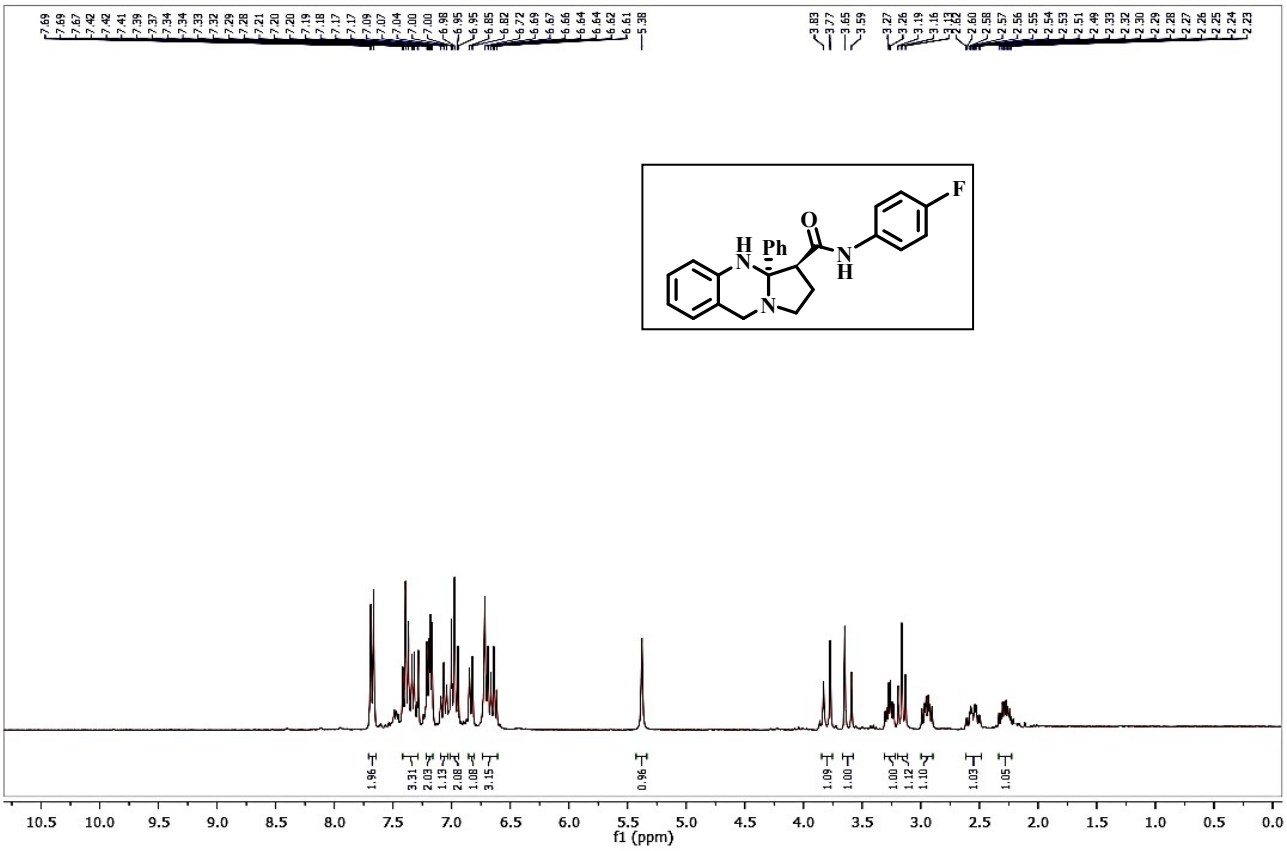
^{1}H NMR of Compound 3d



^{13}C NMR of Compound 3d



^{1}H NMR of Compound 3e



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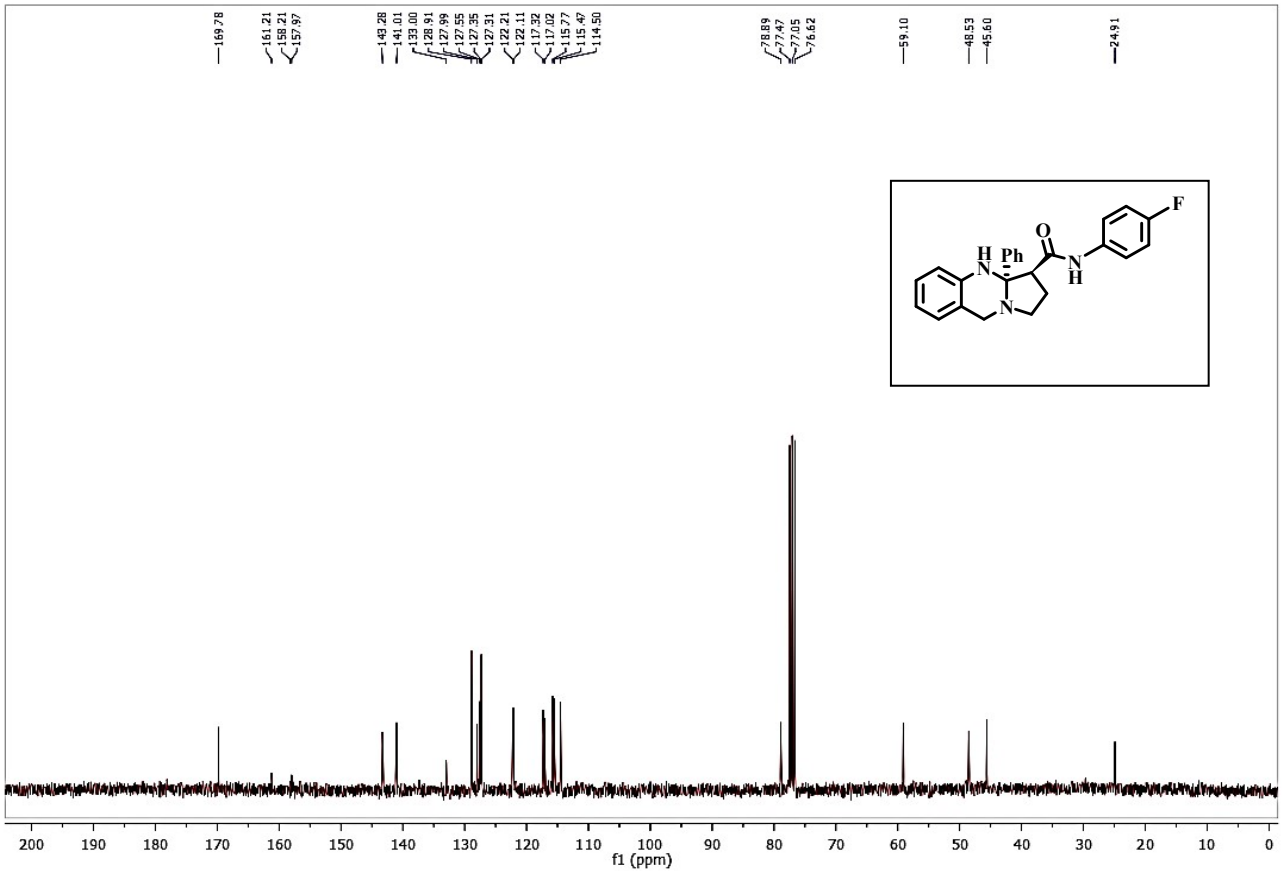
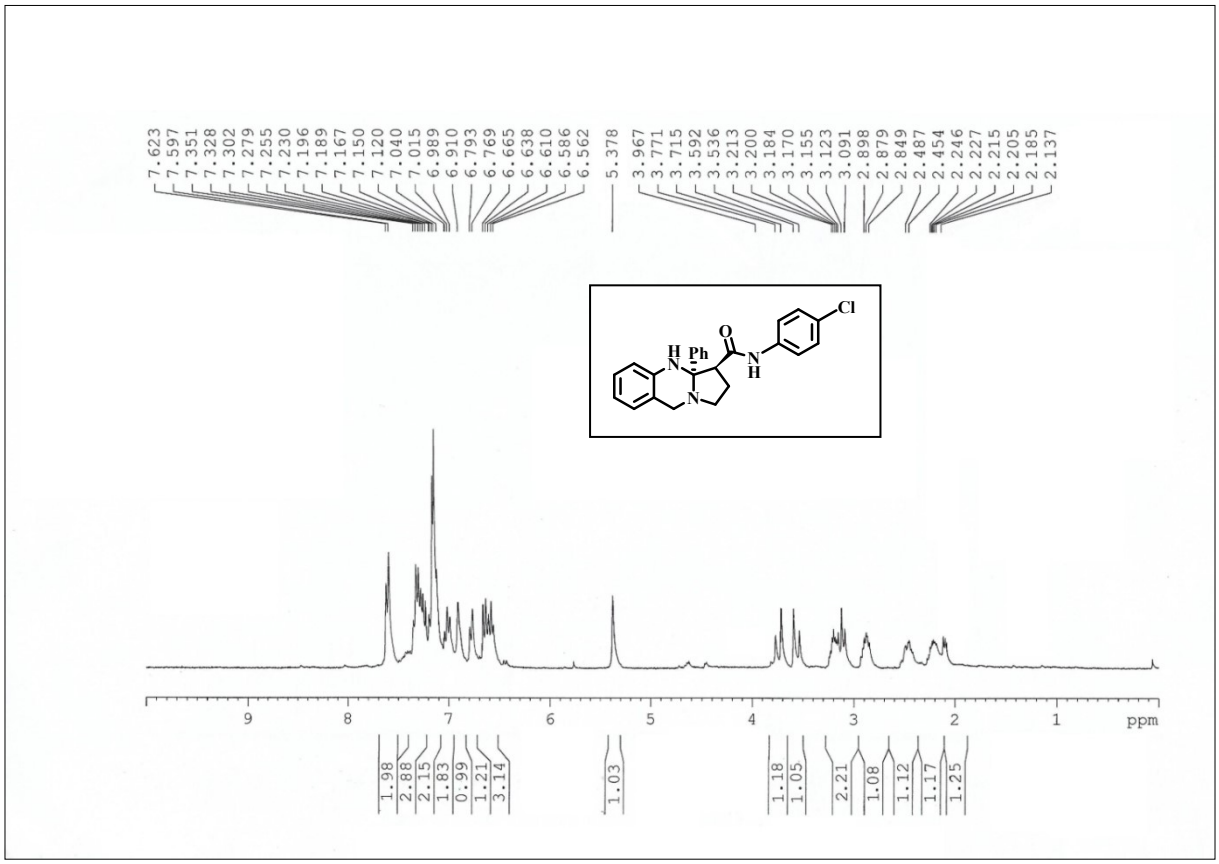


[1]H NMR of Compound 3f



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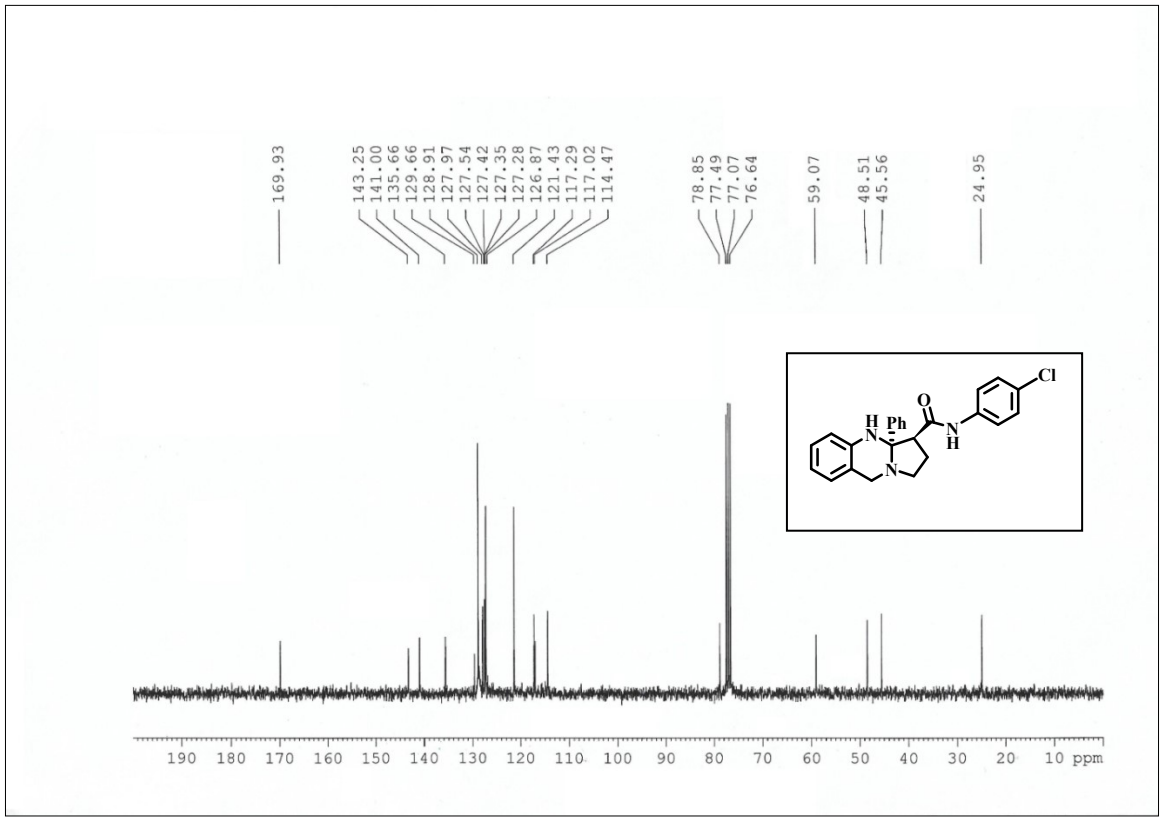
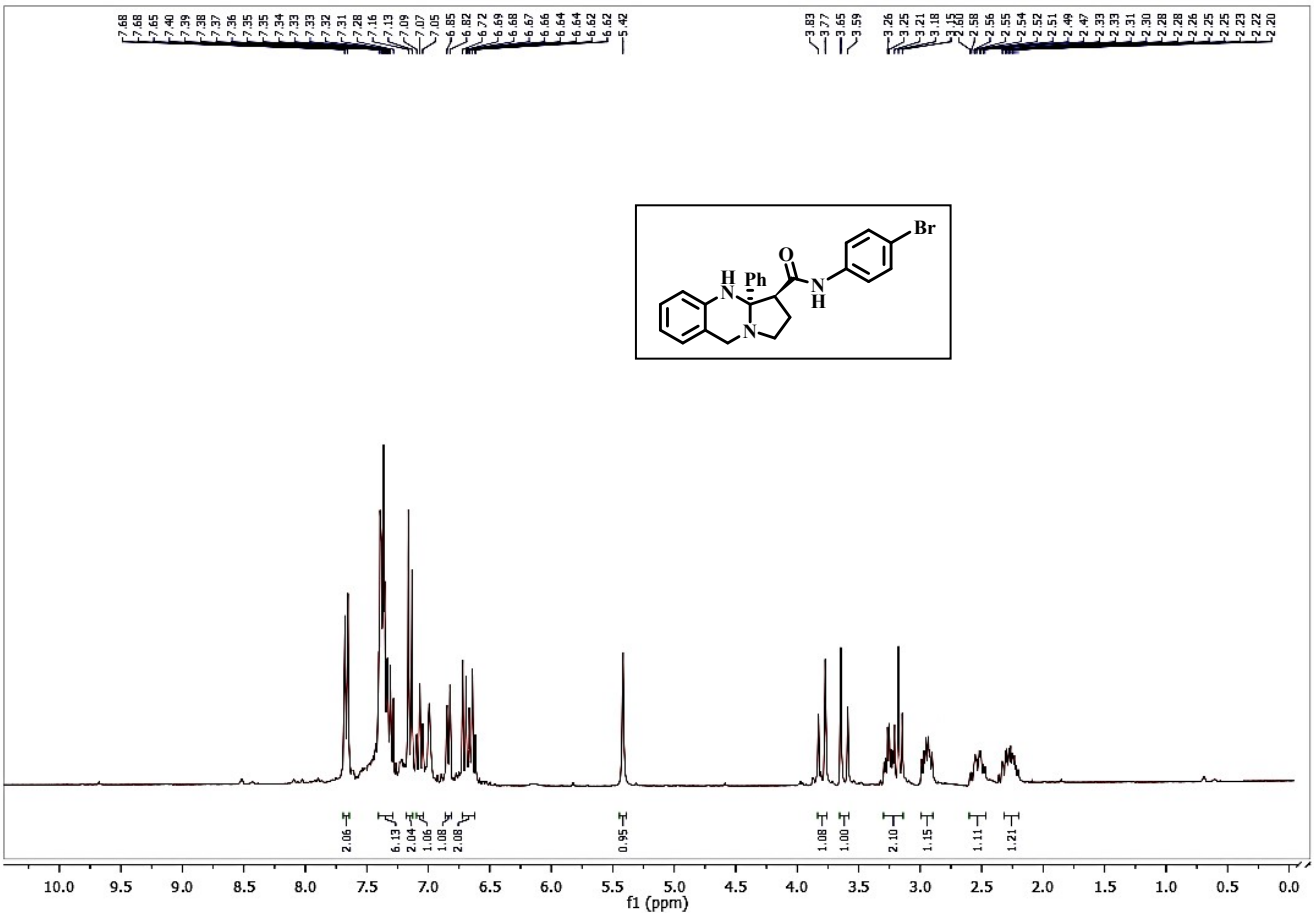
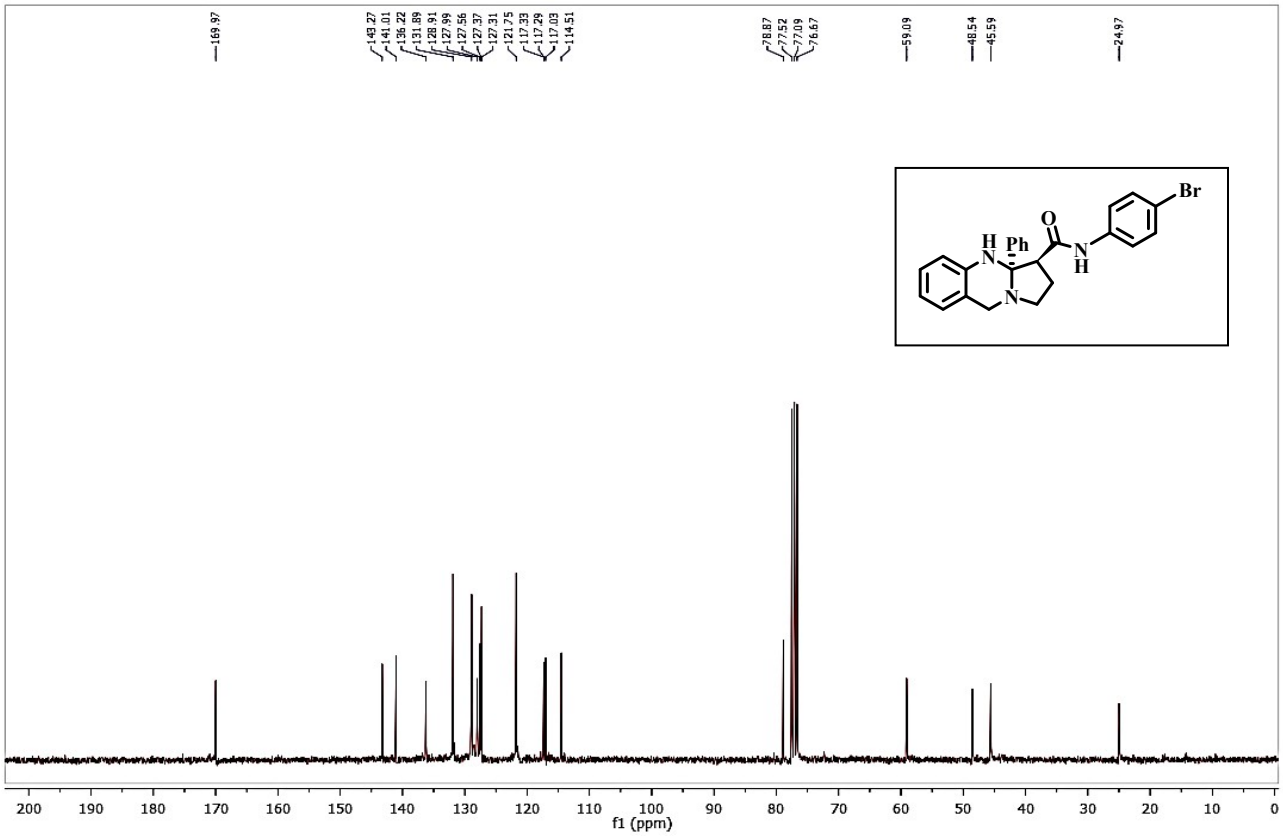


[1]H NMR of Compound 3g



[13]C NMR of Compound 3g



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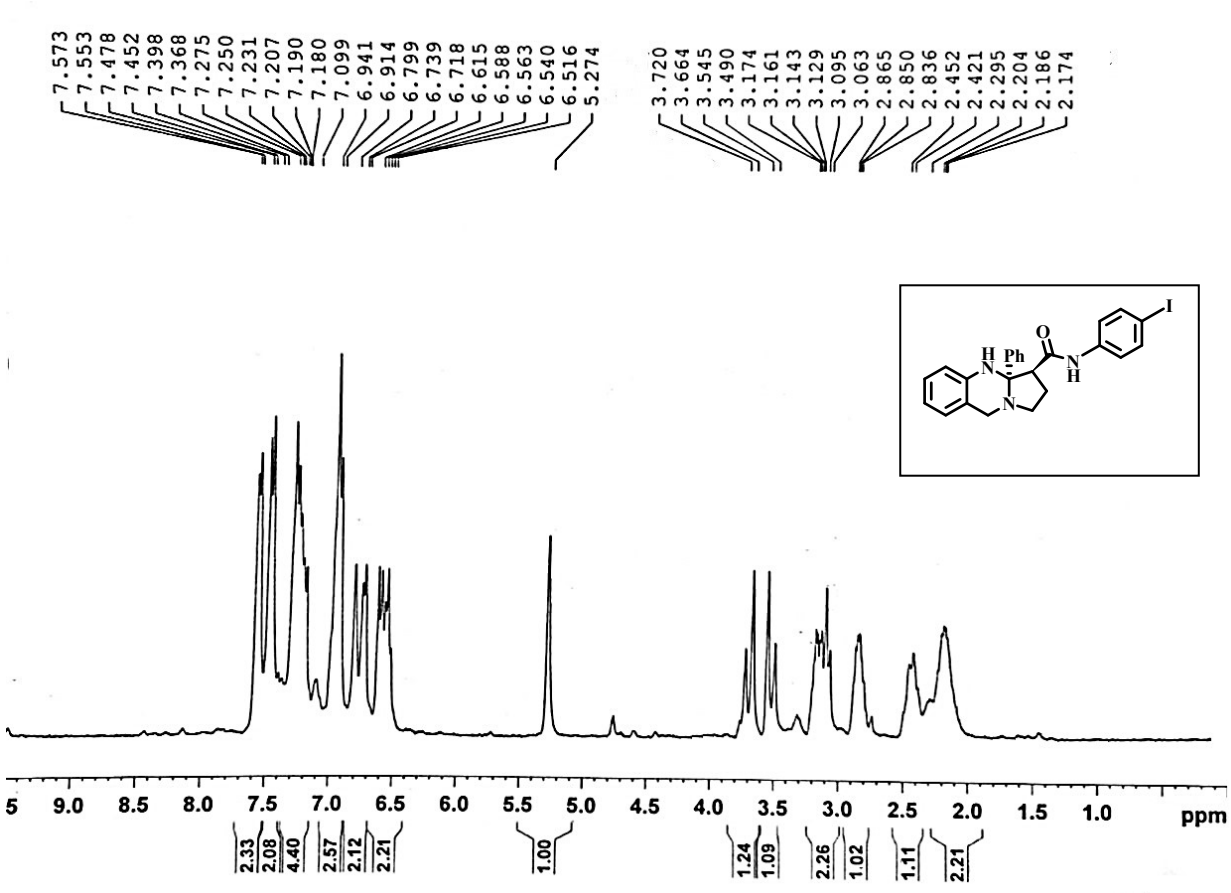
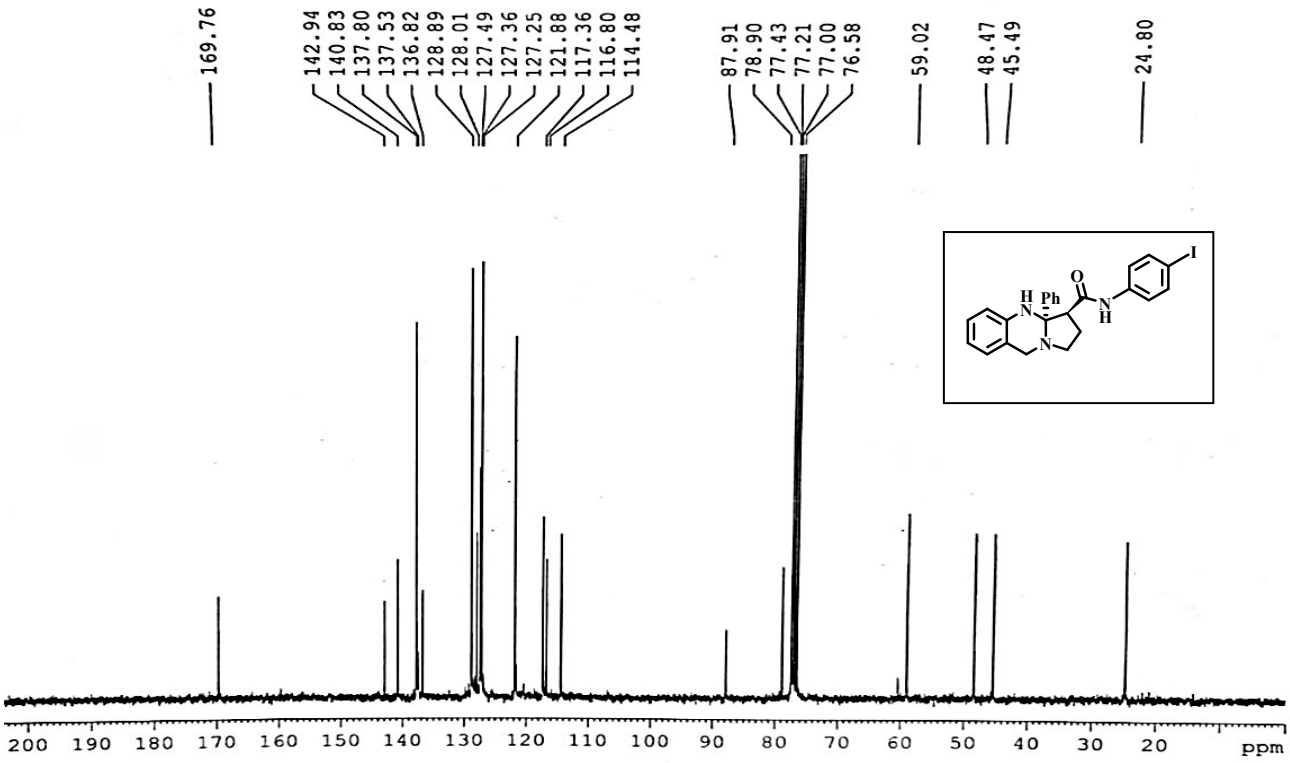
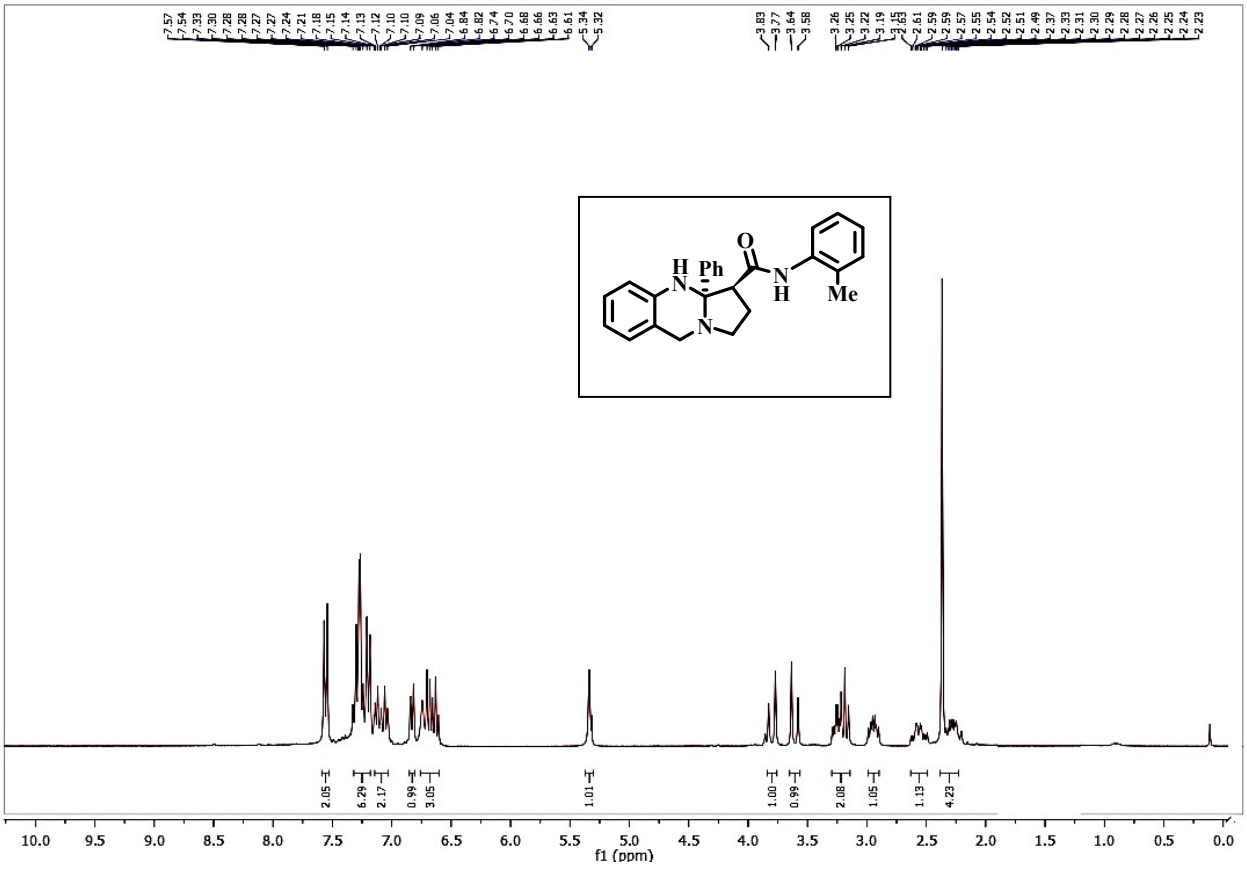


^{13}C NMR of Compound 3h



^{1}H NMR of Compound 3i



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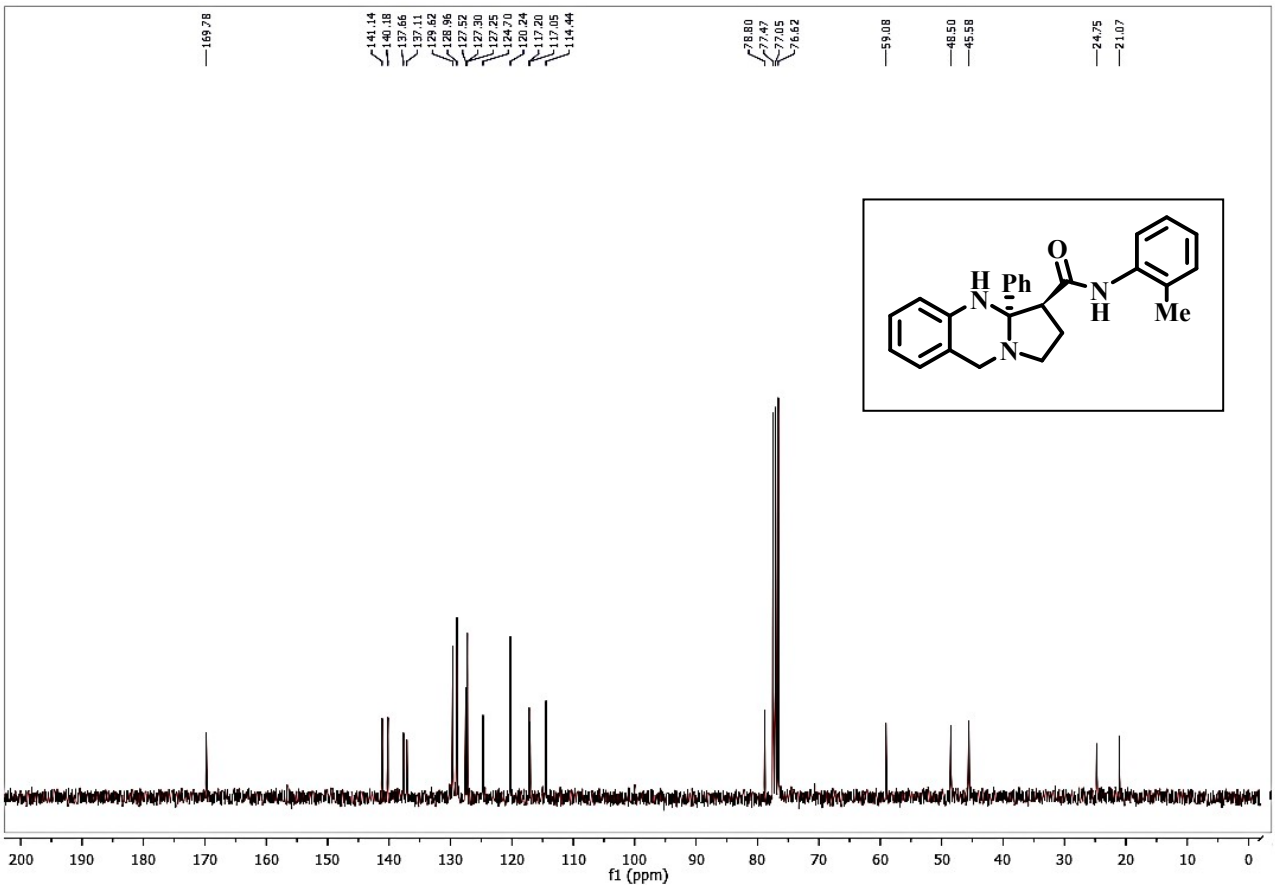

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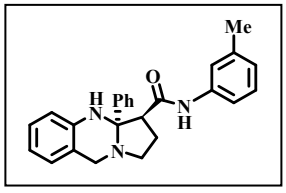

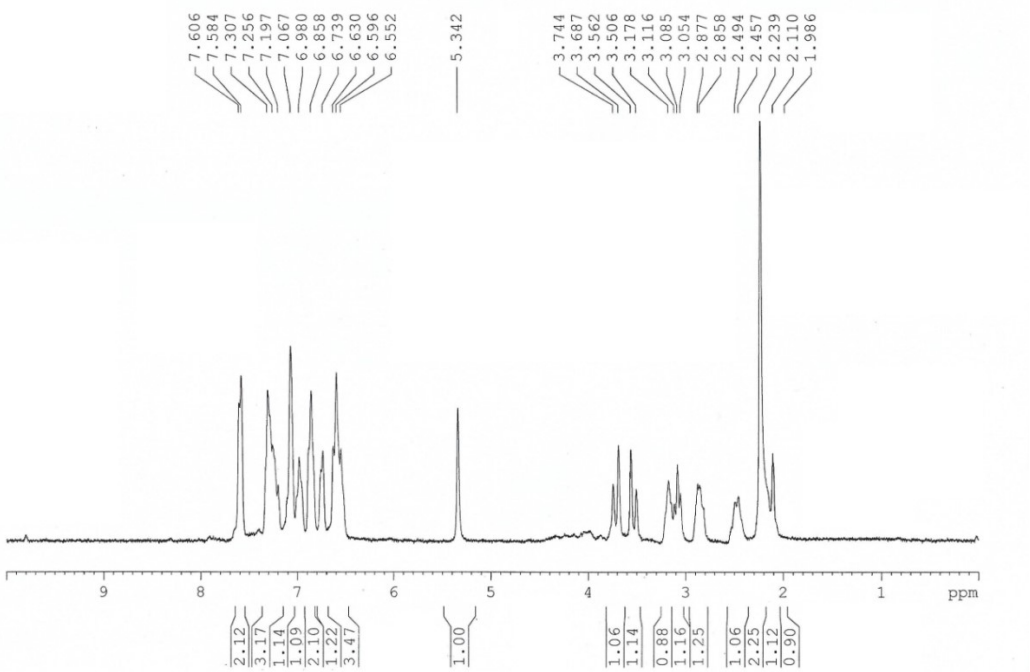

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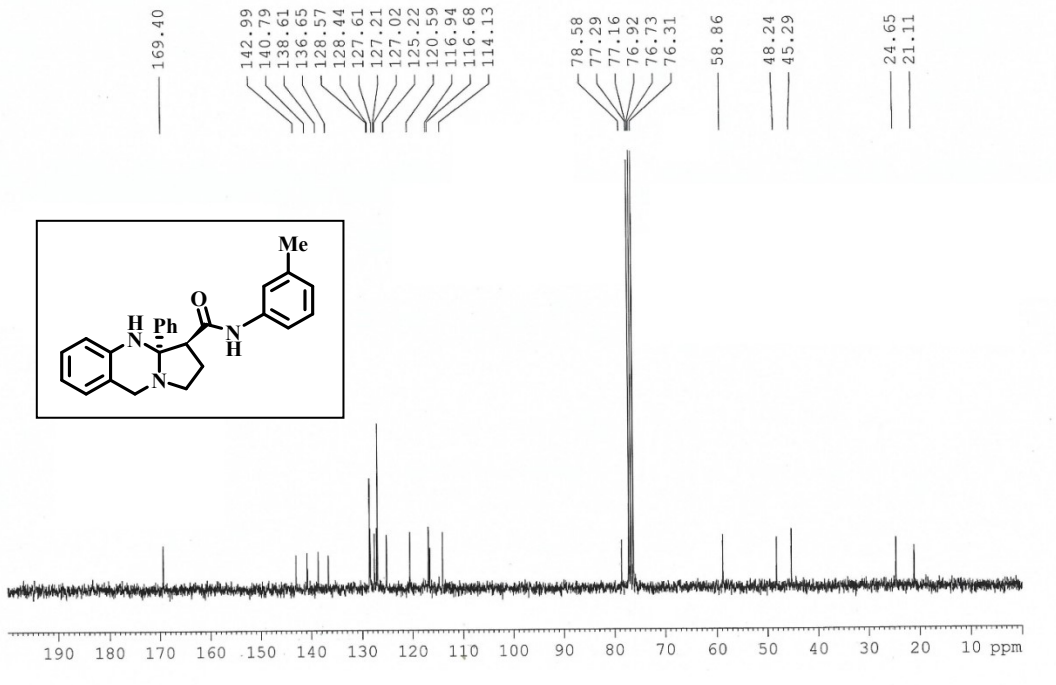

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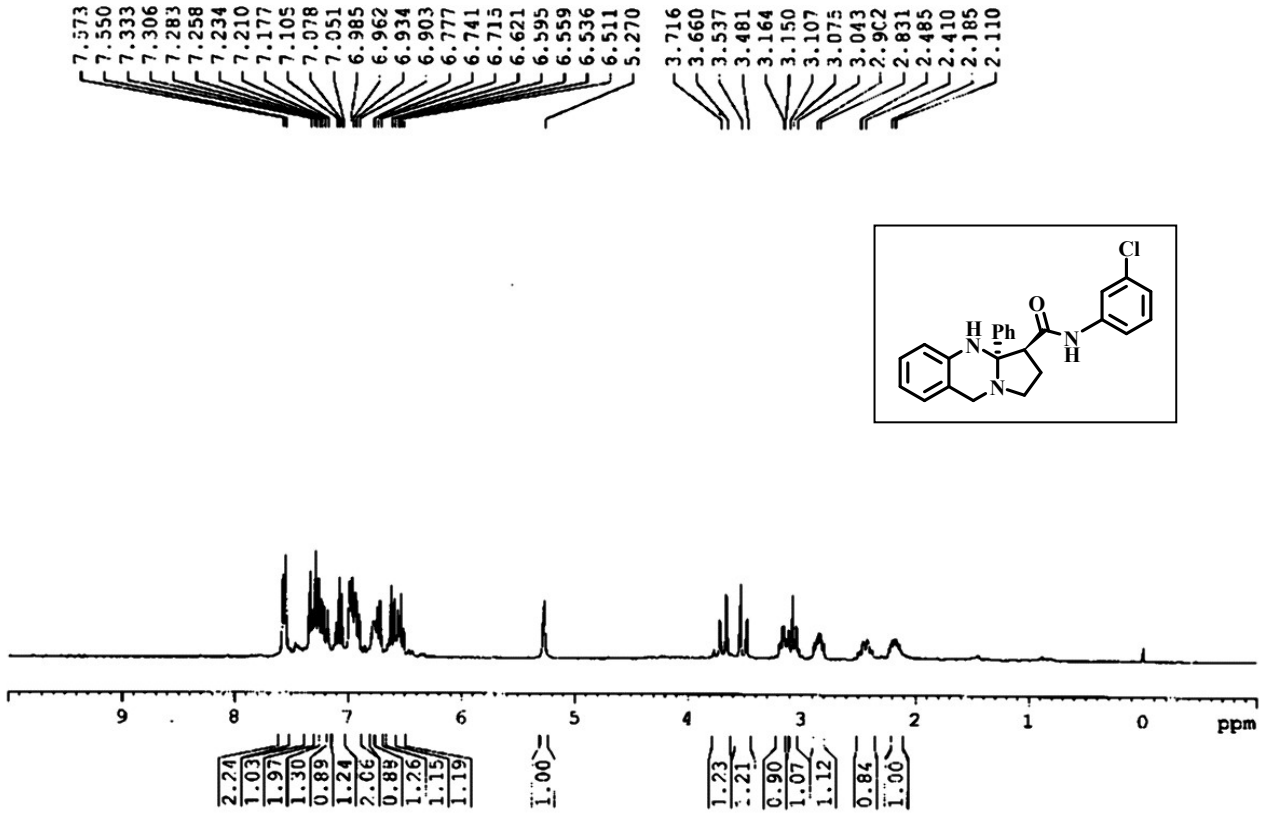

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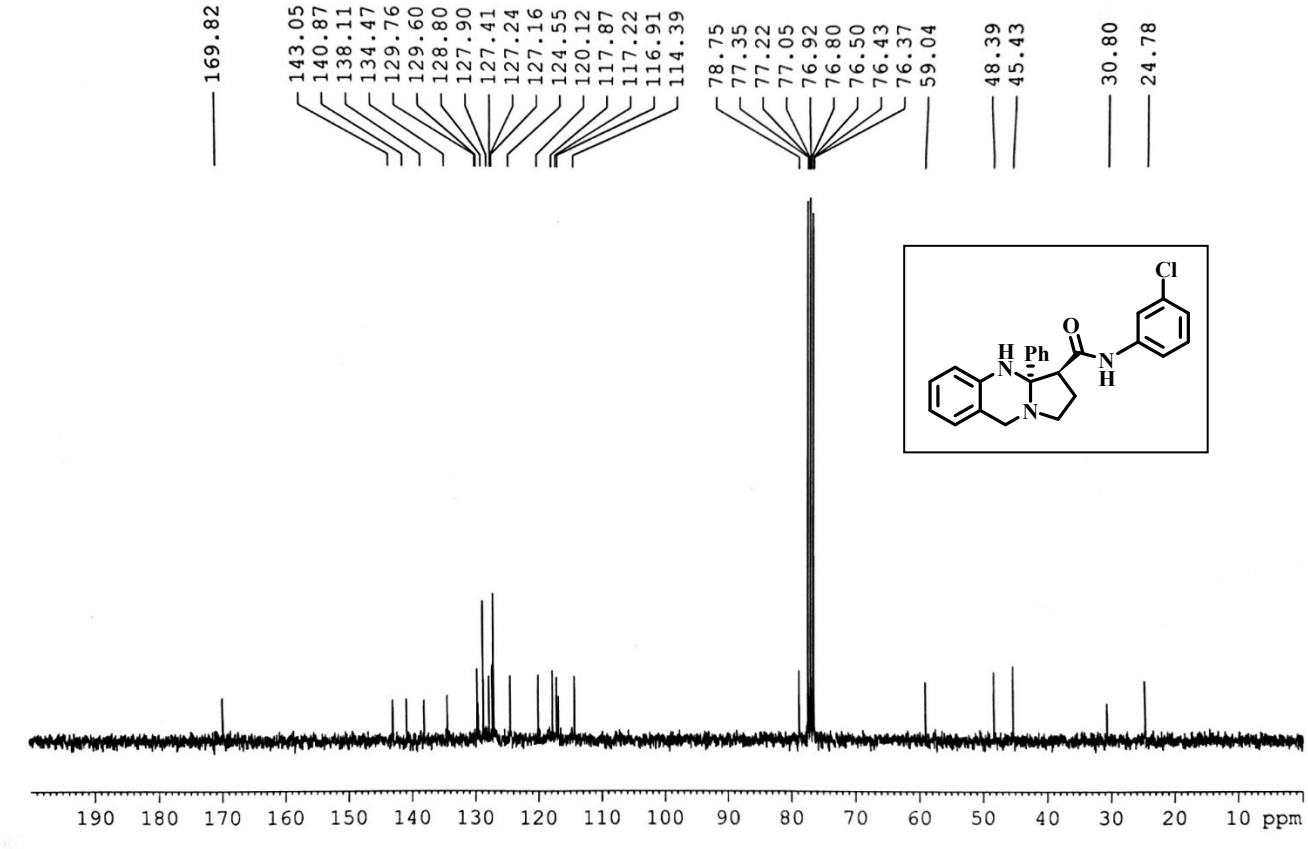

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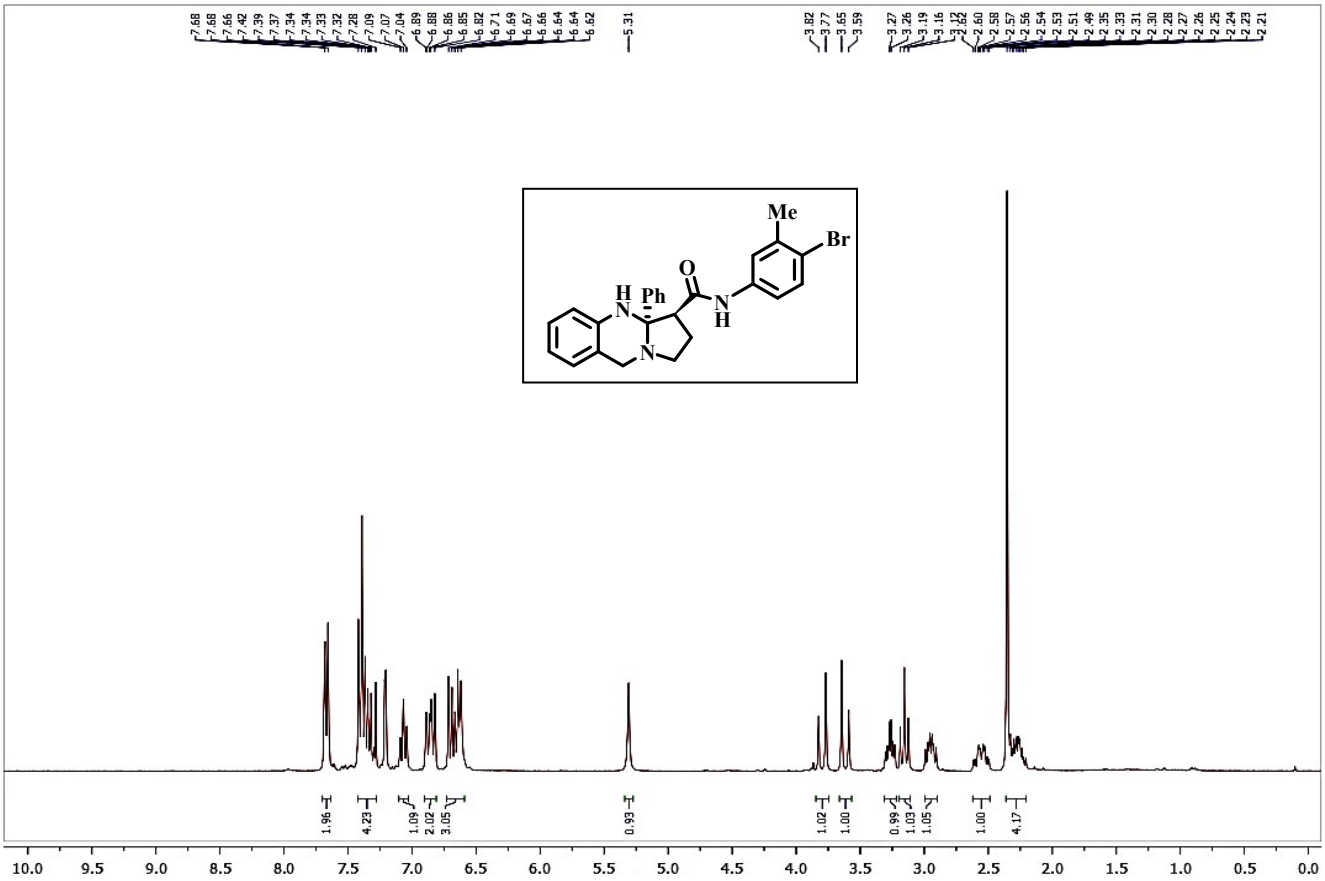

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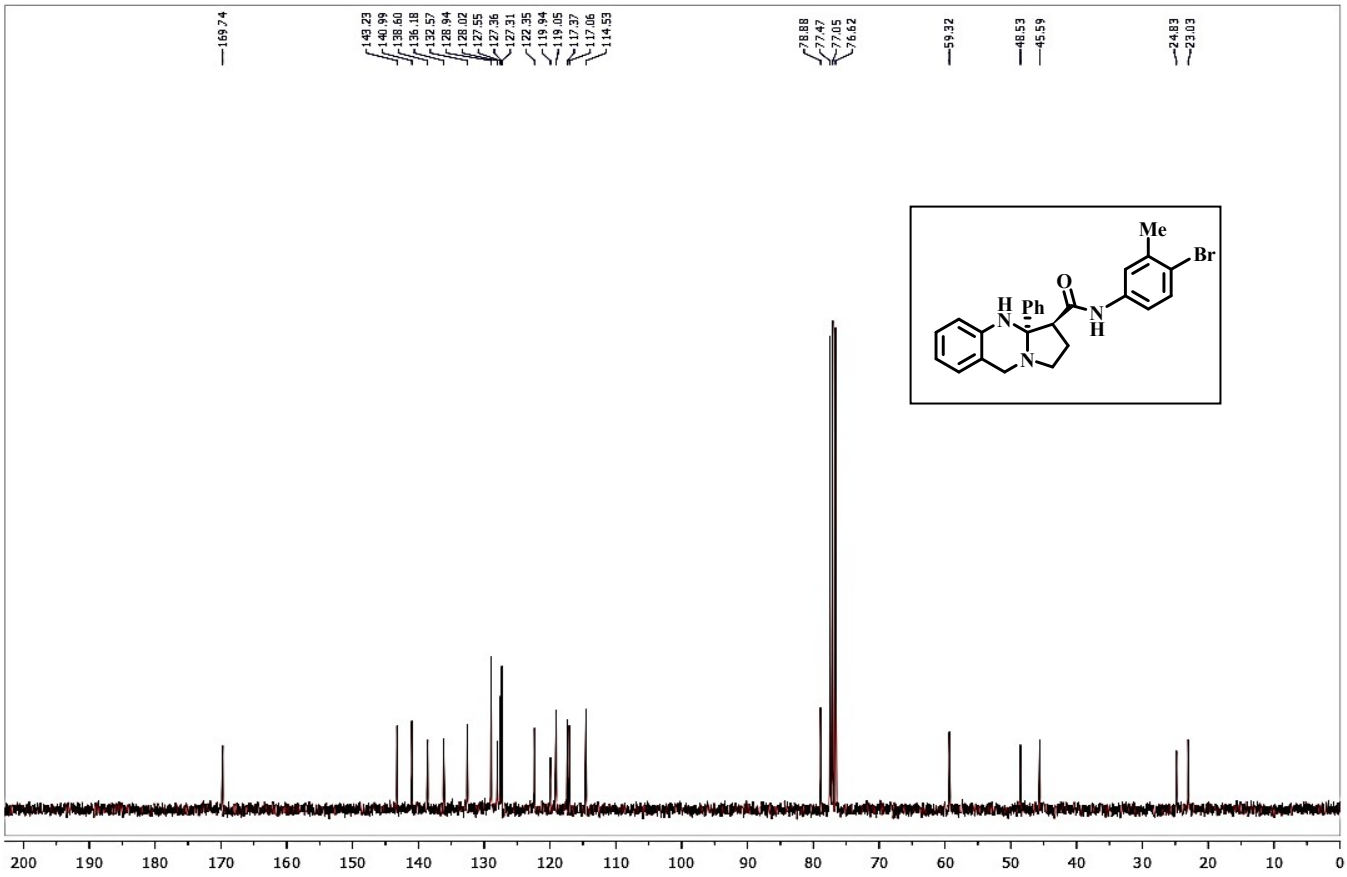

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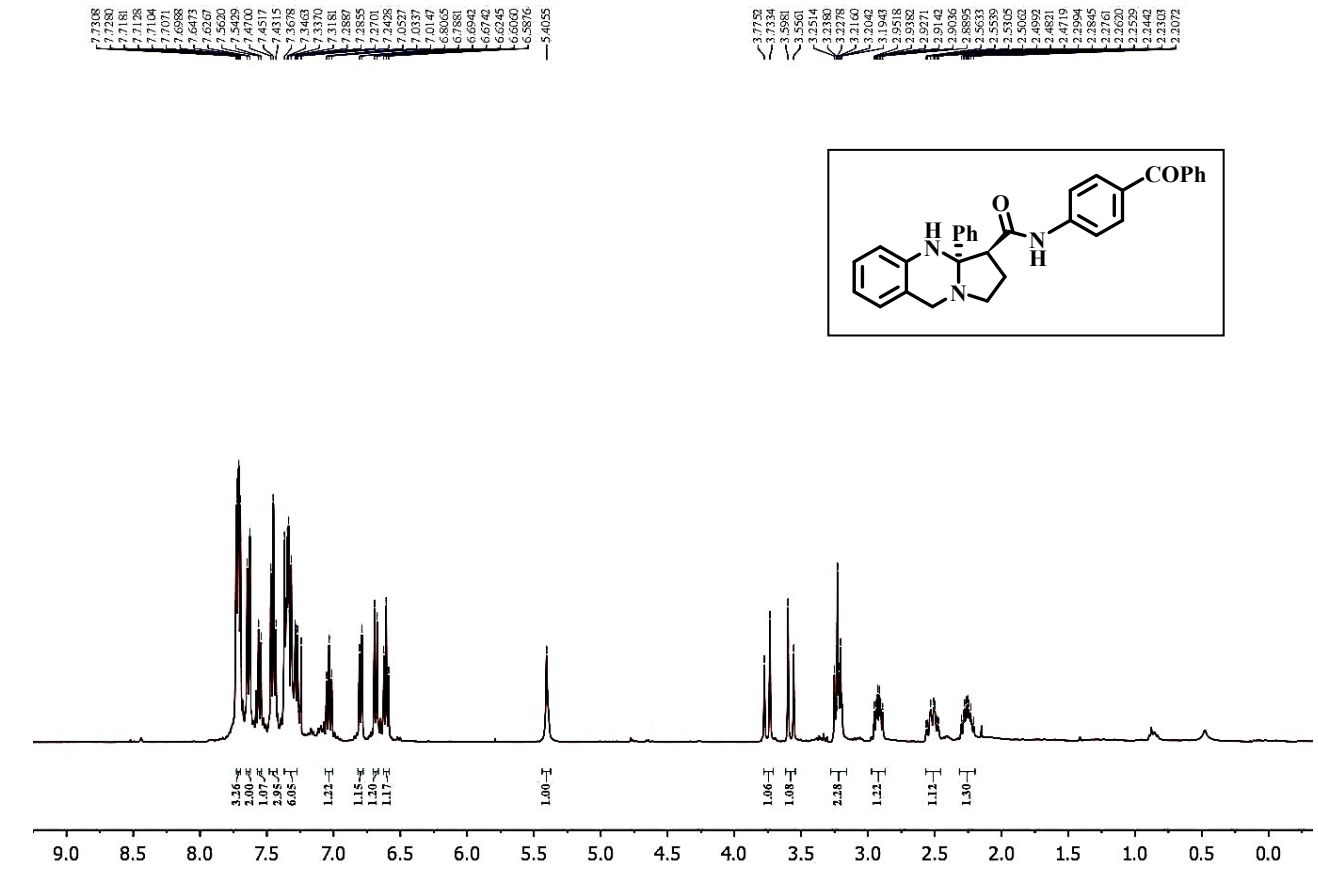

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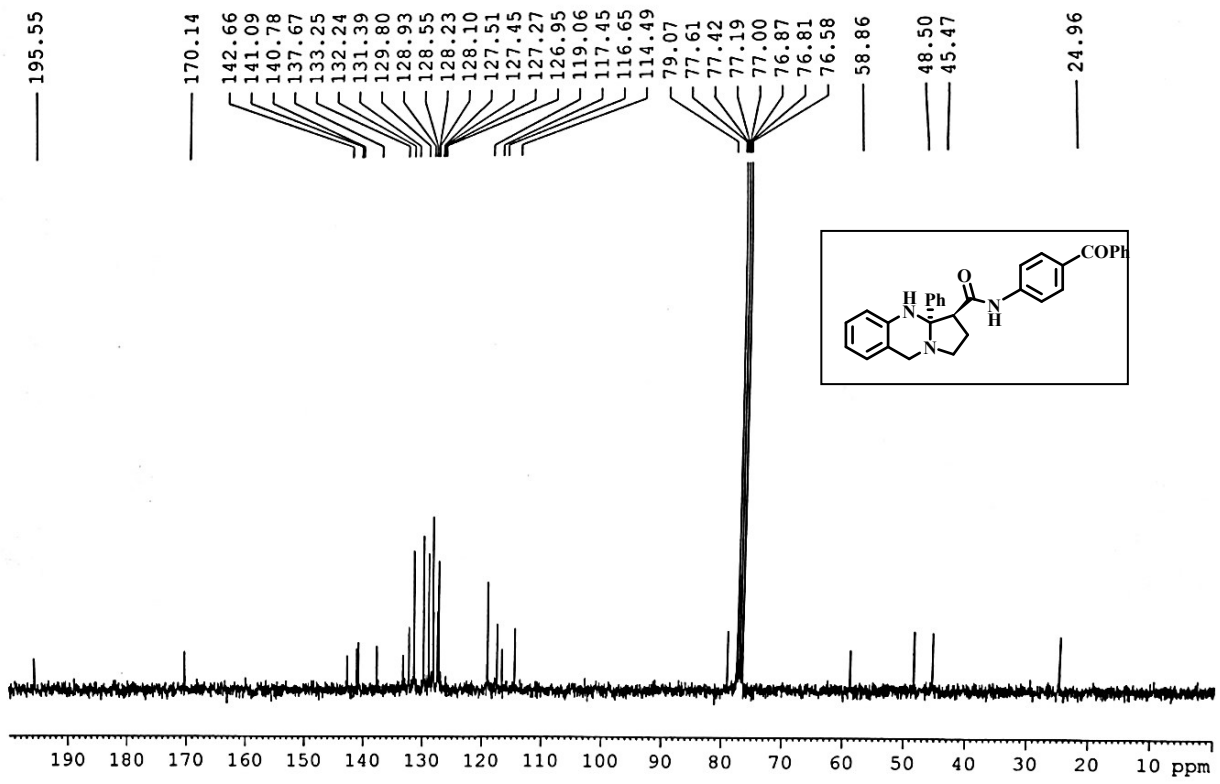

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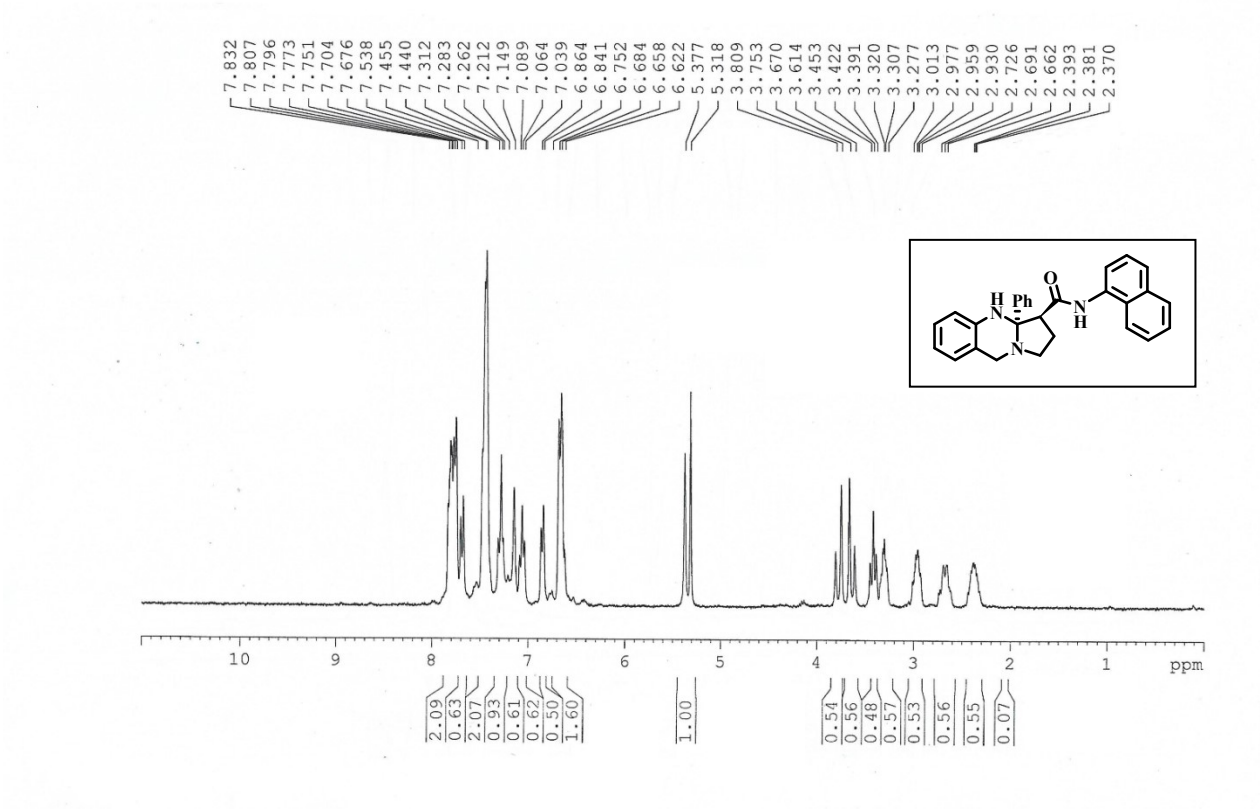

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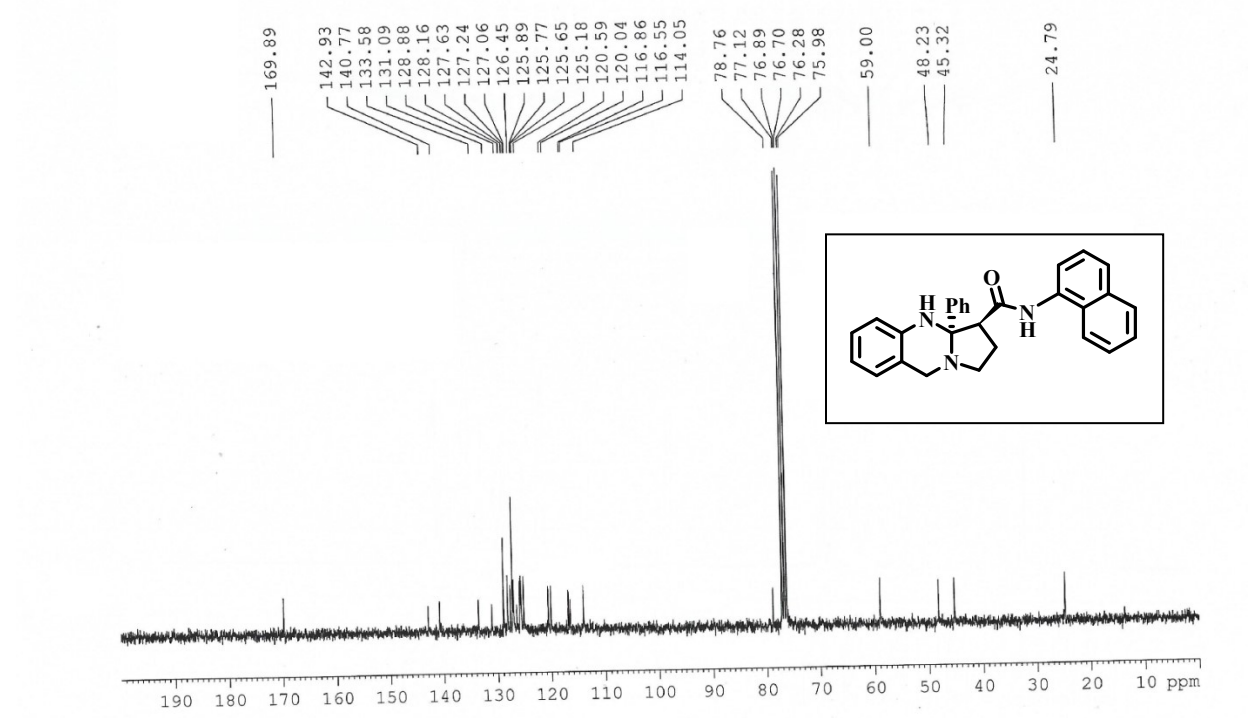
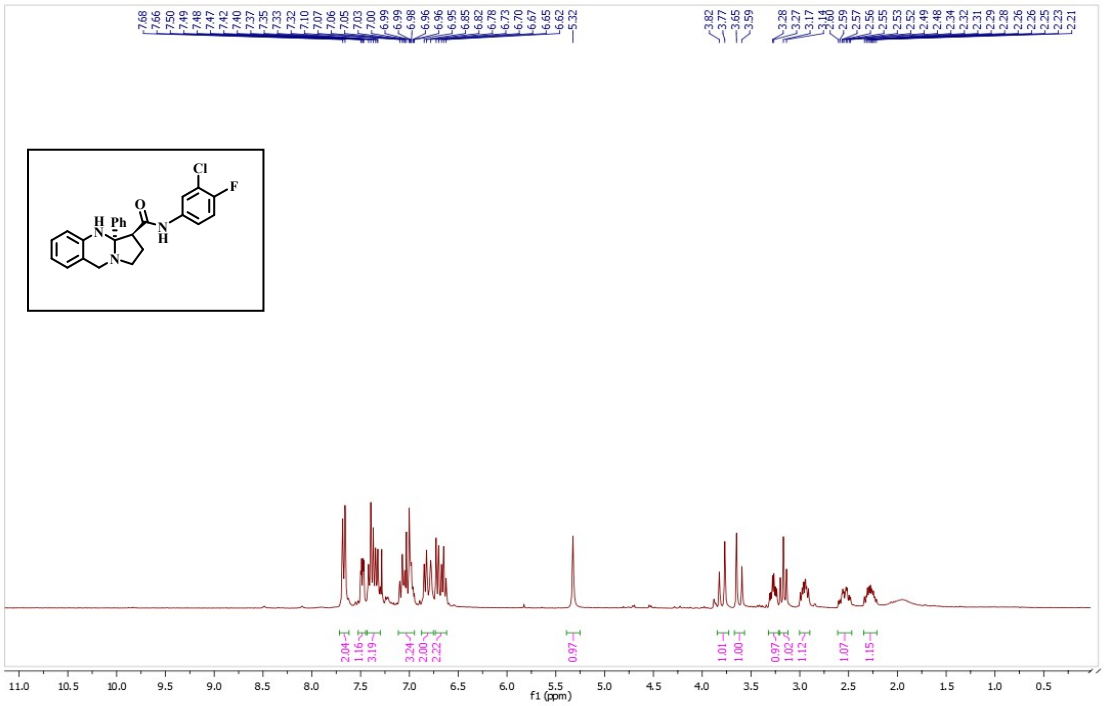


^{1}H NMR of Compound 3o



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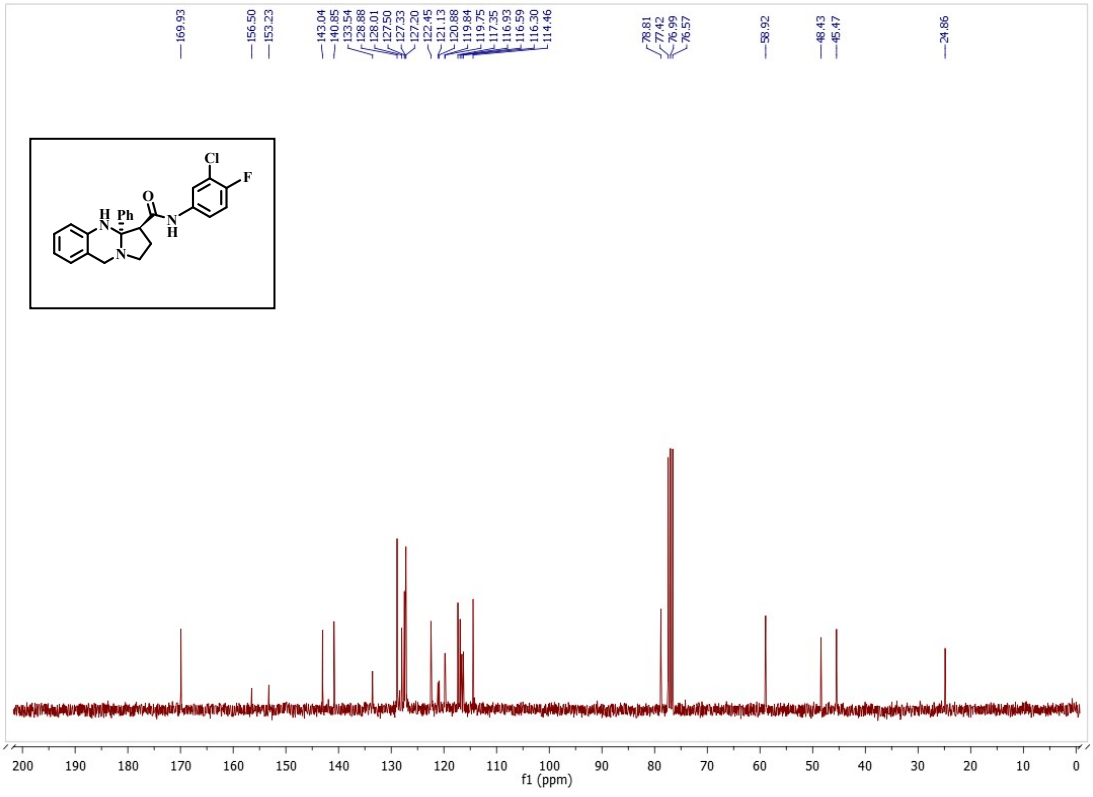

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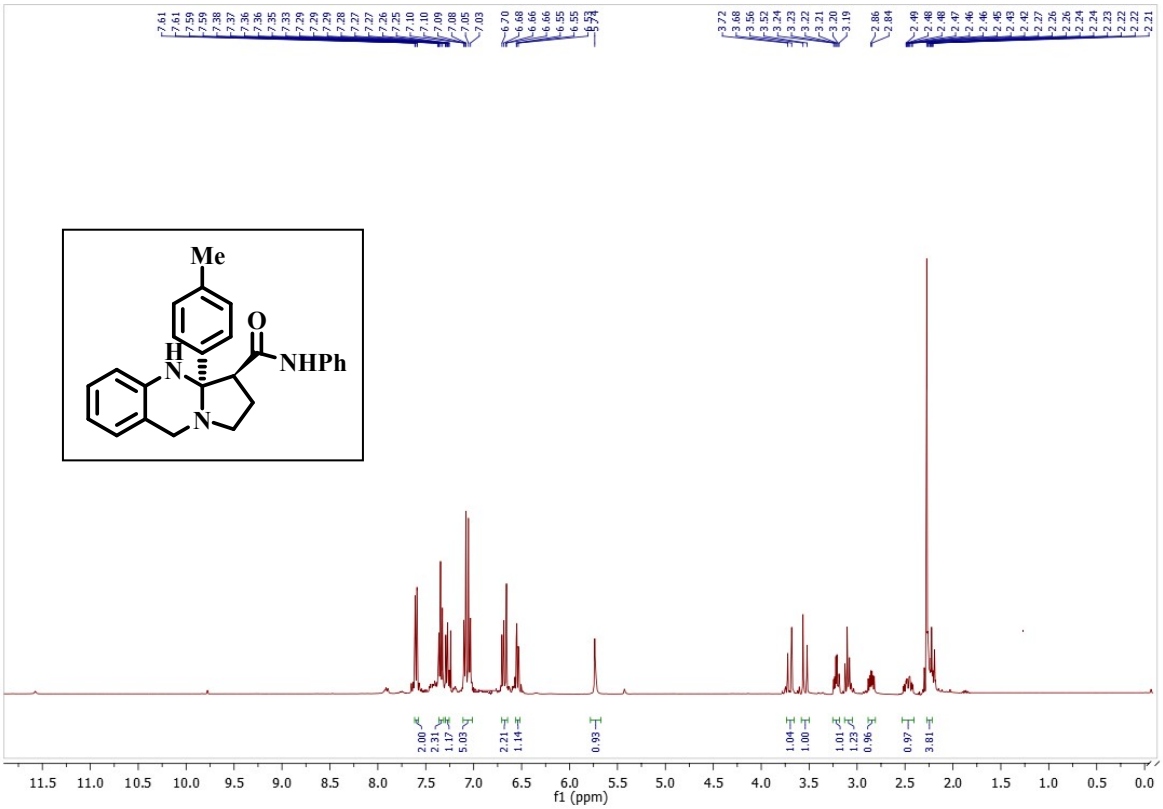

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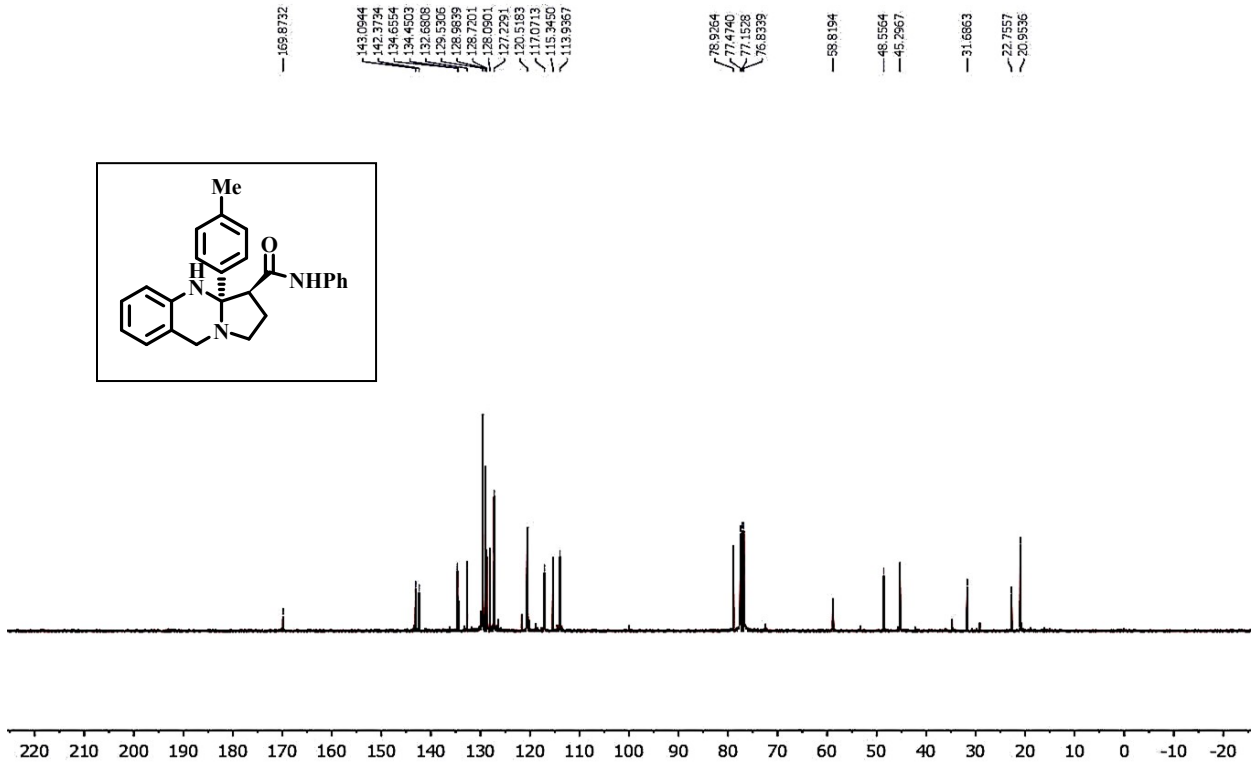
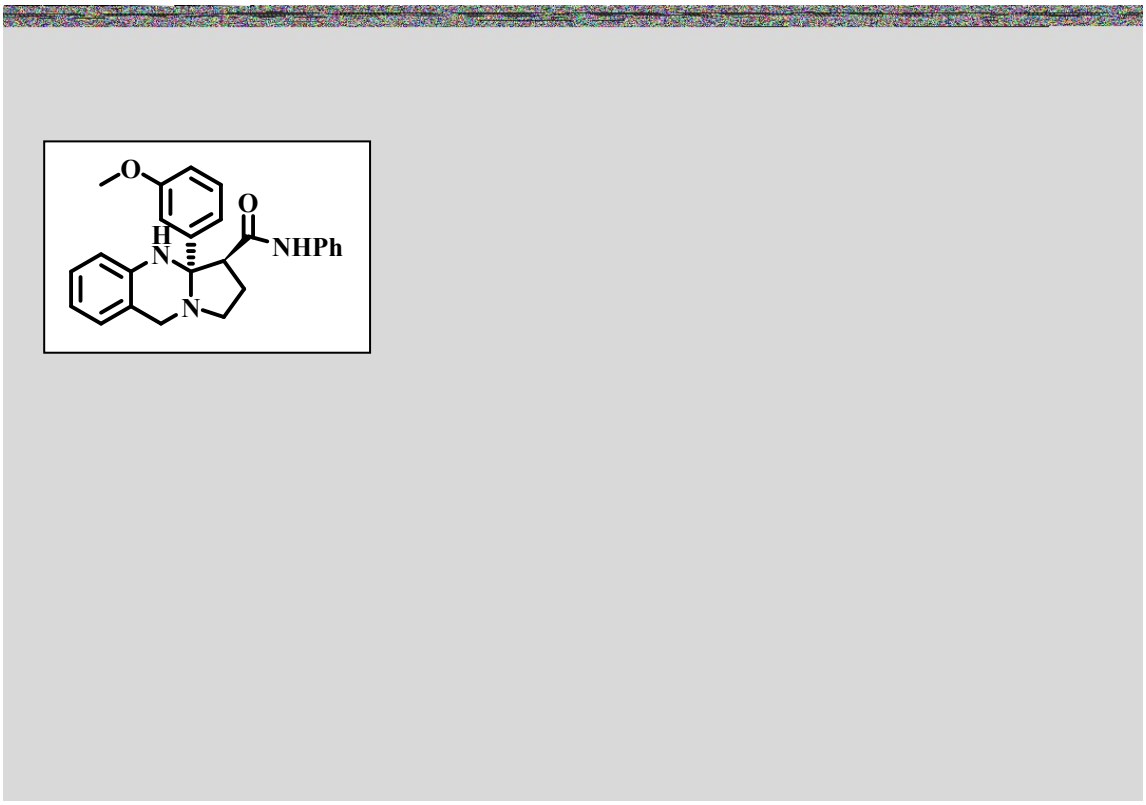


[1]H NMR of Compound 3q



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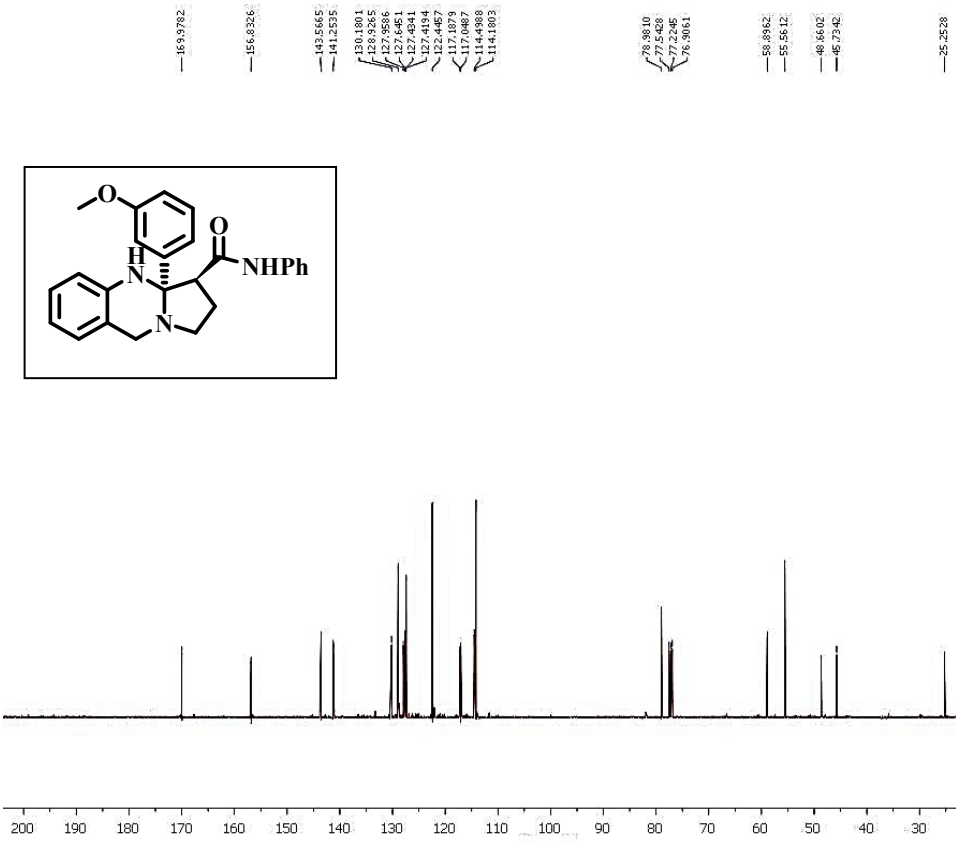

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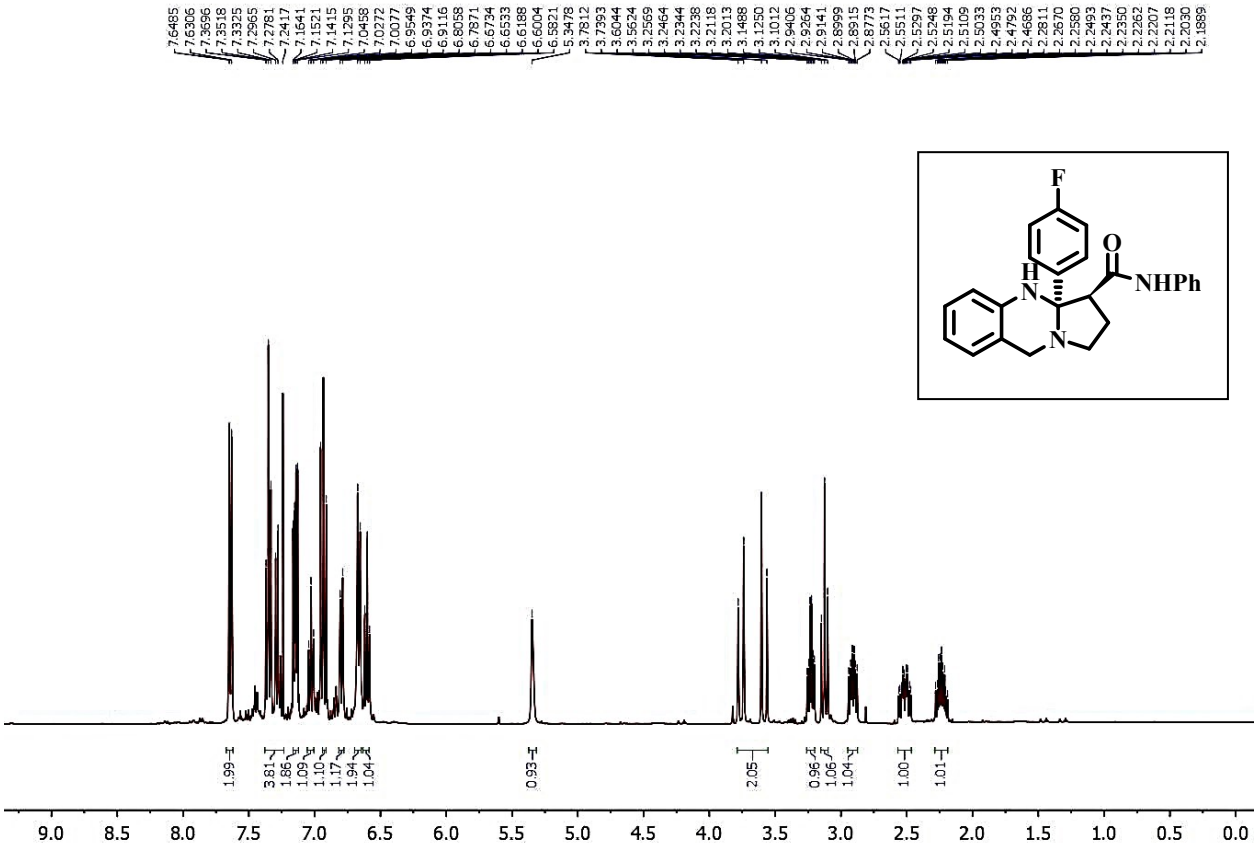

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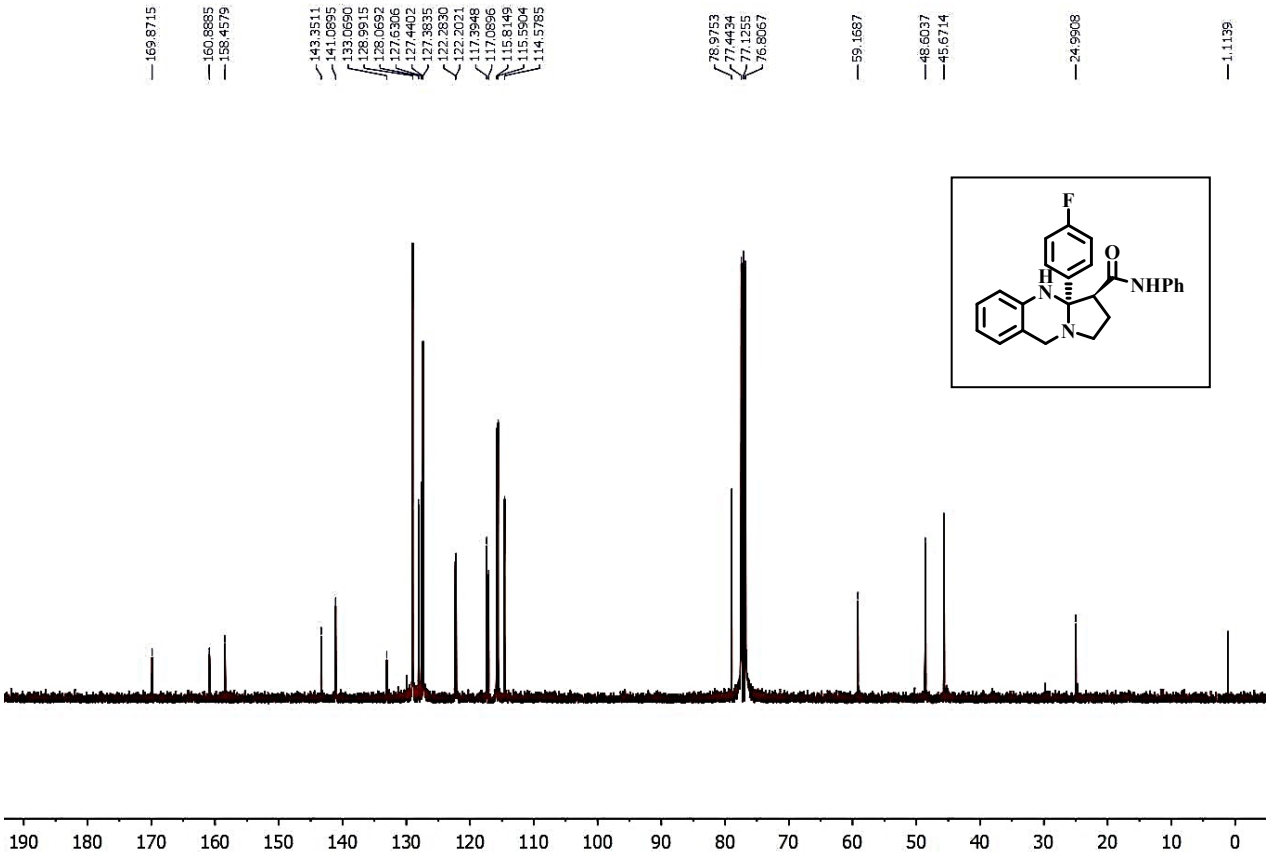

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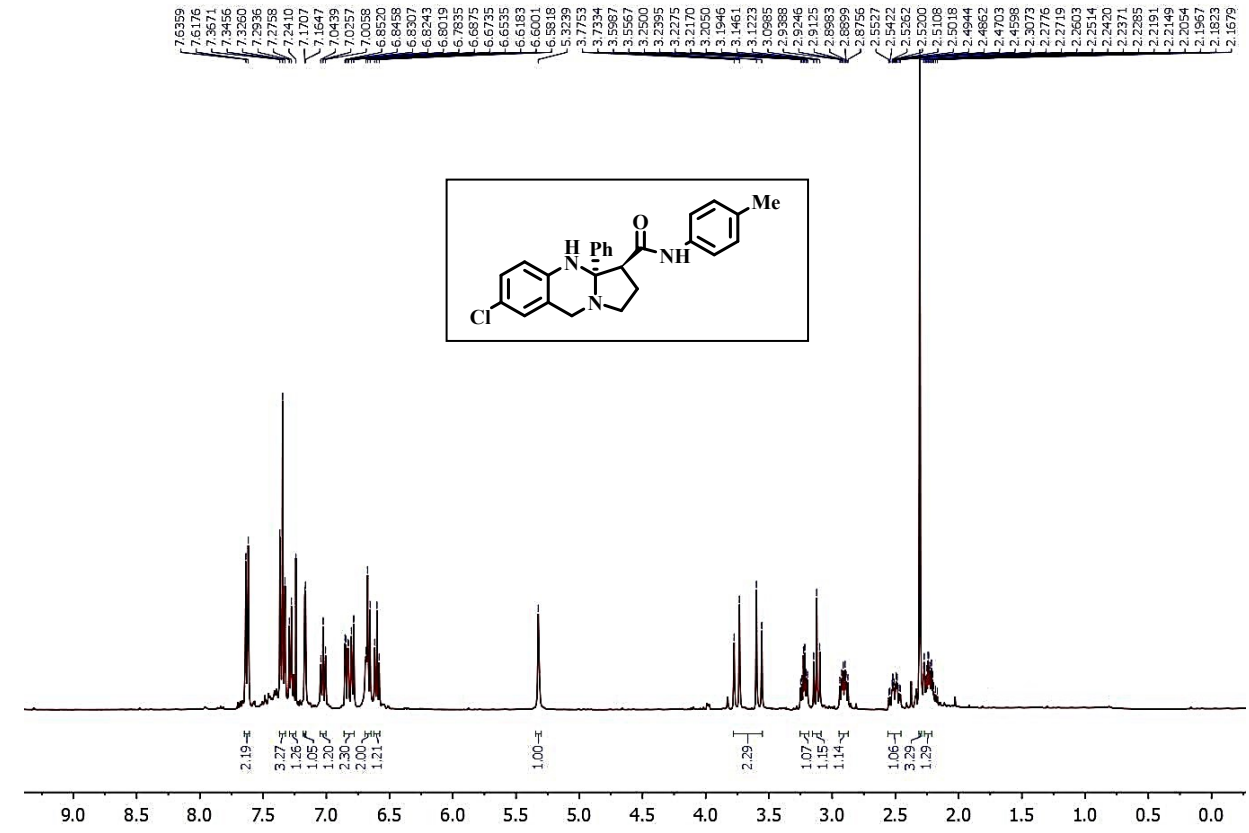

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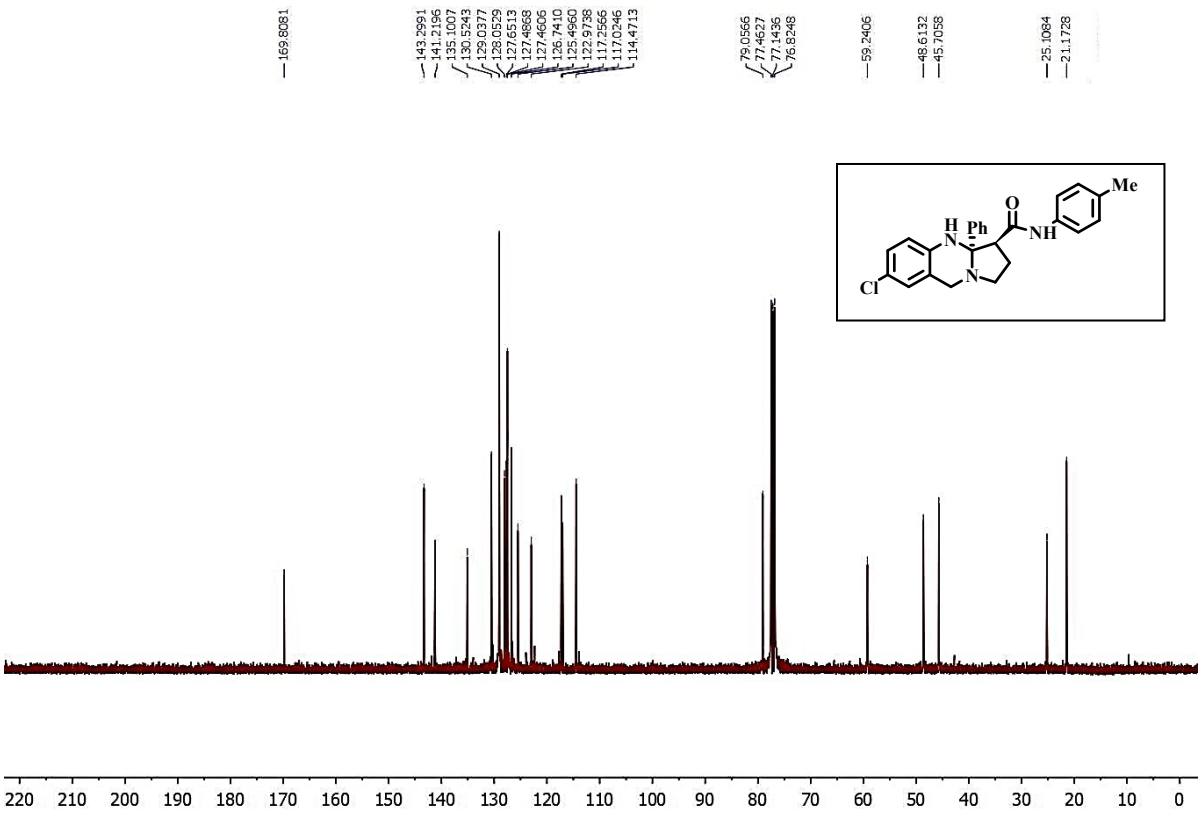

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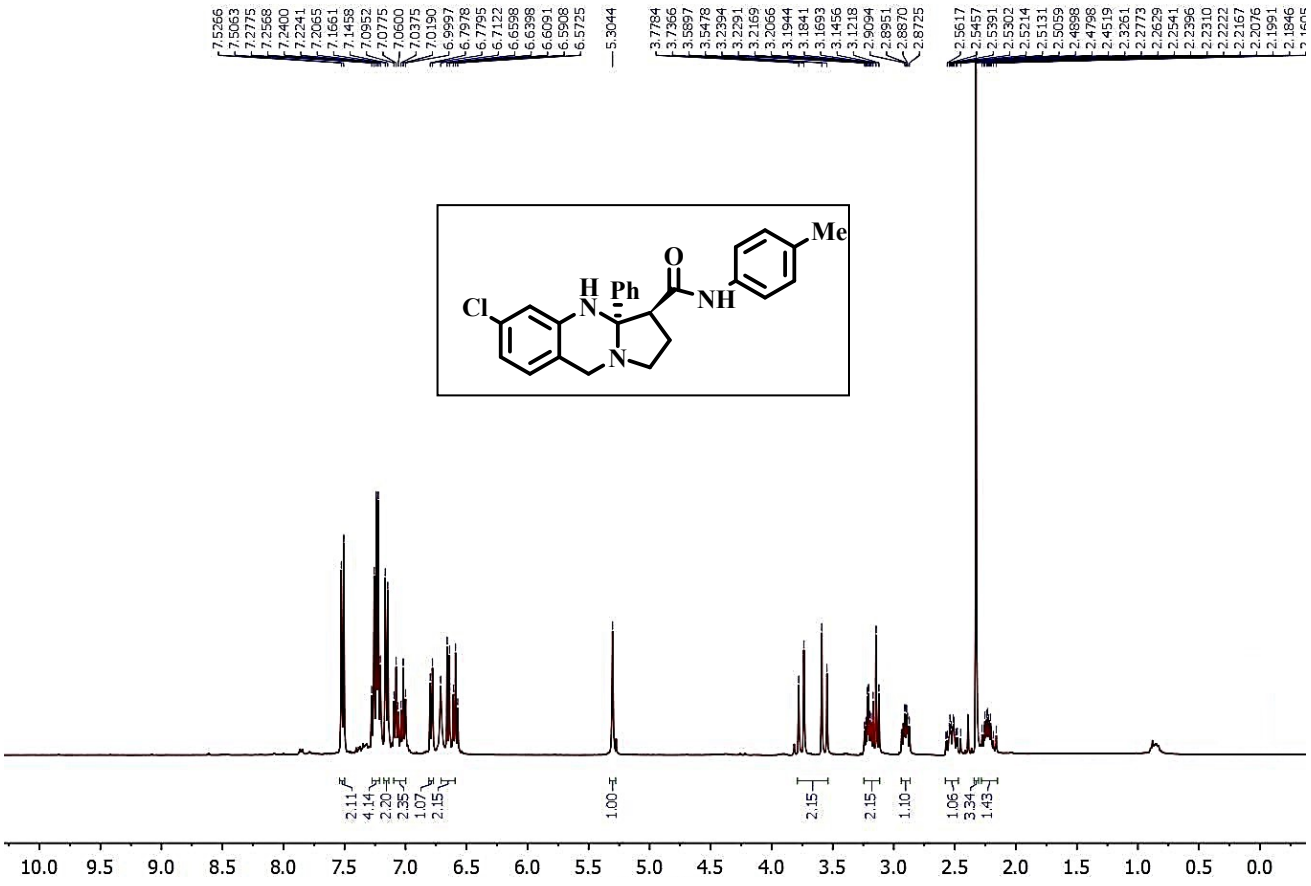

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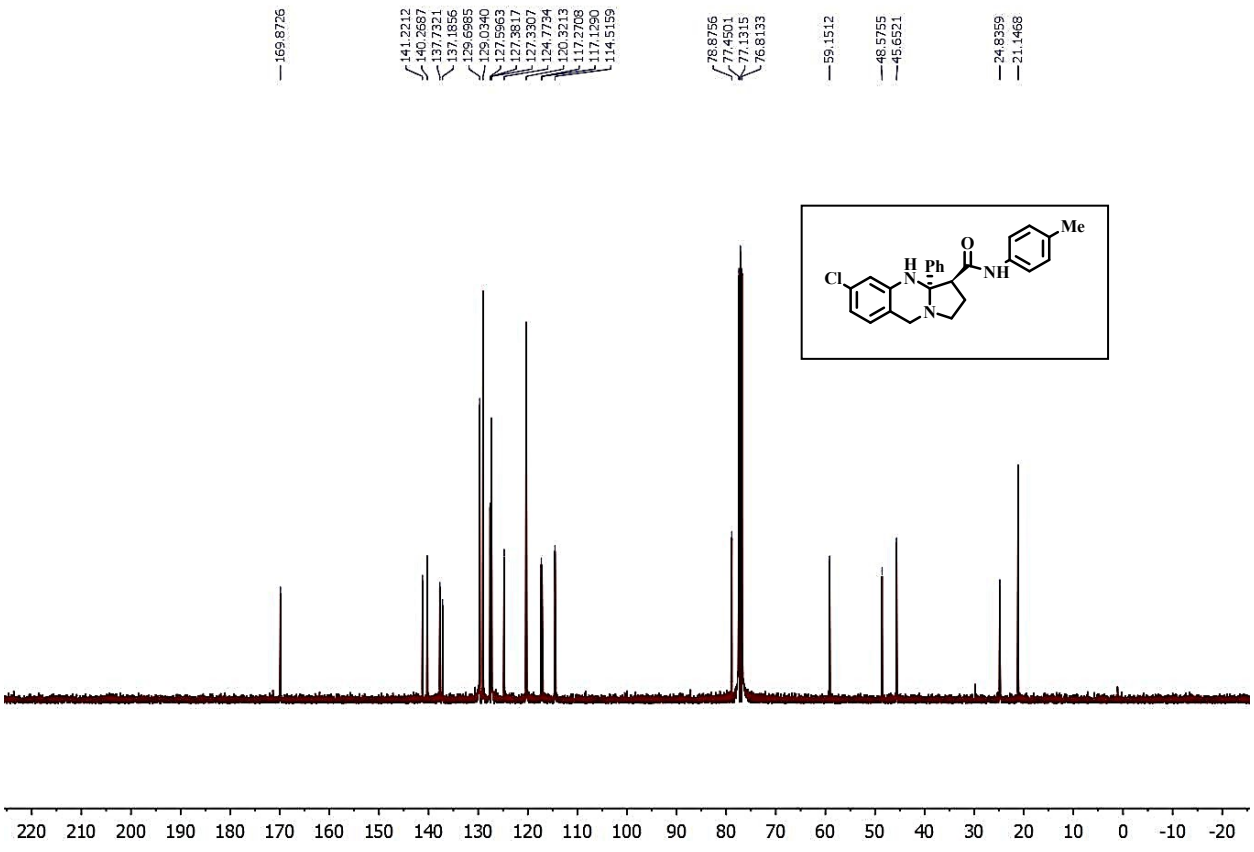

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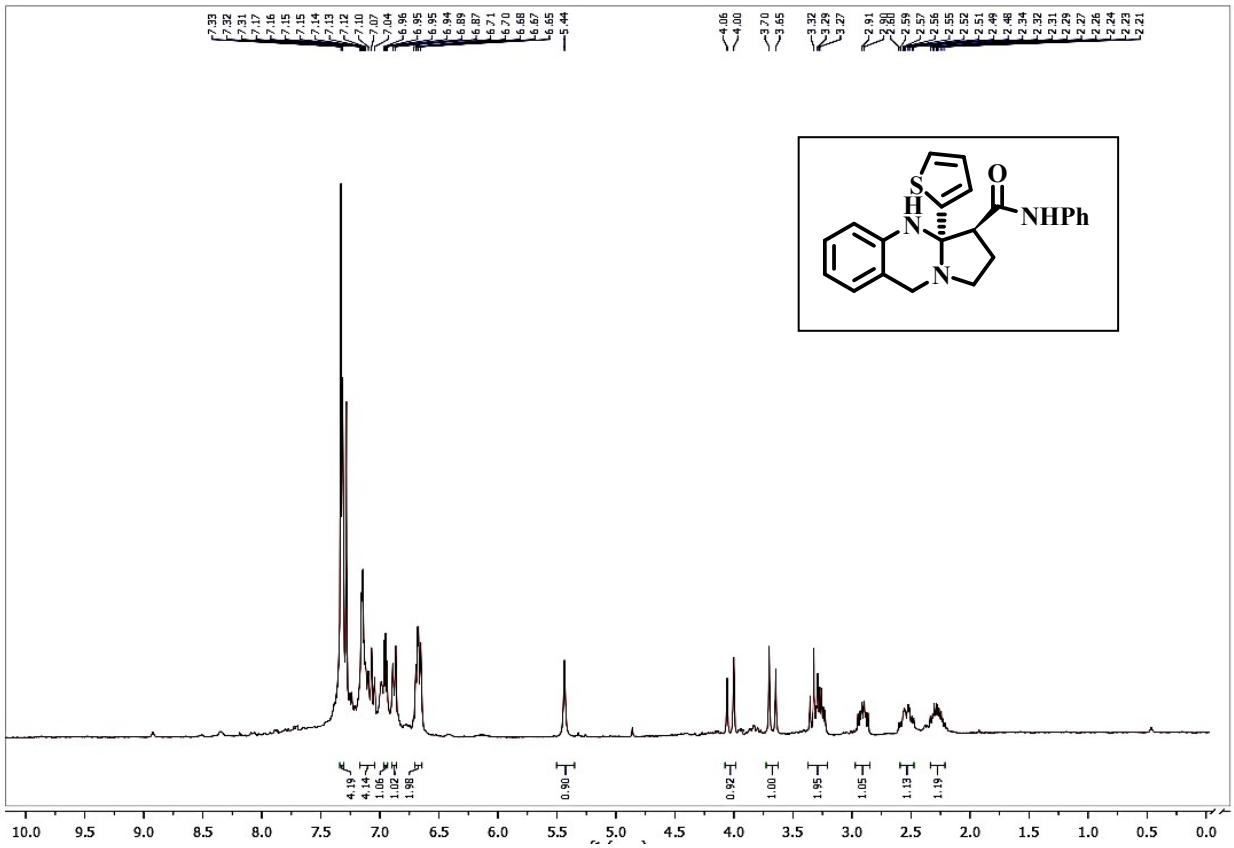

^{13}C NMR of Compound 3u