Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting information

for

A greener approach for the synthesis of 3-cyanoacetamide pyrrole catalyzed by amorphous carbon-supported sulfonic acid

Hai Truong Nguyen,[a,b] Tan Van Le,[a,b] Phat Ngoc Nguyen,[a,b] Khanh Ha Nguyen,[a,b] Linh Ho Thuy Nguyen,[b,c] Tan Le Hoang Doan,[b,c] and Phuong Hoang Tran[a,b]*

[a] Department of Organic Chemistry, Faculty of Chemistry, University of Science, Vietnam National University, Ho Chi Minh City 700000, Viet Nam.

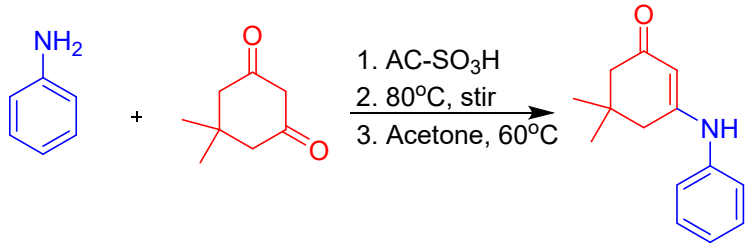
Email: thphuong@hcmus.edu.vn, Phone number: +84903706762

[b] Vietnam National University, Ho Chi Minh City 700000, Viet Nam.

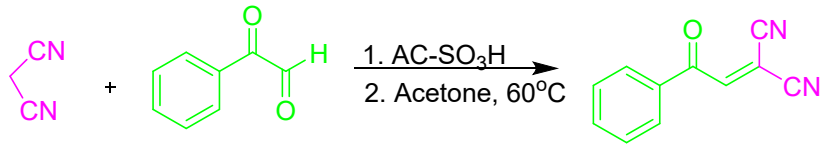
[c] Center for Innovative Materials and Architectures, Ho Chi Minh City 700000, Viet Nam.

Table of contents

Section S1. Control experiments



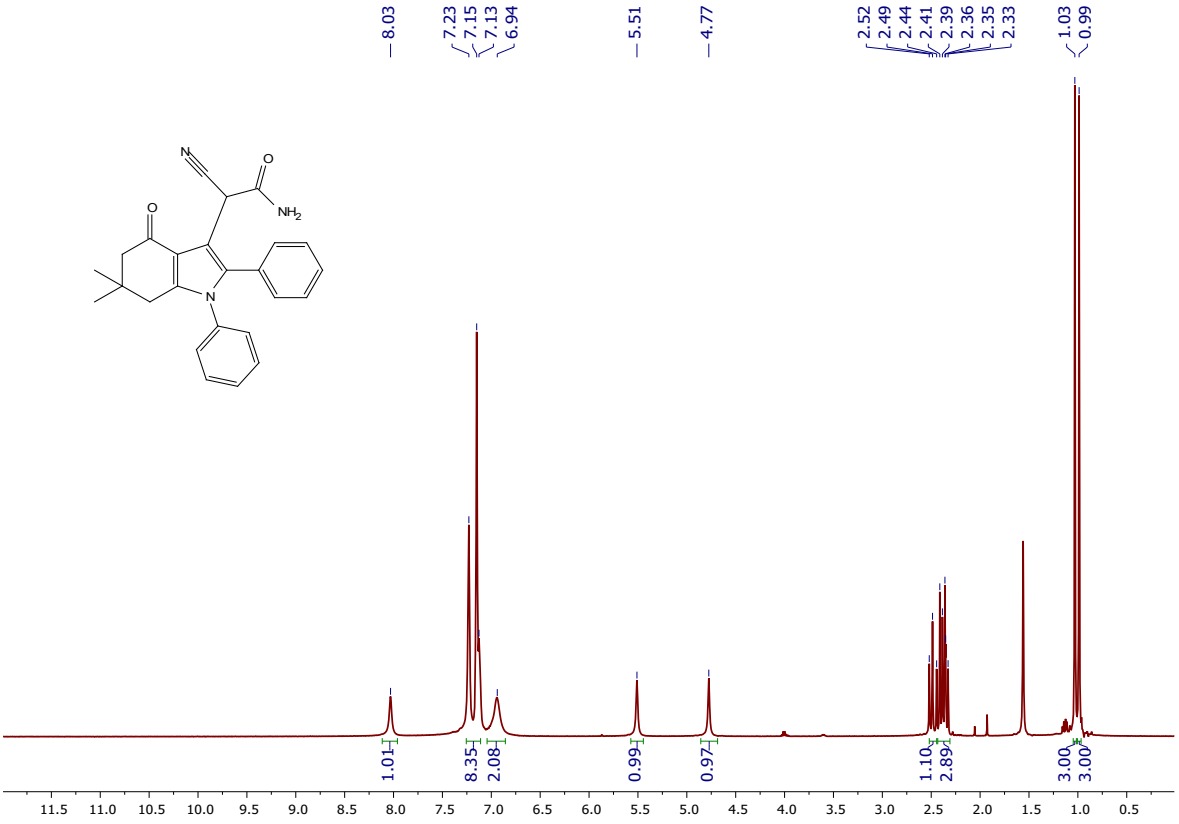
(55%)

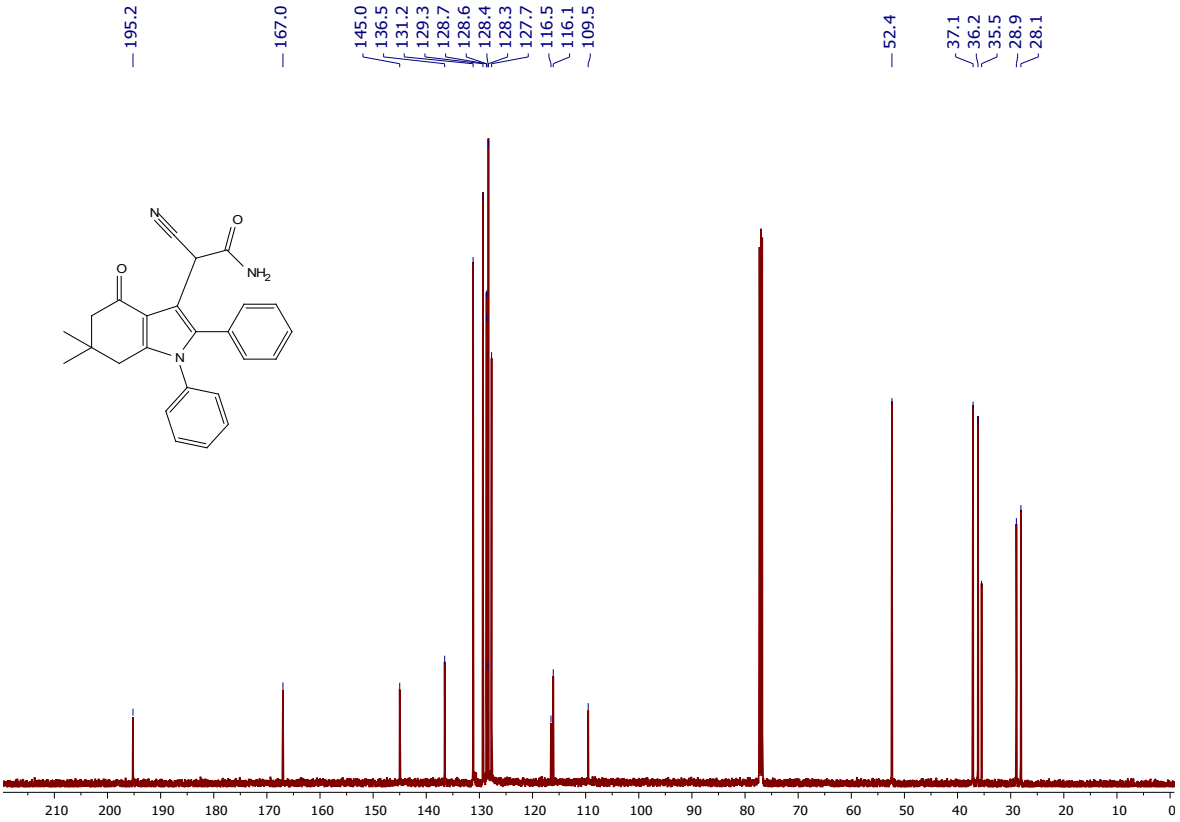


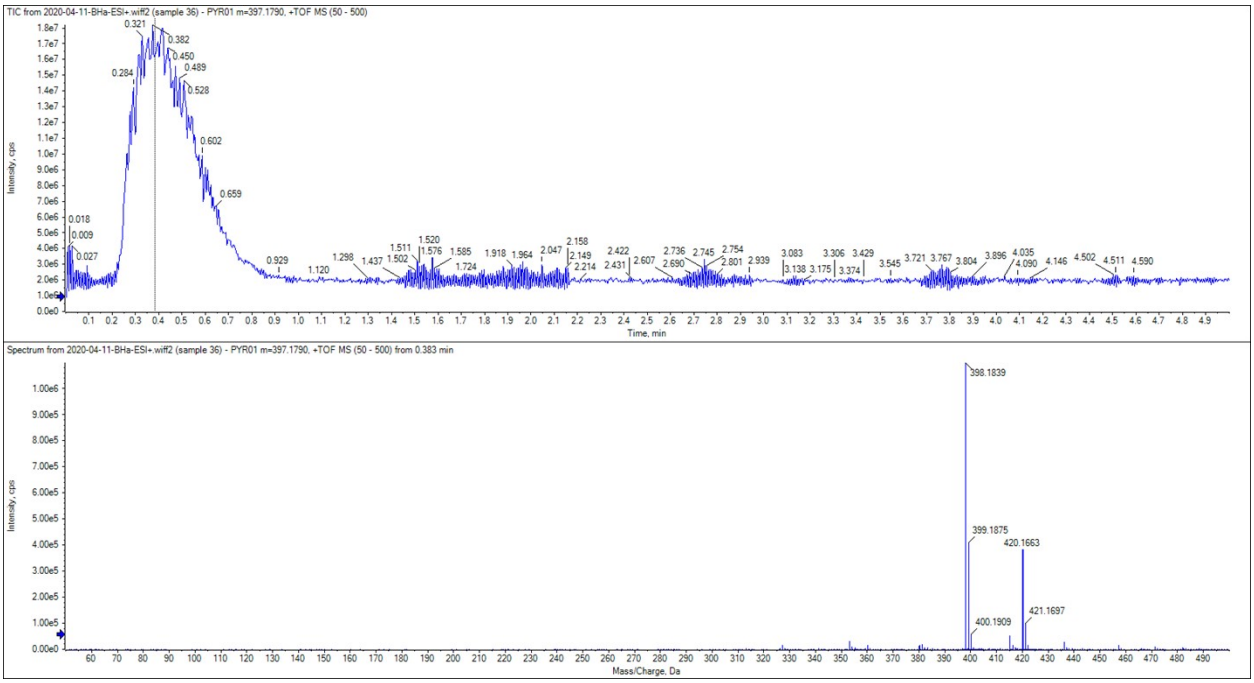
(10%)

Section S2. Spectral data

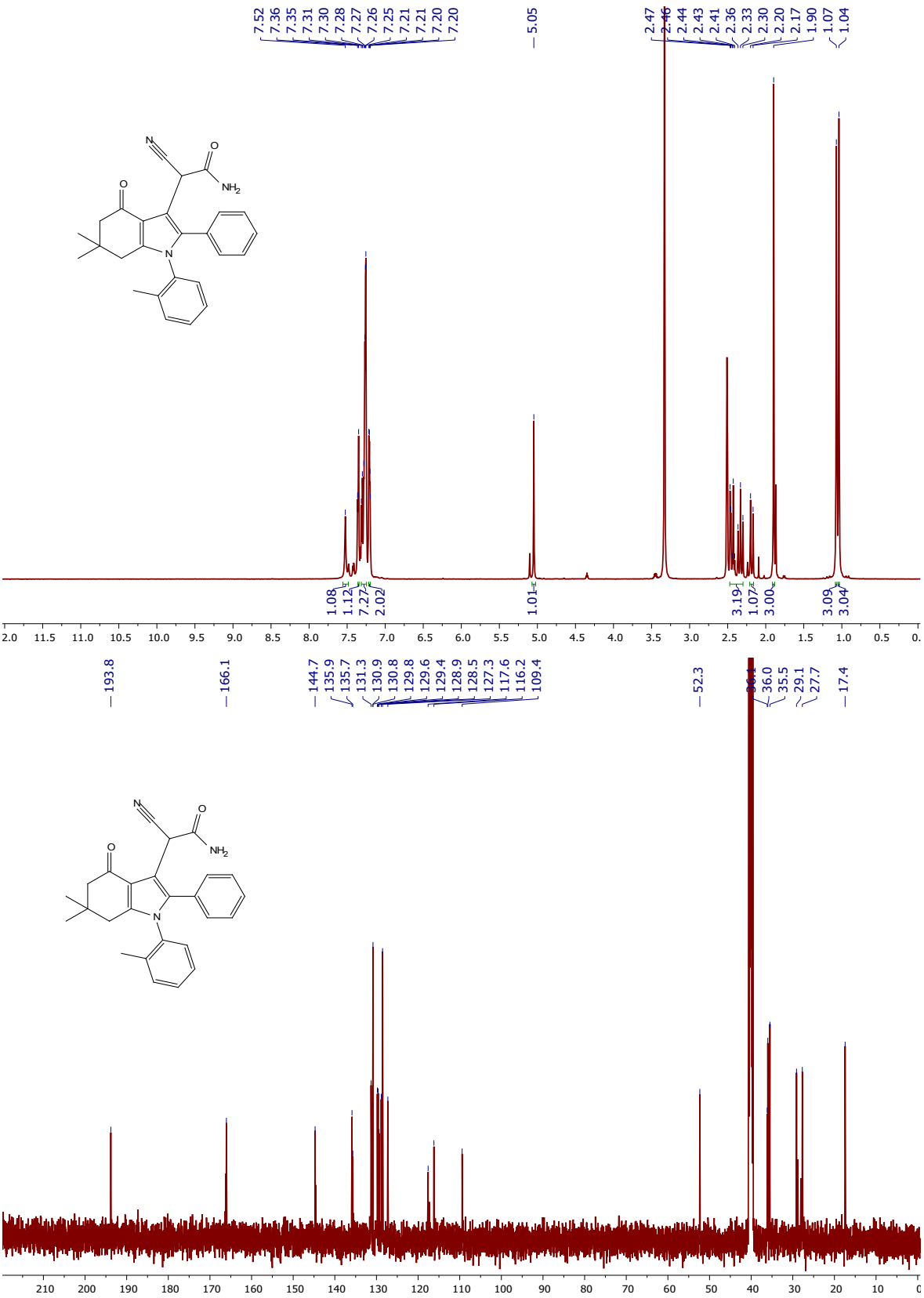
^{1}H, ^{13}C NMR spectrum and HRMS of 2-Cyano-2-(6,6-dimethyl-4-oxo-1,2-diphenyl-4,5,6,7-tetrahydro-1*H*-indol-3-yl)acetamide (1a)



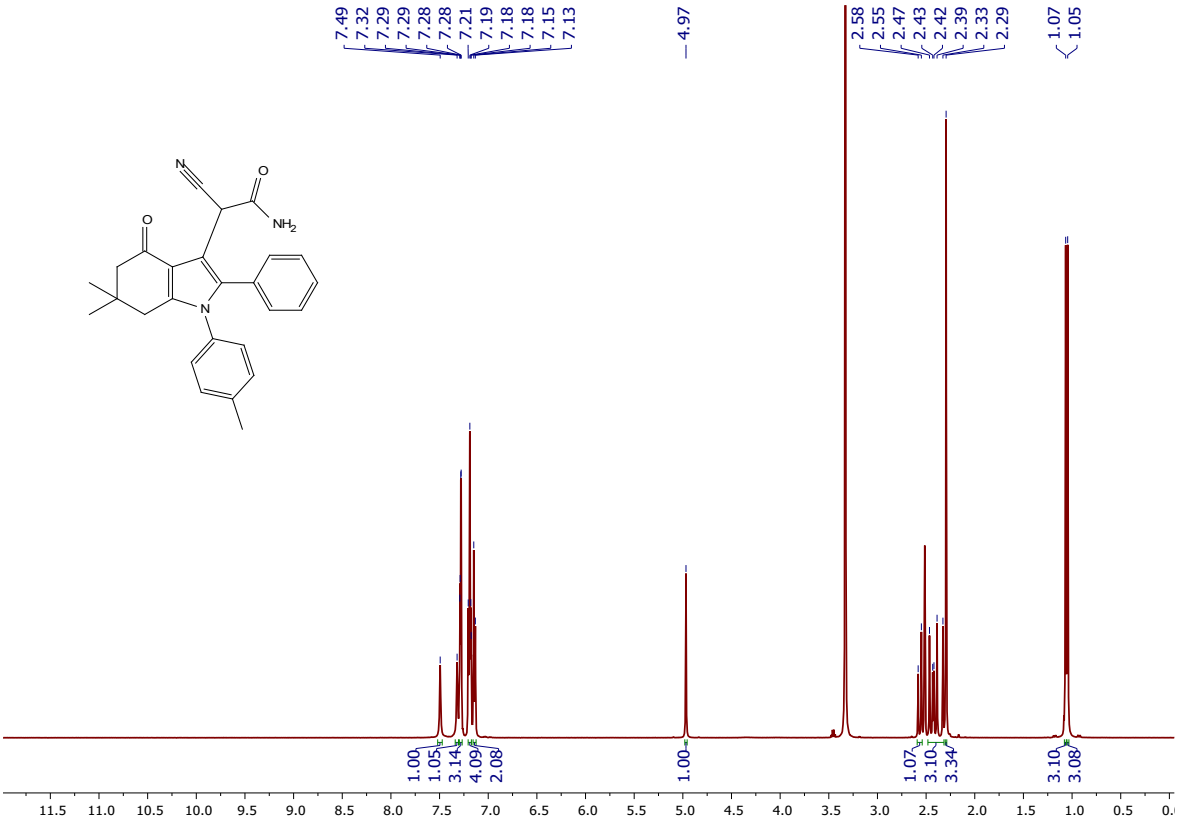

195.2
167.0
145.0
136.5
131.2
129.3
128.7
128.6
128.4
128.3
127.7
116.5
116.1
109.5
52.4
37.1
36.2
35.5
28.9
28.1
O
N
O
NH2
O
N

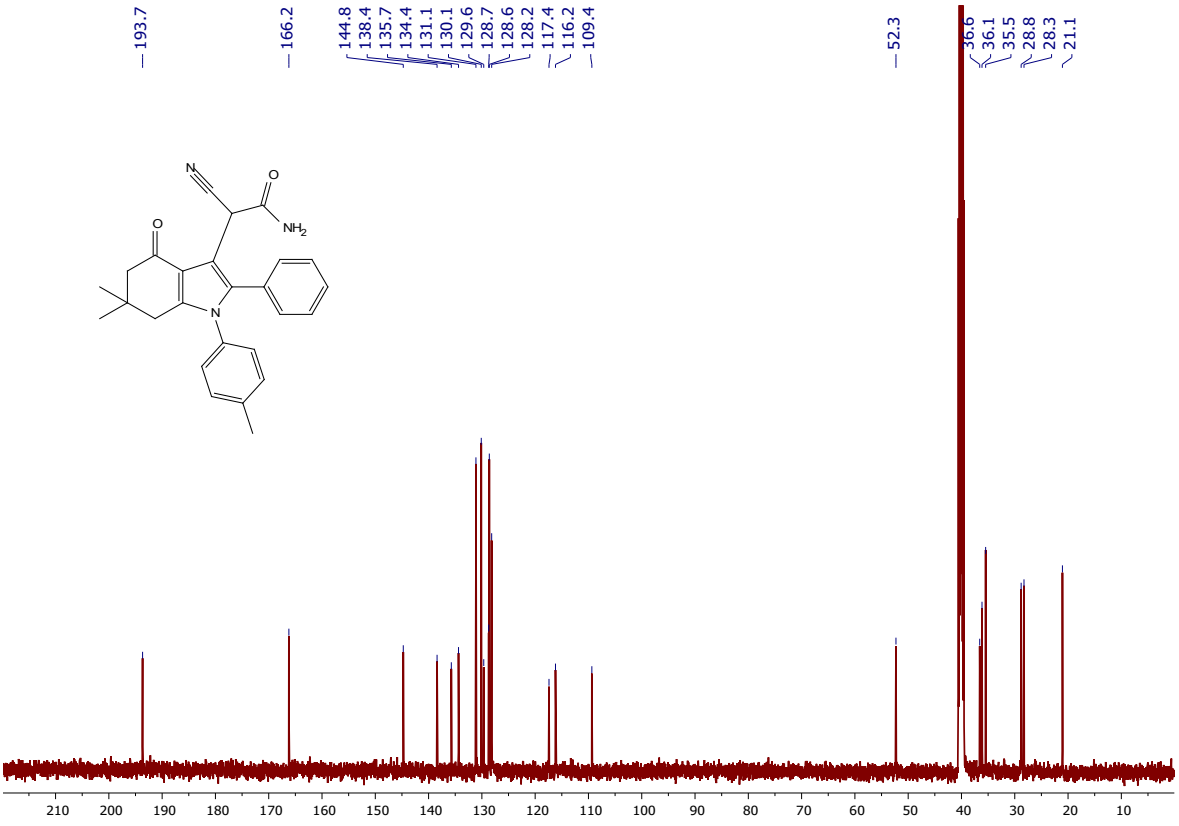

TIC from 2020-04-11-BHa-ESI+.wiff2 (sample 36) - PYR01 m=397.1790, +TOF MS (50 - 500)
Intensity, cps
Time, min
Spectrum from 2020-04-11-BHa-ESI+.wiff2 (sample 36) - PYR01 m=397.1790, +TOF MS (50 - 500) from 0.383 min
398.1839
399.1875
420.1663
400.1909
421.1697
Mass/Charge, Da

^{1}H, ^{13}C NMR spectrum of 2-Cyano-2-(6,6-dimethyl-4-oxo-2-phenyl-1-(*o*-tolyl)-4,5,6,7-tetrahydro-1*H*-indol-3-yl)acetamide (2a)

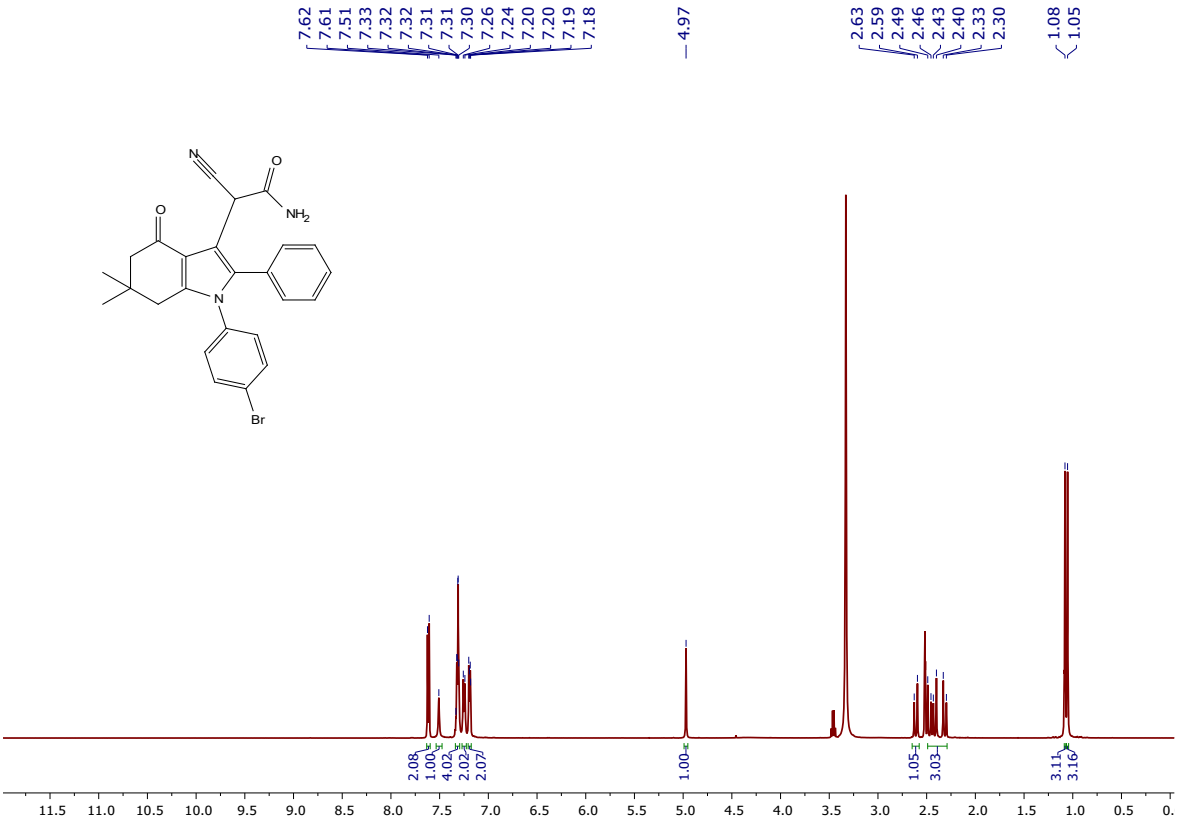


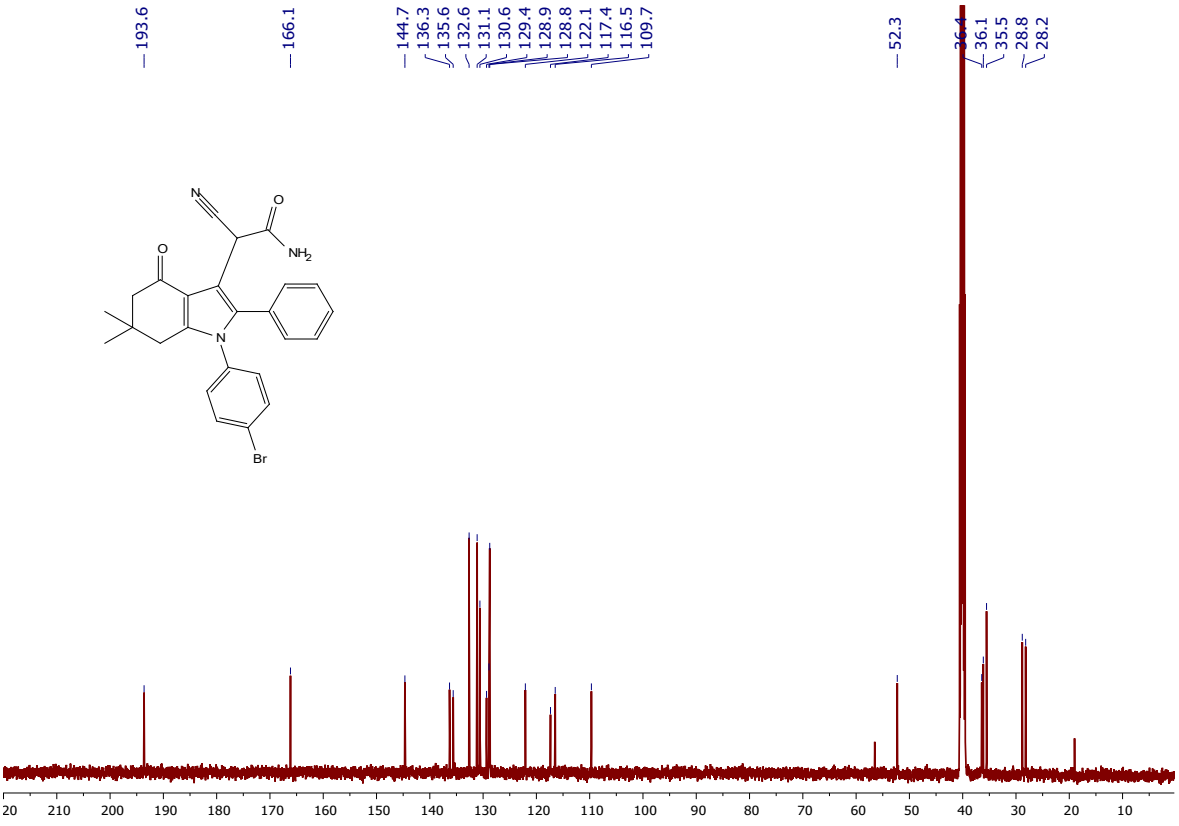
^{1}H, ^{13}C NMR spectrum of 2-Cyano-2-(6,6-dimethyl-4-oxo-2-phenyl-1-(*p*-tolyl)-4,5,6,7-tetrahydro-1*H*-indol-3-yl)acetamide (3a)



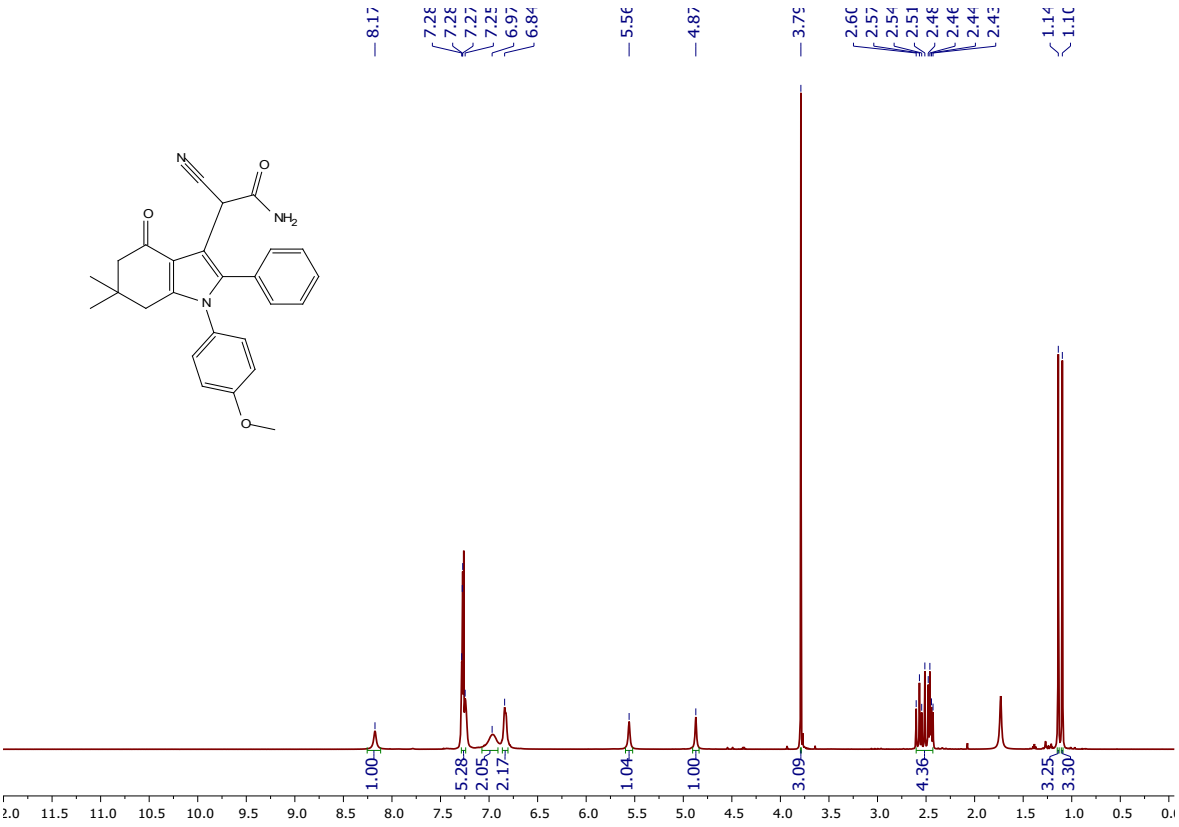


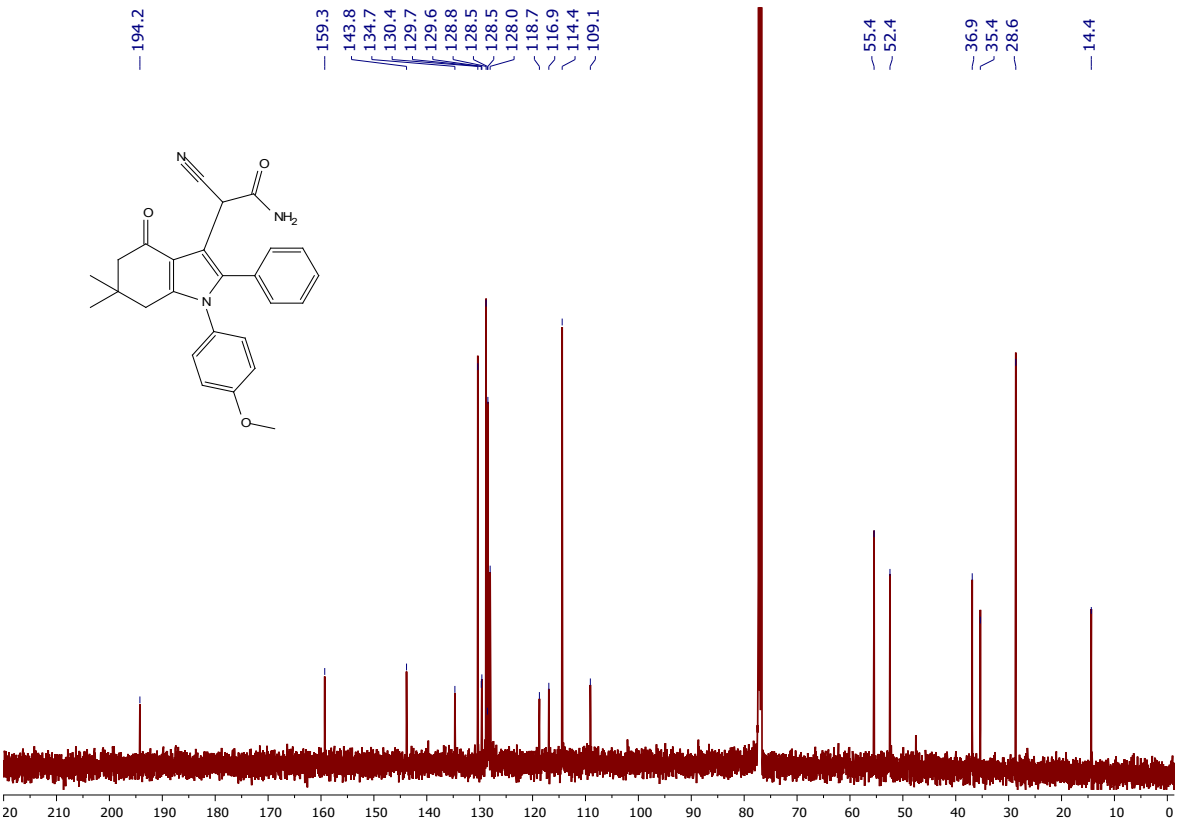
^{1}H, ^{13}C NMR spectrum of 2-(1-(4-Bromophenyl)-6,6-dimethyl-4-oxo-2-phenyl-4,5,6,7-tetrahydro-1*H*-indol-3-yl)-2-cyanoacetamide (4a)



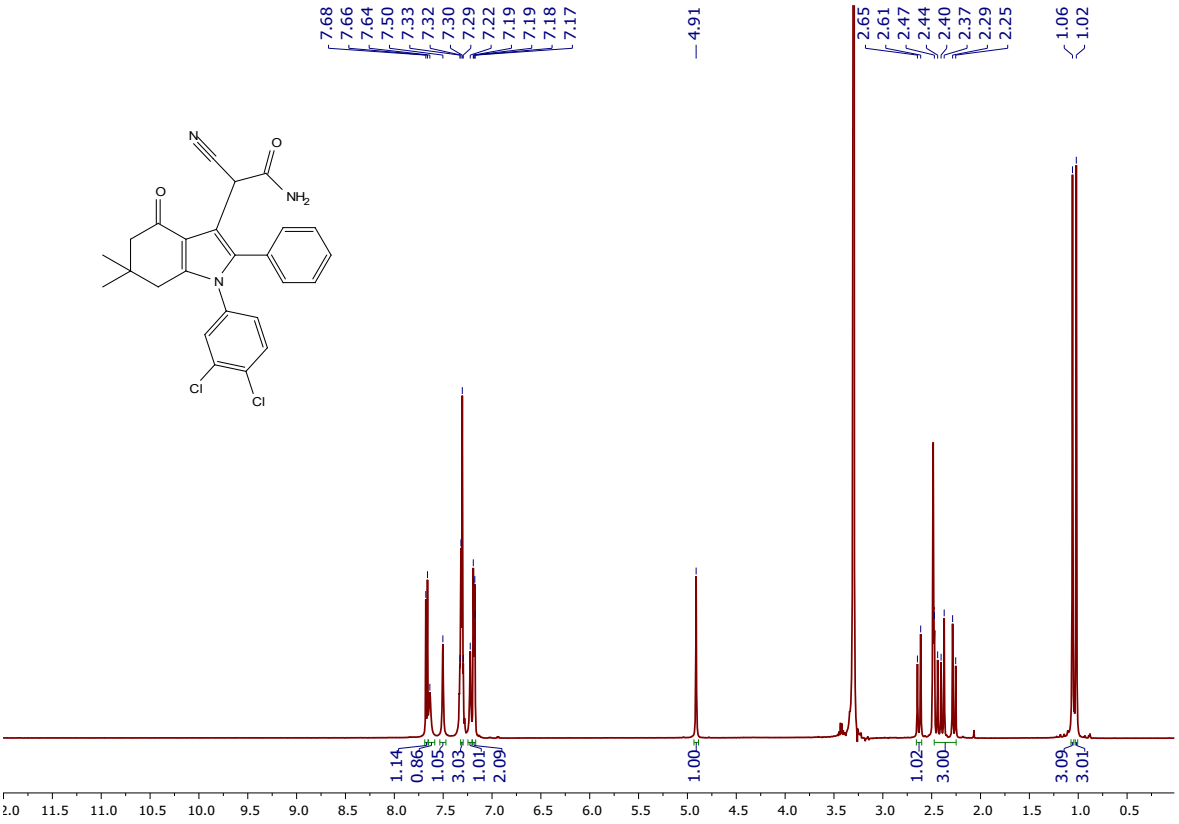


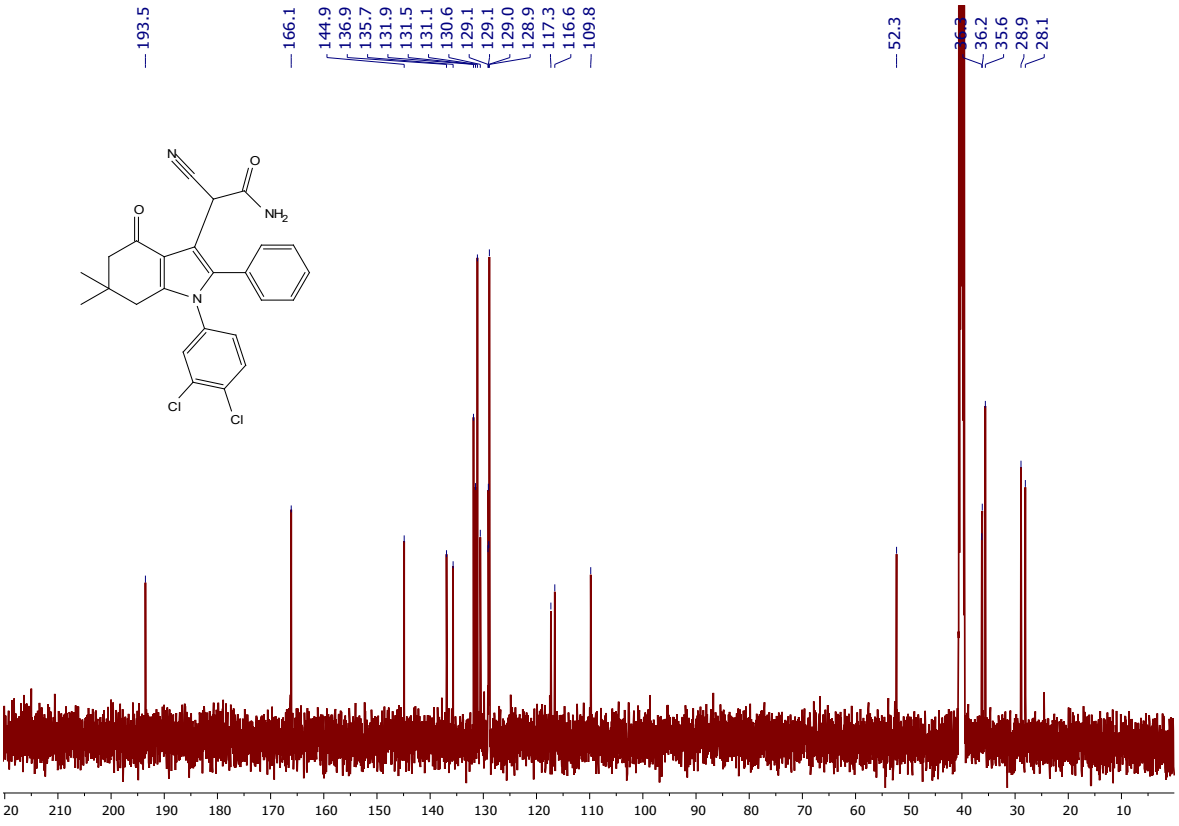
^{1}H, ^{13}C NMR spectrum of 2-Cyano-2-(1-(4-methoxyphenyl)-6,6-dimethyl-4-oxo-2-phenyl-4,5,6,7-tetrahydro-1*H*-indol-3-yl)acetamide (5a).



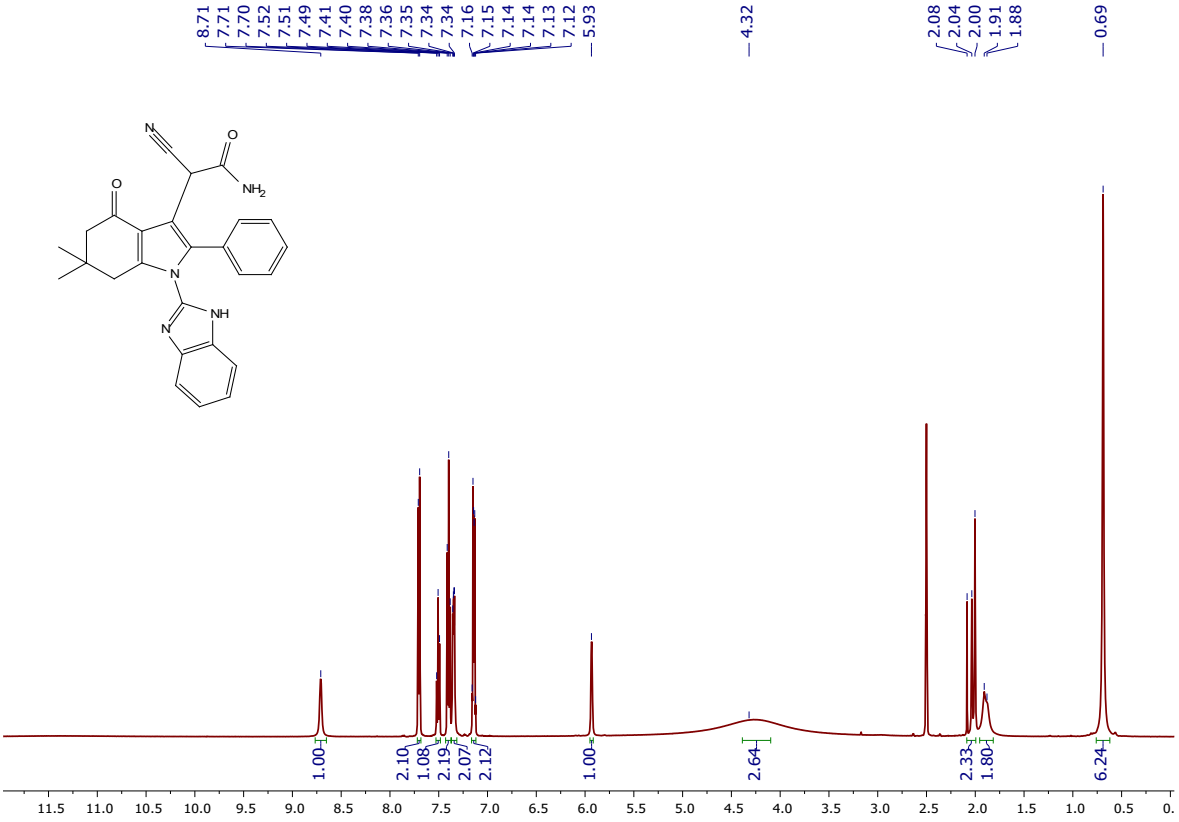


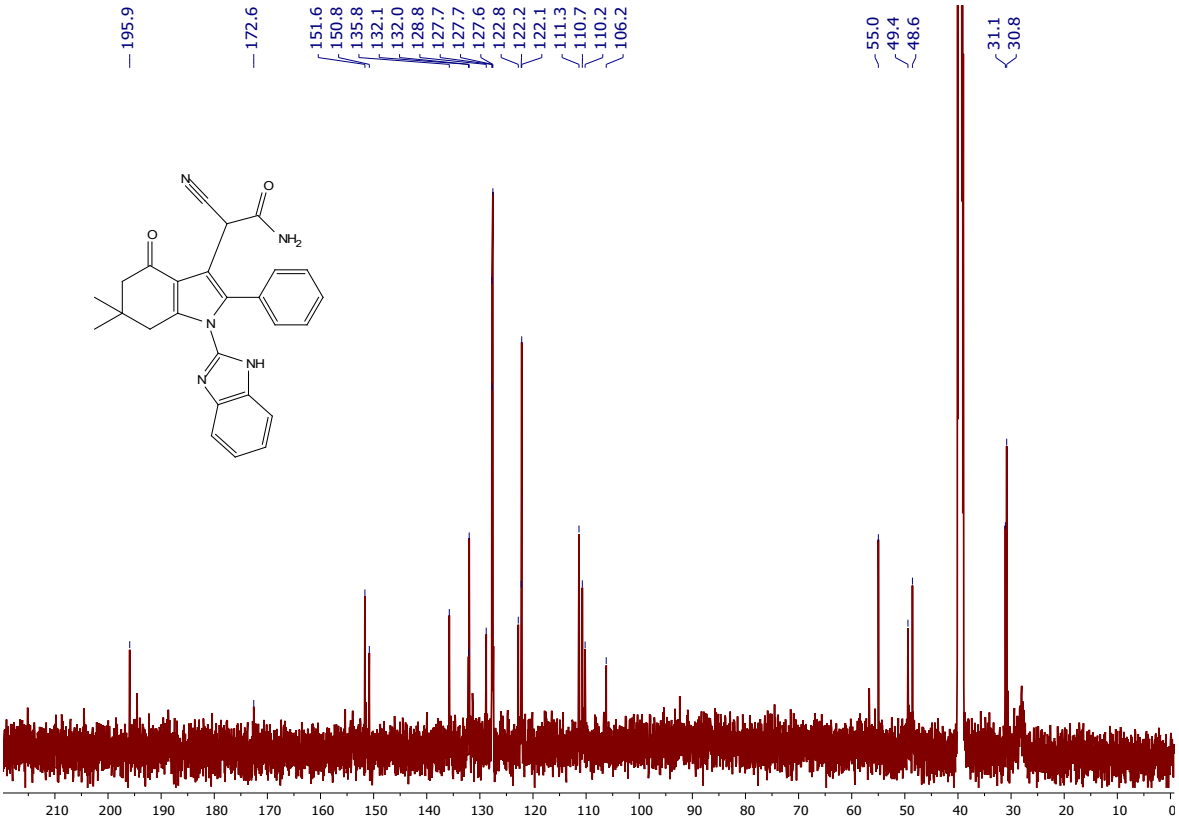
^{1}H, ^{13}C NMR spectrum of 2-Cyano-2-(1-(3,4-dichlorophenyl)-6,6-dimethyl-4-oxo-2-phenyl-4,5,6,7-tetrahydro-1*H*-indol-3-yl)acetamide (6a)



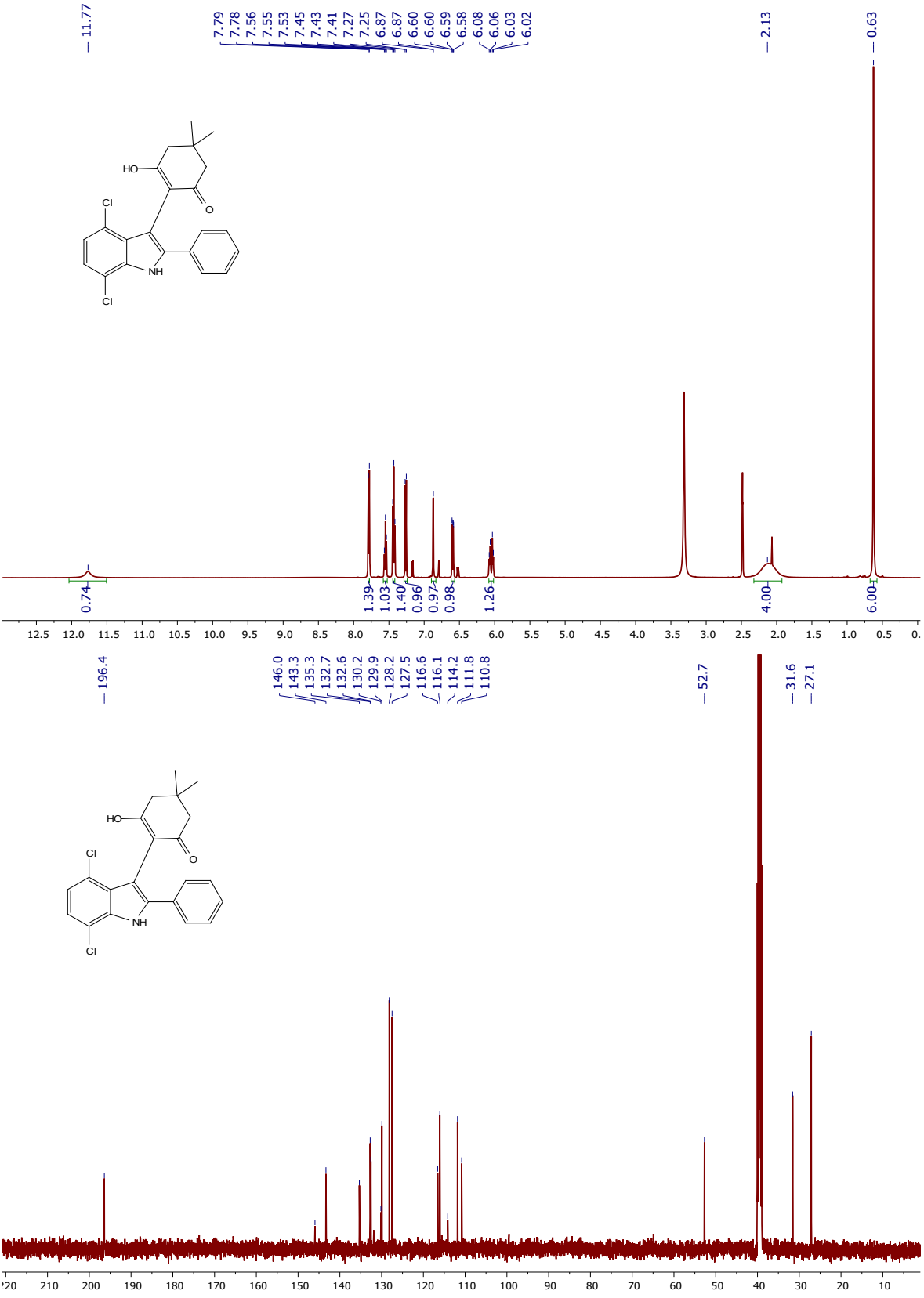


^{1}H, ^{13}C NMR spectrum of 2-(1-(1*H*-Benzo[*d*]imidazol-2-yl)-6,6-dimethyl-4-oxo-2-phenyl-4,5,6,7-tetrahydro-1*H*-indol-3-yl)-2-cyanoacetamide (7a)

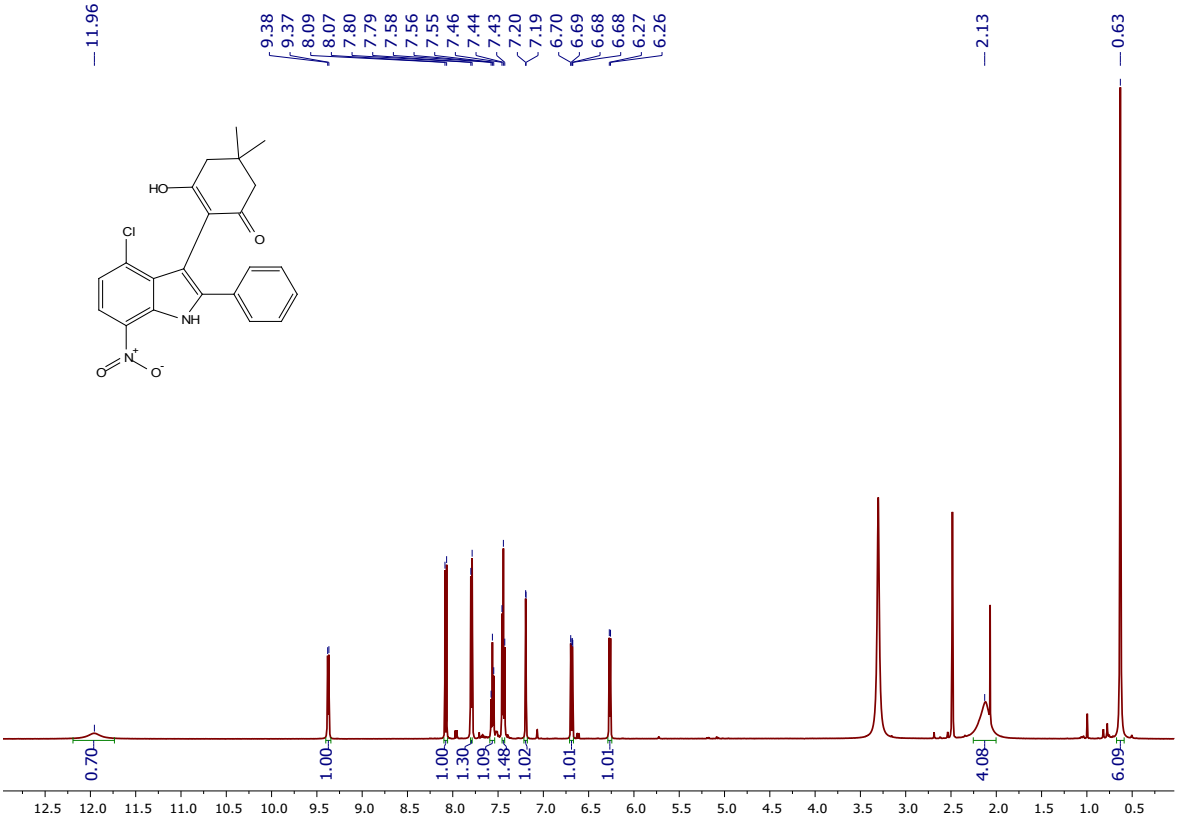


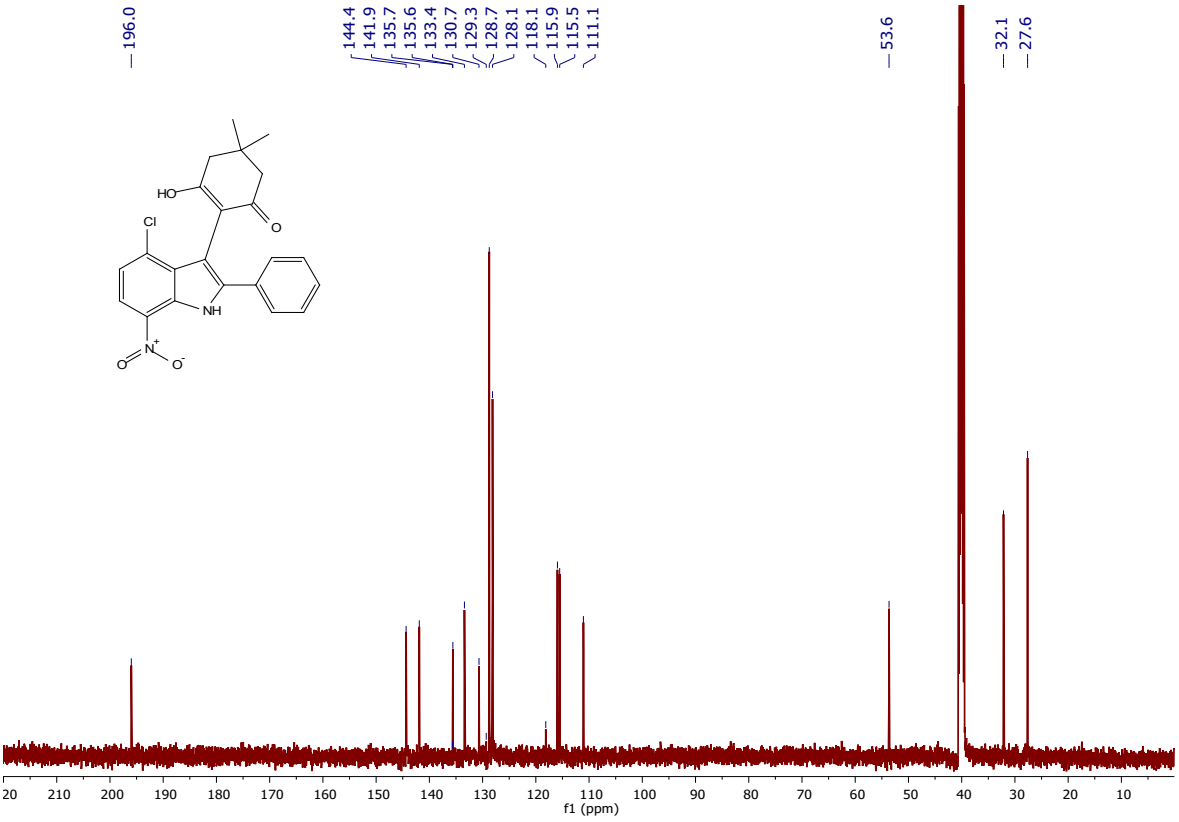


^{1}H, ^{13}C NMR spectrum of 2-(4,7-Dichloro-2-phenyl-1*H*-indol-3-yl)-3-hydroxy-5,5-dimethylcyclohex-2-en-1-one (8c).

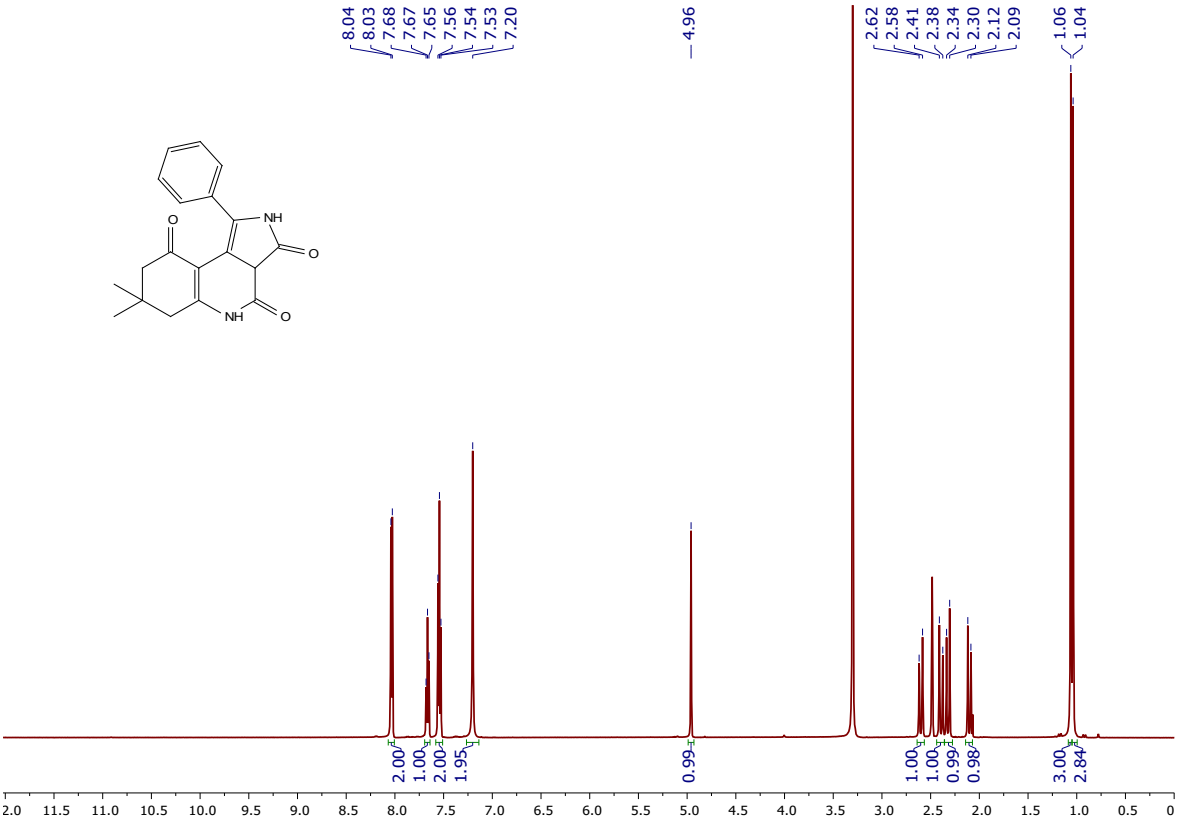


^{1}H, ^{13}C NMR spectrum of 2-(4-Chloro-7-nitro-2-phenyl-1*H*-indol-3-yl)-3-hydroxy-5,5-dimethylcyclohex-2-en-1-one (9c).

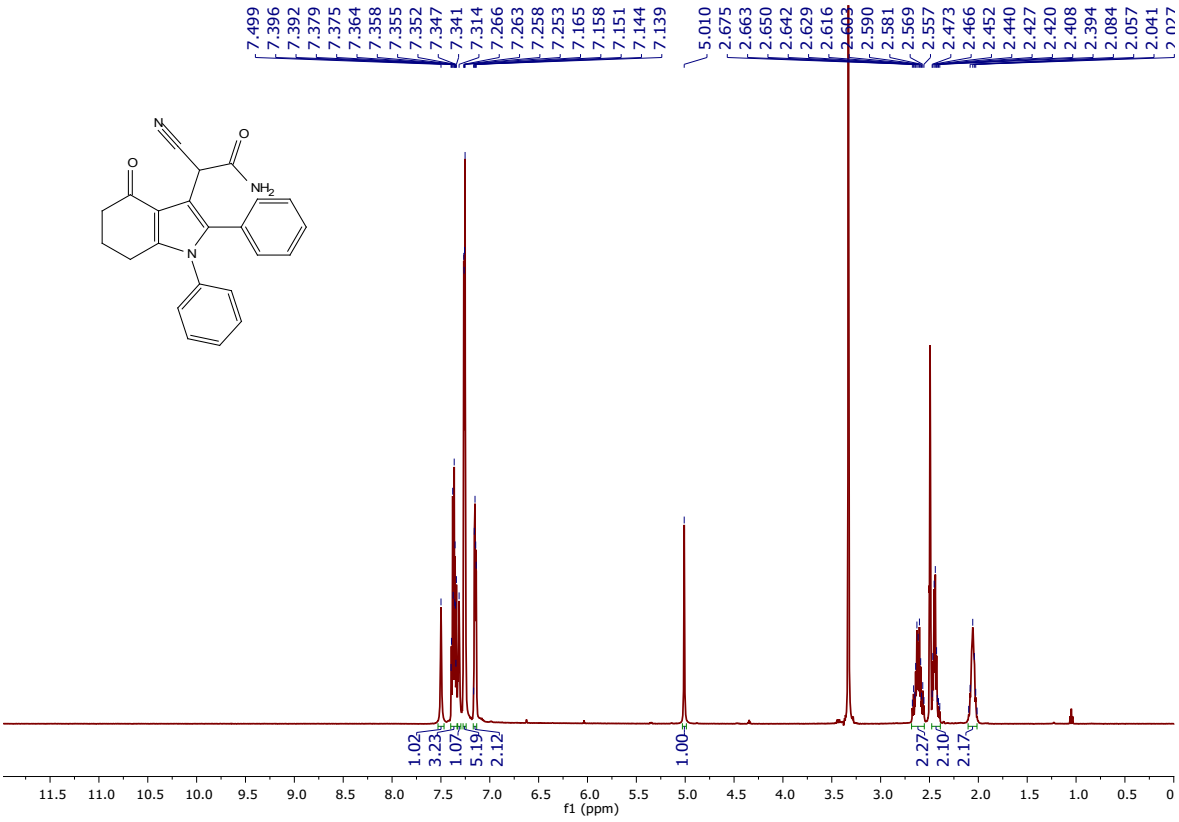


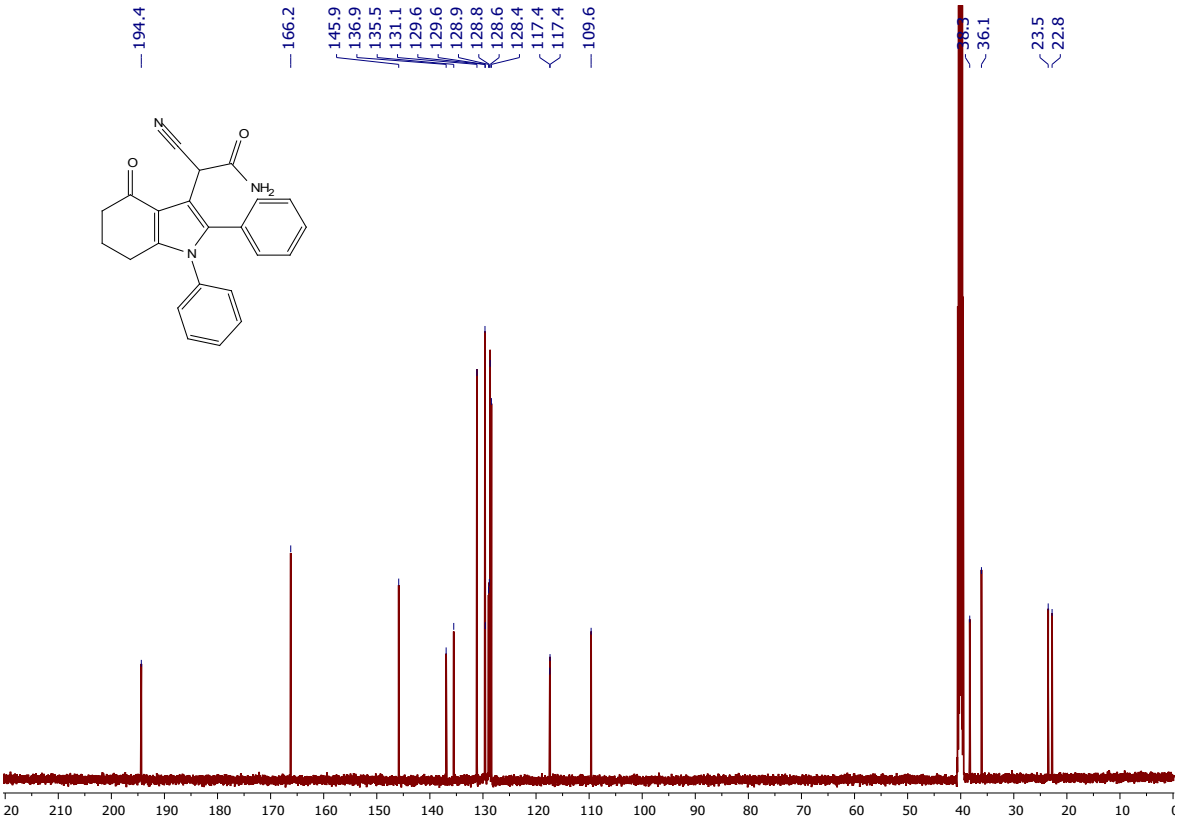


^{1}H NMR spectrum of 7,7-Dimethyl-1-phenyl-2,6,7,8-tetrahydro-3*H*-pyrrolo[3,4-*c*]quinoline-3,4,9(3a*H*,5*H*)-trione (10b)

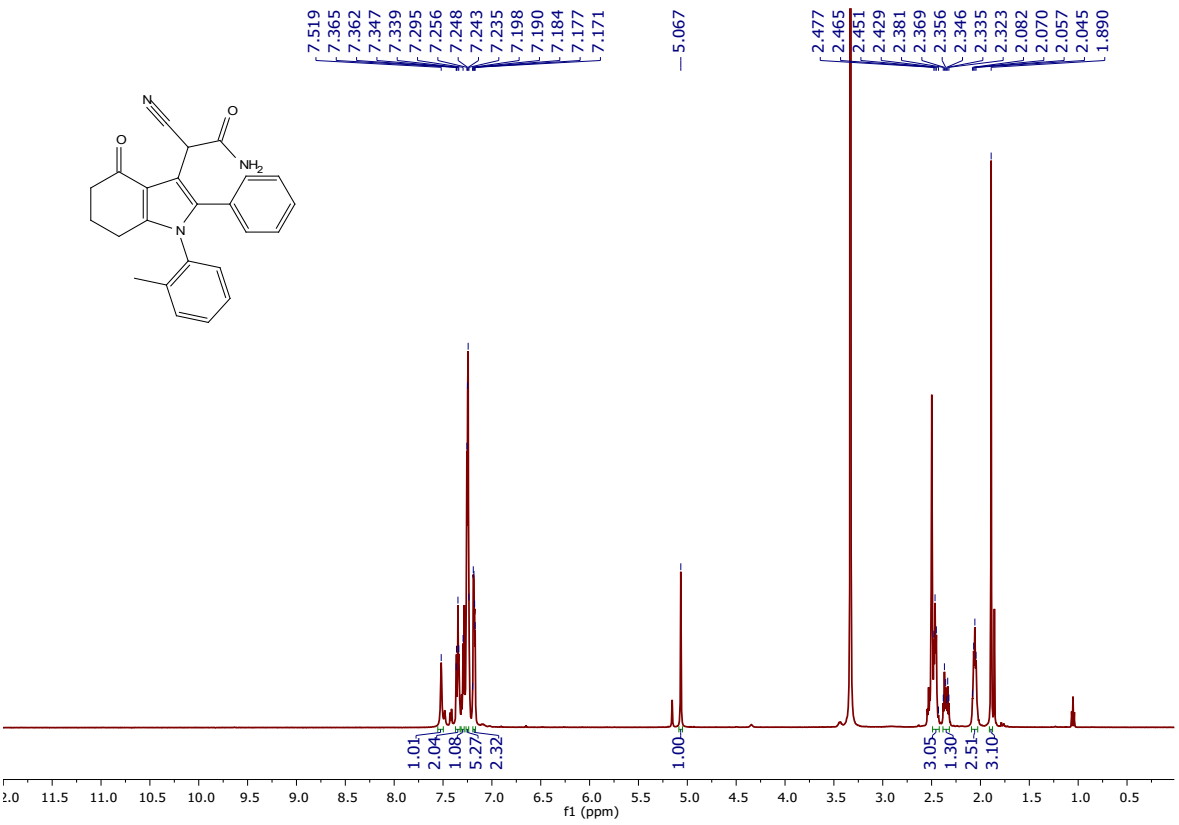


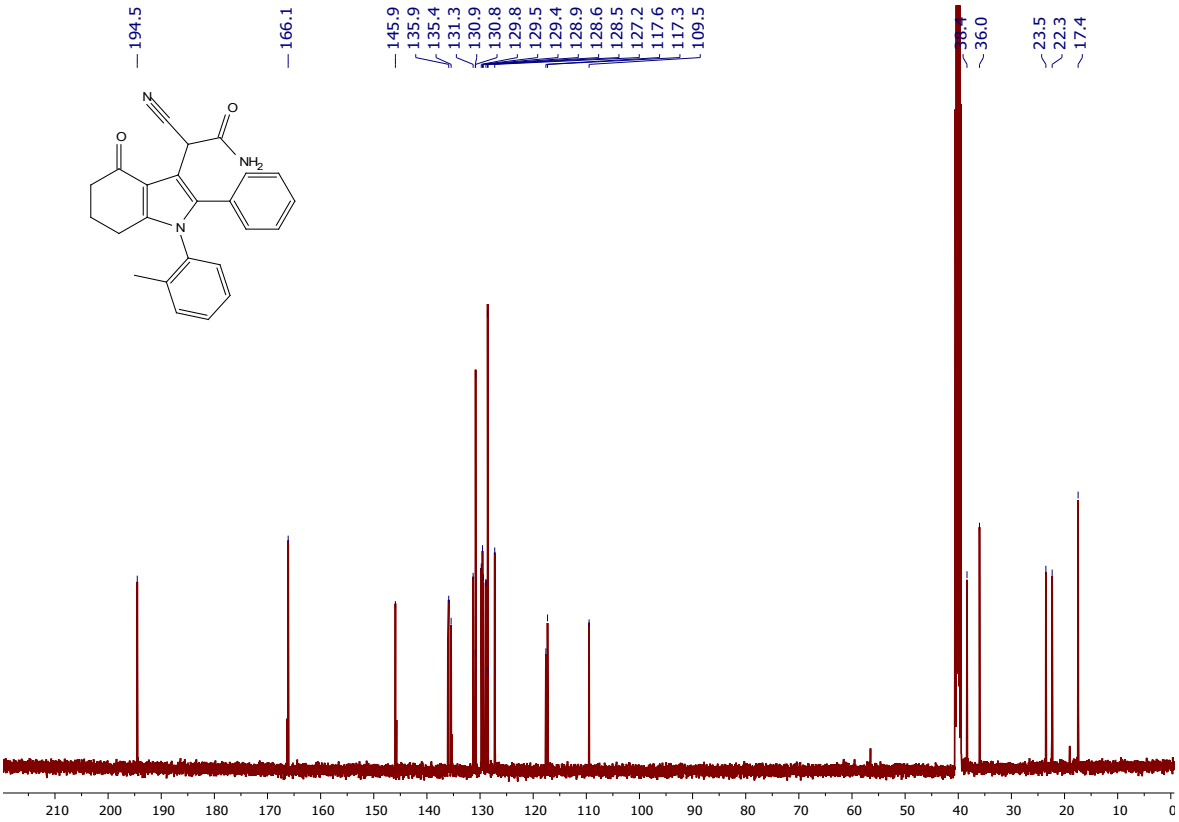
^{1}H, ^{13}C NMR spectrum of 2-Cyano-2-(4-oxo-1,2-diphenyl-4,5,6,7-tetrahydro-1*H*-indol-3-yl)acetamide (12a)



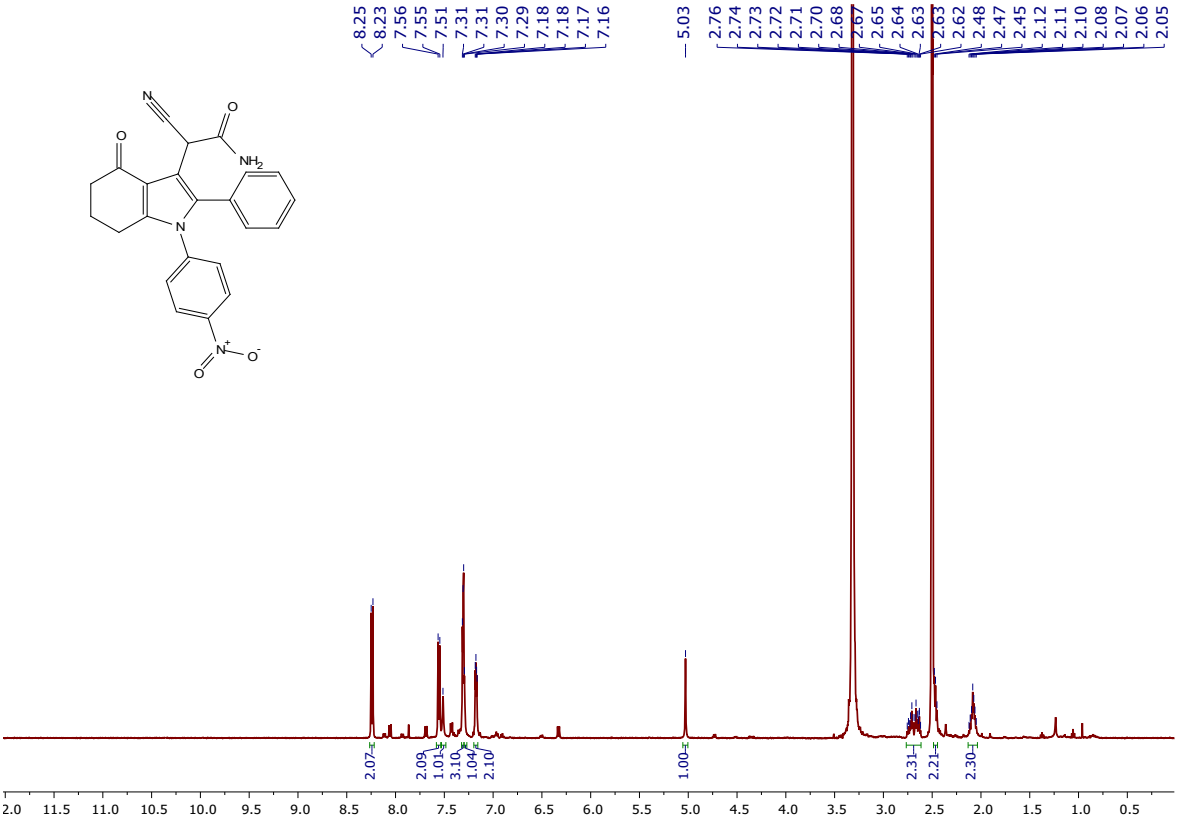


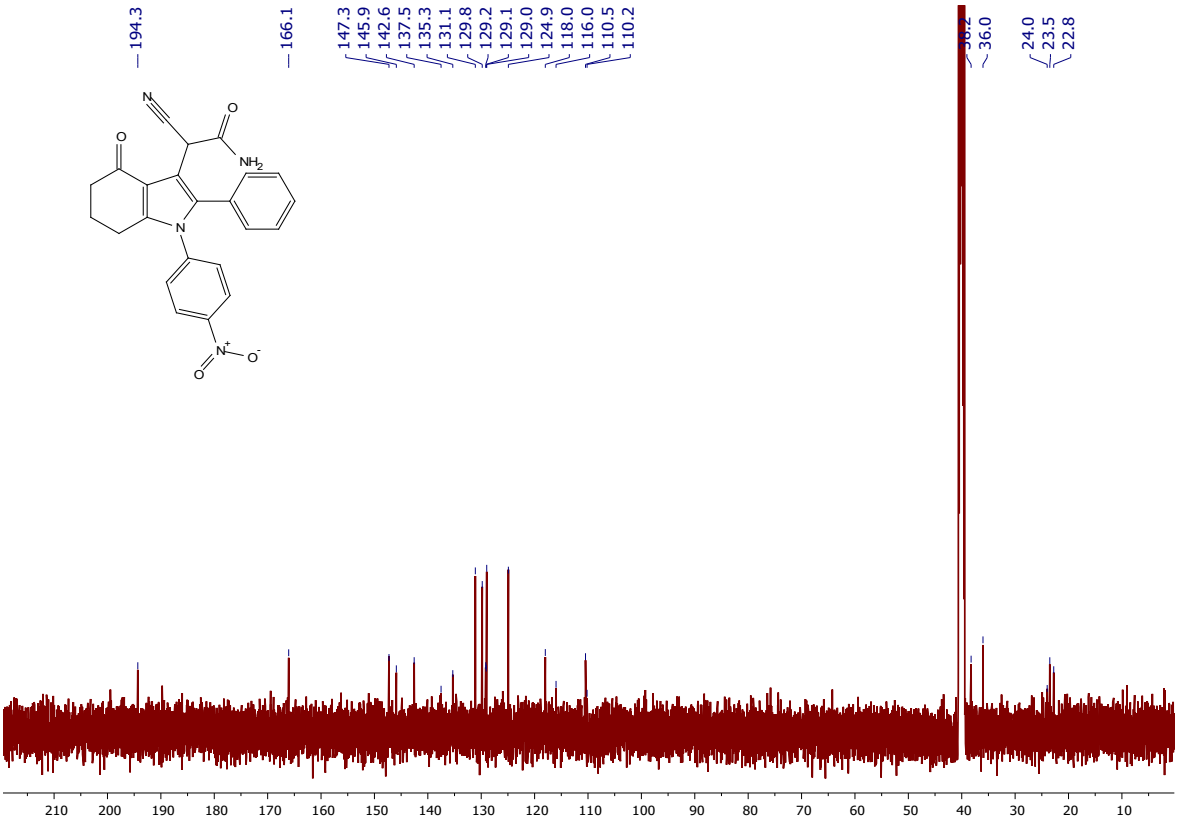
^{1}H, ^{13}C NMR spectrum of 2-Cyano-2-(4-oxo-2-phenyl-1-(*o*-tolyl)-4,5,6,7-tetrahydro-1*H*-indol-3-yl)acetamide (13a)





^{1}H, ^{13}C NMR spectrum of 2-Cyano-2-(1-(4-nitrophenyl)-4-oxo-2-phenyl-4,5,6,7-tetrahydro-1*H*-indol-3-yl)acetamide (14a).





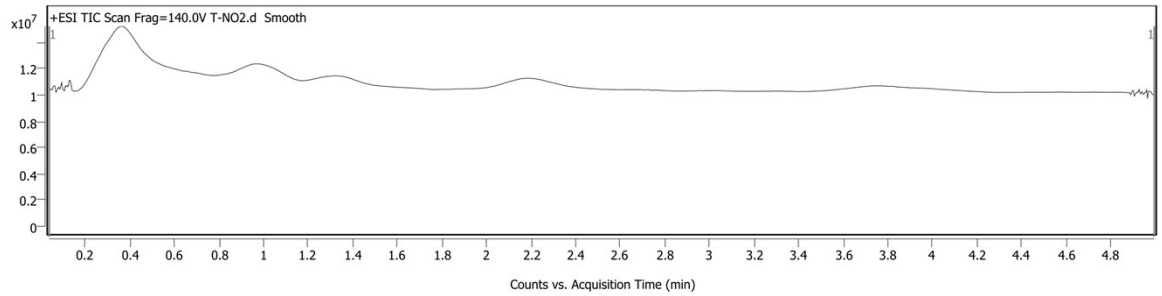
Analysis Report

Agilent | Trusted Answers

Sample Information

Name		**Data File Path**	D:\MassHunter\Data\DP\20230425\T-NO2.d
Sample ID		**Acq. Time (Local)**	25/04/23 7:15:35 PM (UTC+07:00)
Instrument	LCQTOF	**Method Path (Acq)**	D:\DP\DPTEST\DP-20230329.m
MS Type	QTOF	**Version (Acq SW)**	6200 series TOF/6500 series Q-TOF 10.1 (48.0)
Inj. Vol. (ul)	2	**IRM Status**	Success
Position	P1-B1	**Method Path (DA)**	
Plate Pos.		**Target Source Path**	
Operator		**Result Summary**	

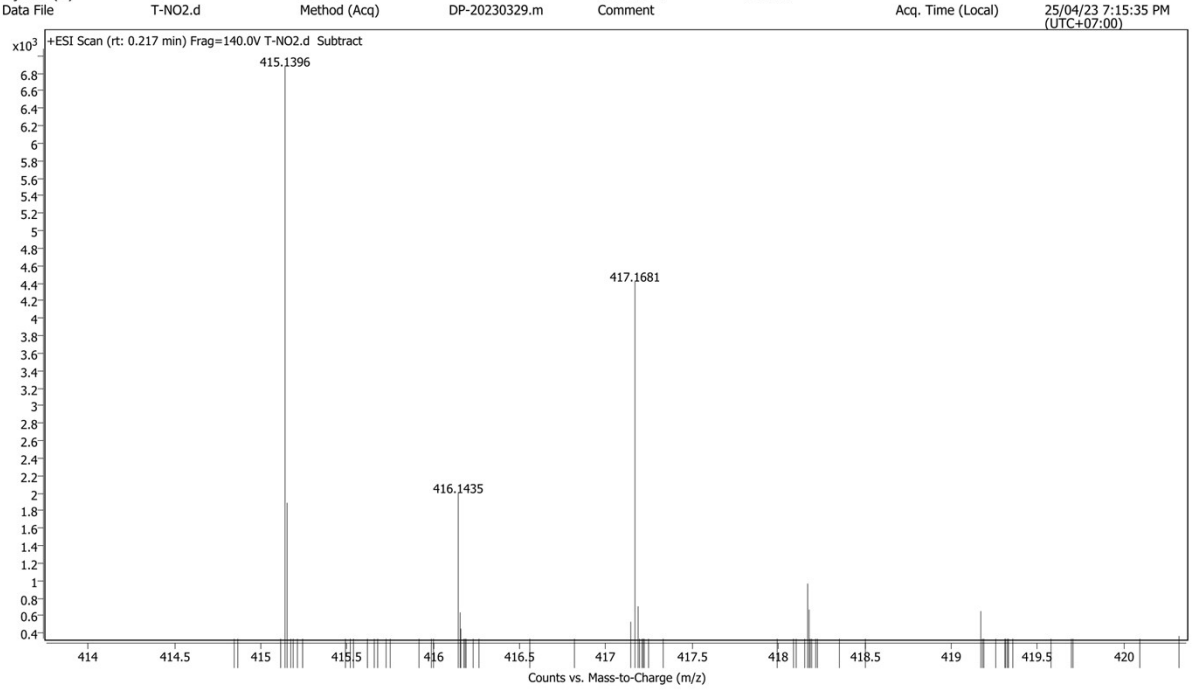
Sample Chromatograms



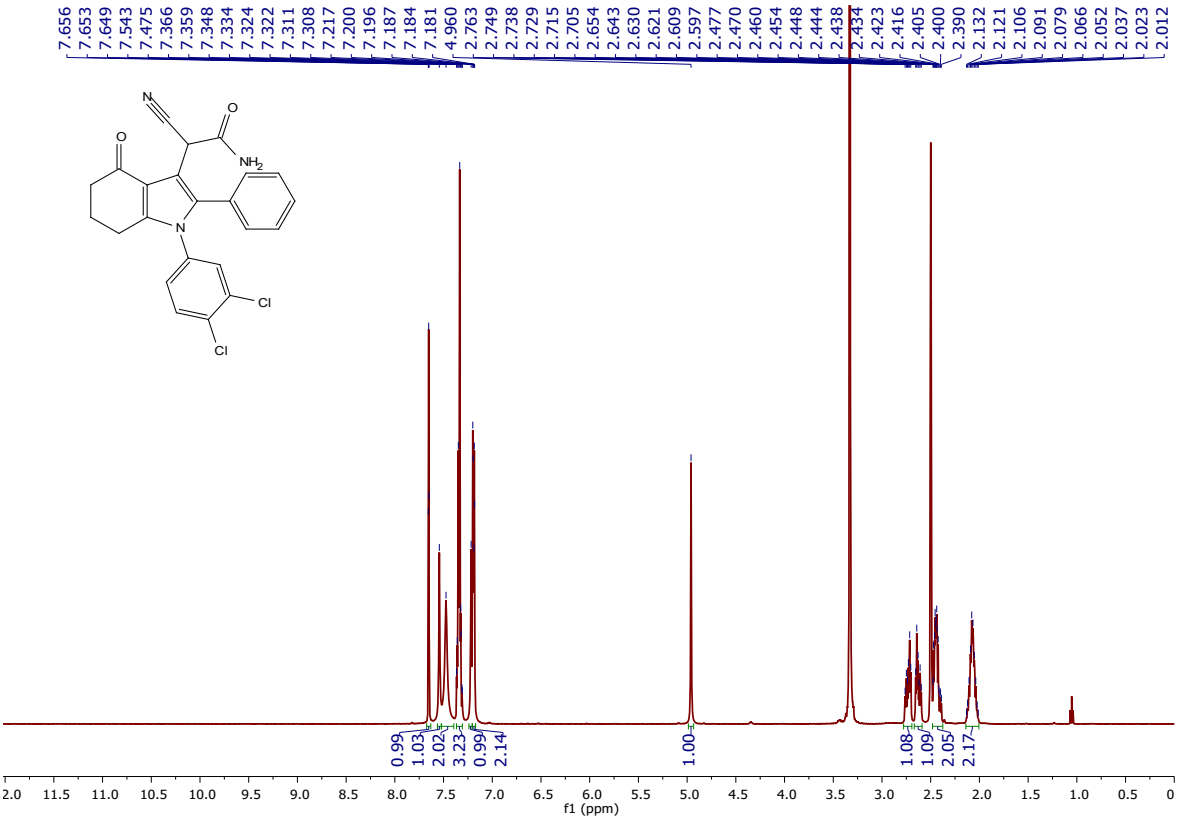
Spectrum Plot Report

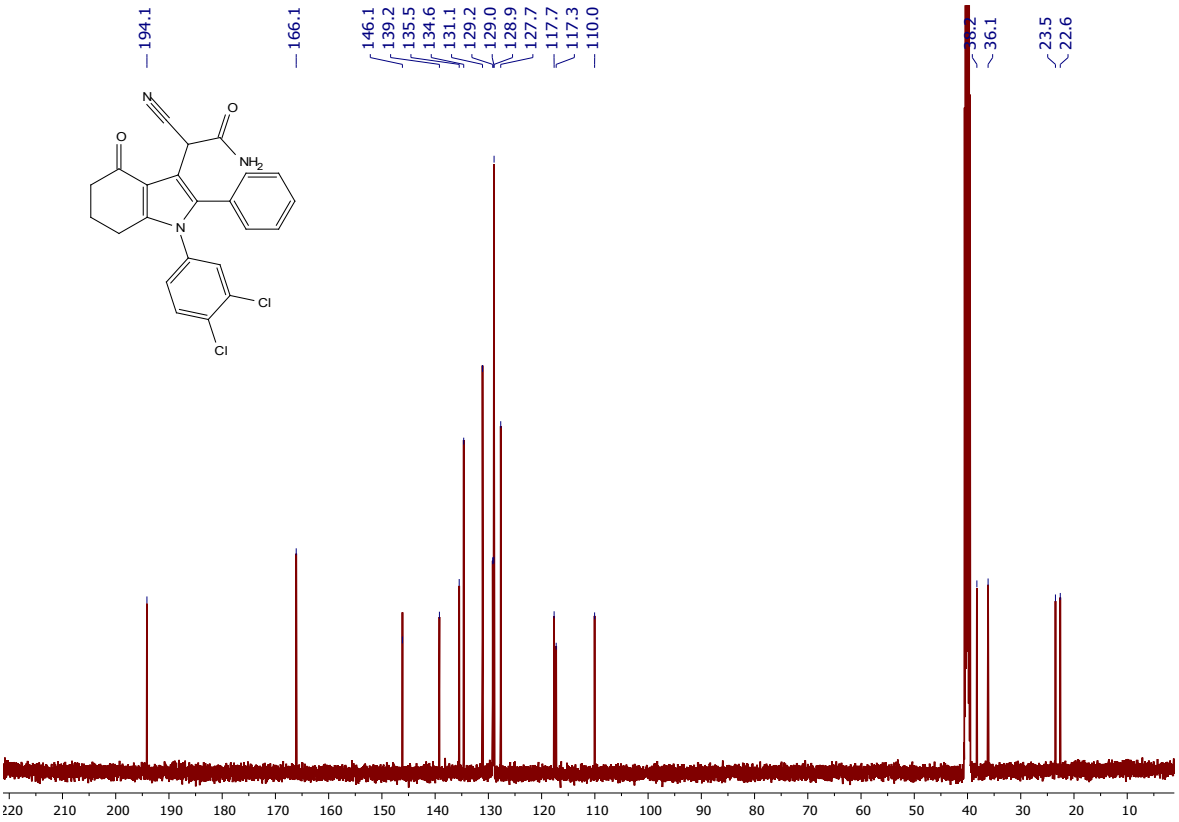
Agilent | Trusted Answers

Name		Rack Pos.		Instrument	LCQTOF	Operator	
Inj. Vol. (ul)	2	Plate Pos.		IRM Status	Success		
Data File	T-NO2.d	Method (Acq)	DP-20230329.m	Comment		Acq. Time (Local)	25/04/23 7:15:35 PM (UTC+07:00)



^{1}H, ^{13}C NMR spectrum of 2-Cyano-2-(1-(3,4-dichlorophenyl)-4-oxo-2-phenyl-4,5,6,7-tetrahydro-1*H*-indol-3-yl)acetamide (15a).





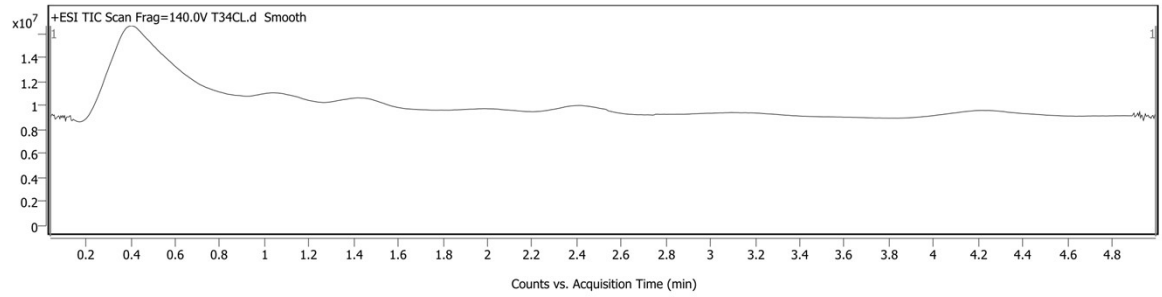
Analysis Report

Agilent | Trusted Answers

Sample Information

Name		**Data File Path**	D:\MassHunter\Data\DP\20230425\T34CL.d
Sample ID		**Acq. Time (Local)**	25/04/23 8:20:14 PM (UTC+07:00)
Instrument	LCQTOF	**Method Path (Acq)**	D:\DP\DPTEST\DP-20230329.m
MS Type	QTOF	**Version (Acq SW)**	6200 series TOF/6500 series Q-TOF 10.1 (48.0)
Inj. Vol. (ul)	2	**IRM Status**	All ions missed
Position	P1-C1	**Method Path (DA)**	
Plate Pos.		**Target Source Path**	
Operator		**Result Summary**	

Sample Chromatograms



Spectrum Plot Report

Agilent | Trusted Answers

Name		Rack Pos.		Instrument	LCQTOF	Operator	
Inj. Vol. (ul)	2	Plate Pos.		IRM Status	All ions missed		
Data File	T34CL.d	Method (Acq)	DP-20230329.m	Comment		Acq. Time (Local)	25/04/23 8:20:14 PM (UTC+07:00)