

Supporting Information

Metal-Free and Regioselective Synthesis of Substituted and Fused Chromenopyrrole Scaffolds *via* the Divergent Reactivity of α -Azido Ketones in Water

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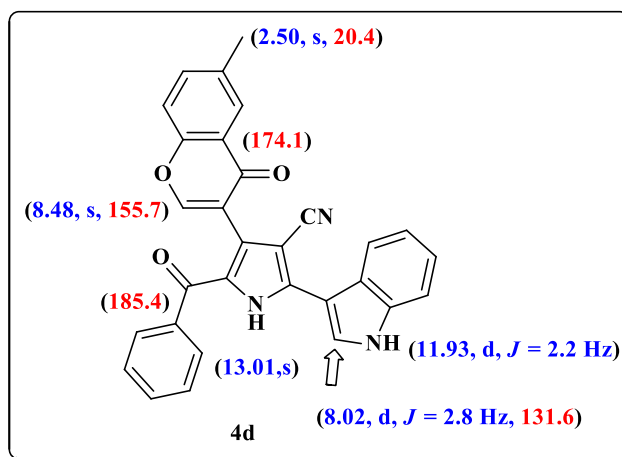
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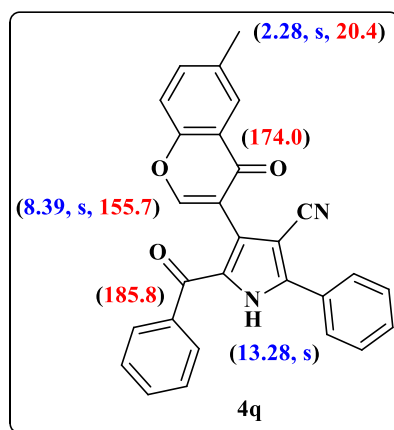
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I. A brief discussion of the spectral characterization of compounds 4d, 4q, 8a, 10a, 12b, 15a, 17b and 18a

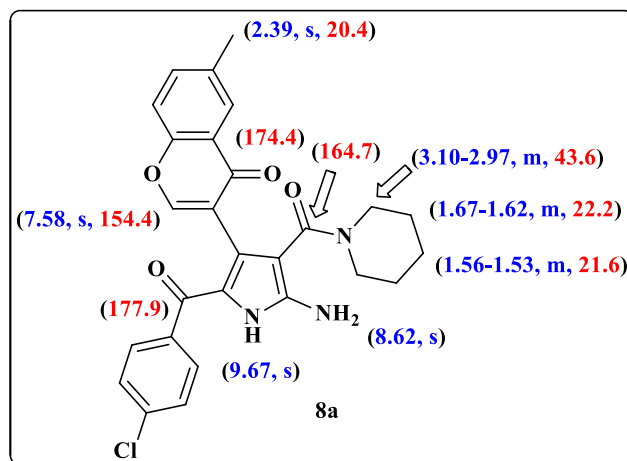


In the ^1H NMR spectra of a compound **4d**, a peak that appears at 13.01 ppm for one proton belongs to the pyrrole $-\text{NH}$, a doublet that appears at 11.93 ppm with the coupling constant of 2.2 Hz for one proton belongs to the indole $-\text{NH}$, a singlet appears at 8.48 ppm for one proton belongs to the $-\text{CH}$ of chromone ring, a doublet appears at 8.02 ppm with the coupling constant of 2.8 Hz for one proton belongs to $-\text{CH}$ of indole ring and a peak appears as a singlet at 2.50 ppm for three protons belongs to the $-\text{CH}_3$ of chromone ring. Similarly in ^{13}C NMR spectra of a compound **4d**, a peak appears at 185.4 ppm belongs to the carbonyl carbon of benzoyl group, a peak appears at 174.1 ppm belongs to the carbonyl carbon of chromone ring, a peak appears at 155.7 ppm belongs to the $-\text{CH}$ carbon of chromone ring and a peak that appears at 20.4 ppm belongs to the $-\text{CH}_3$ of chromone ring. Further, the structure of **4d** was confirmed by high resolution mass (HRMS-ESI) spectra of the molecular ion peak $[\text{M} + \text{H}]^+$ appears at 470.1533 indicate that the confirmation of product formation.

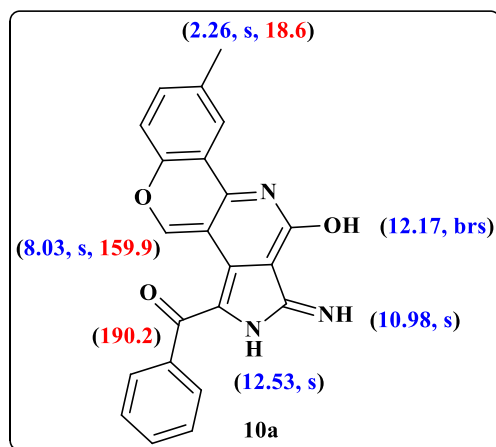


In the ^1H NMR spectra of a compound **4q**, a peak that appears at 13.28 ppm for one proton belongs to the pyrrole $-\text{NH}$, a singlet appears at 8.39 ppm for one proton belongs to the $-\text{CH}$ of chromone ring and a peak appears as a singlet at 2.28 ppm for three protons that belongs

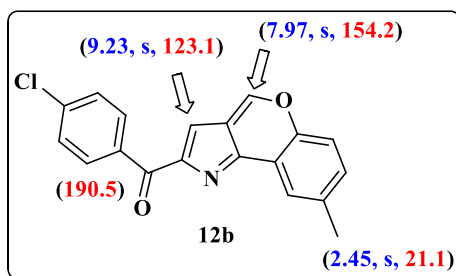
to the $-\text{CH}_3$ of chromone ring. Similarly in ^{13}C NMR spectra of a compound **4q**, a peak appears at 185.8 ppm belongs to the carbonyl carbon of benzoyl group, a peak appears at 174.0 ppm belongs to the carbonyl carbon of chromone ring, a peak appears at 155.7 ppm belongs to the $-\text{CH}$ carbon of chromone ring and a peak that appears at 20.4 ppm belongs to the $-\text{CH}_3$ of chromone ring. Further, the structure of **4q** was confirmed by high resolution mass (HRMS-ESI) spectra of the molecular ion peak $[\text{M} + \text{H}]^+$ appears at 431.1396 indicate that the confirmation of product formation.



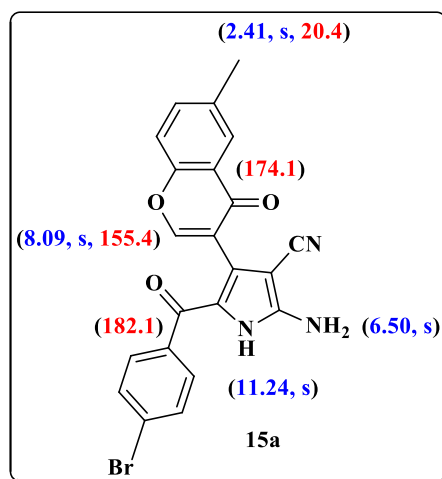
In the ^1H NMR spectra of a compound **8a**, a singlet appears at 9.67 ppm for one proton belongs to the pyrrole $-\text{NH}$, a broad singlet appears at 8.62 ppm for two protons belongs to the $-\text{NH}_2$ of pyrrole, a singlet appears at 7.58 ppm for one proton belongs to the $-\text{CH}$ of chromone ring, a multiplet appears at 3.10 – 2.97 ppm for four protons belong to $-\text{CH}_2$ of piperidine ring (Adjacent to ring nitrogen), a singlet appears at 2.39 ppm belongs to the $-\text{CH}_3$ protons from chromone ring, a multiplet appears at 1.67 – 1.62 ppm for four protons belong to $-\text{CH}_2$ protons of piperidine ring and a multiplet appears at 1.56 - 1.53 ppm for two protons belong to $-\text{CH}_2$ protons of the piperidine ring. Similarly in ^{13}C NMR spectra of a compound **8a**, a peak appears at 177.9 ppm belongs to the carbonyl carbon of benzoyl group, a peak appears at 174.4 ppm belongs to the carbonyl carbon of chromone ring, a peak appears at 164.7 ppm belongs to the carbonyl group attached with piperidine ring, a peak appears at 154.4 ppm belongs to the $-\text{CH}$ of chromone ring, a peak appears at 43.6 belong to two aliphatic $-\text{CH}_2$ of piperidine ring (Adjacent to ring nitrogen), a peak appears at 22.2 ppm belong to two aliphatic $-\text{CH}_2$ of piperidine ring, a peak appears at 21.6 ppm belong to one aliphatic $-\text{CH}_2$ of piperidine ring and a peak appears at 20.4 ppm belongs to the $-\text{CH}_3$ of chromone ring. Further, the structure of **8a** was confirmed by high resolution mass (HRMS-ESI) spectra of the molecular ion peak $[\text{M} + \text{H}]^+$ appears at 490.1516 indicate that the confirmation of product formation.



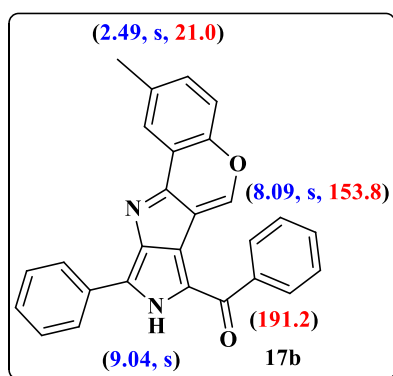
In the ^1H NMR spectra of a compound **10a**, a singlet appears at 12.53 ppm for one proton belongs to the pyrrole $-\text{NH}$, a broad singlet appears at 12.17 ppm for one proton belongs to the $-\text{OH}$ of the pyridine ring, a singlet appears at 10.98 ppm for one proton belongs to the imine $-\text{NH}$ of pyrrole ring and a peak appears at 2.26 ppm for three protons belongs to the $-\text{CH}_3$ of chromone ring. Similarly in ^{13}C NMR spectra of a compound **10a**, a peak appears at 190.2 ppm belongs to the carbonyl carbon of benzoyl group. A peak appears at 159.9 ppm belongs to the $-\text{CH}$ of chromone ring and a peak appears at 18.6 ppm belongs to the $-\text{CH}_3$ of chromone ring.



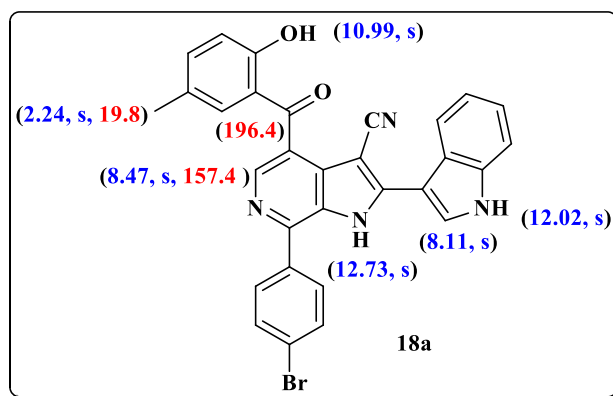
In the ^1H NMR spectra of a compound **12b**, a singlet appears at 9.23 ppm for one proton belongs to the $-\text{CH}$ of pyrrole ring, a singlet appears at 7.97 ppm for one proton belongs to the $-\text{CH}$ of chromone ring and a peak appears at 2.45 ppm for three protons belongs to the $-\text{CH}_3$ of chromone ring. Similarly in ^{13}C NMR spectra of a compound **12b**, a peak appears at 190.5 ppm belongs to the carbonyl carbon of benzoyl group, a peak appears at 154.2 ppm belongs to the $-\text{CH}$ of chromone ring, a peak appears at 123.1 ppm belongs to the $-\text{CH}$ of pyrrole ring and a peak appears at the 21.1 ppm belongs to the $-\text{CH}_3$ of chromone ring. Further, the structure of **12b** was confirmed by high resolution mass (HRMS-ESI) spectra of the molecular ion peak $[\text{M} - \text{H} + \text{H}_2\text{O}]^+$ appears at 338.0599 indicate that the confirmation of product formation.



In the ^1H NMR spectra of a compound **15a**, a singlet appears at 11.24 ppm for one proton belongs to the pyrrole –NH, a singlet appears at 8.09 ppm for one proton belongs to the –CH of chromone ring. A peak appears at 6.50 ppm for two protons belongs to the –NH₂ of pyrrole ring and a peak appears at 2.41 ppm for three protons belongs to the –CH₃ of chromone ring. Similarly in ^{13}C NMR spectra of a compound **15a**, a peak appears at 182.1 ppm belongs to the carbonyl carbon of benzoyl group, a peak appears at 174.1 ppm belongs to the carbonyl group of chromone ring, a singlet appears at 155.4 ppm belongs to the –CH of chromone ring and a peak appears at the 20.4 ppm belongs to the –CH₃ of chromone ring.

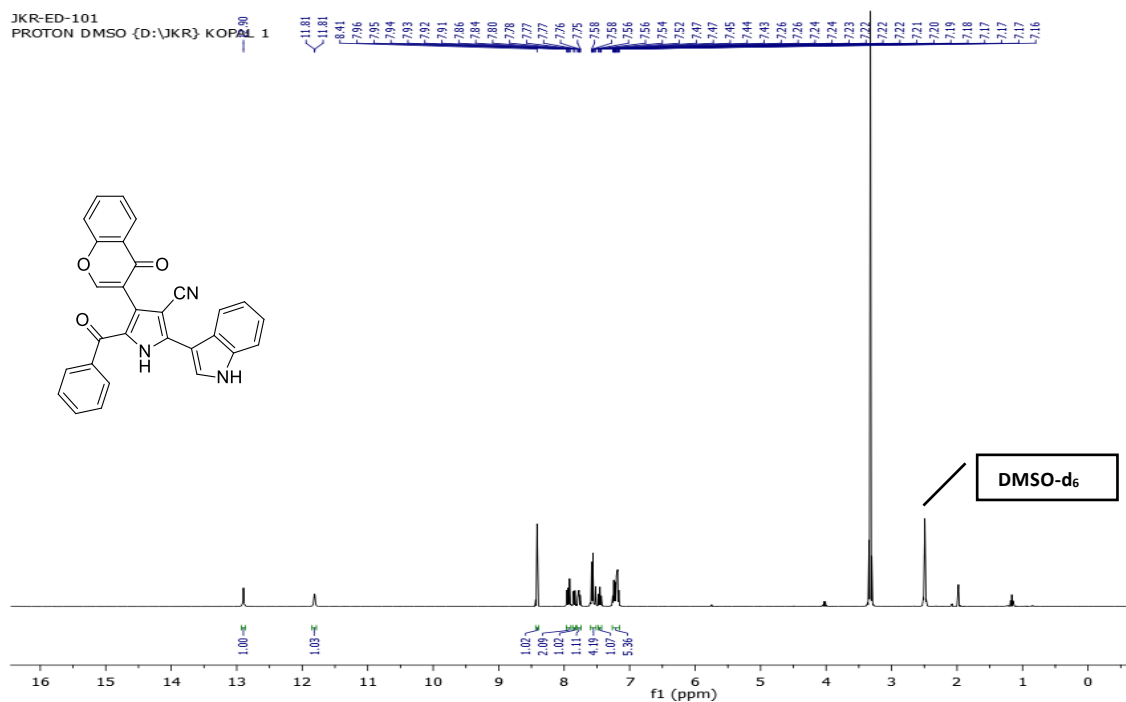


In the ^1H NMR spectra of a compound **17b**, a singlet appears at 9.04 ppm for one proton belongs to the pyrrole ring –NH, a singlet appears at 8.09 ppm for one proton belongs to the –CH of chromone ring and a singlet appears at 2.49 ppm for three protons belongs to the –CH₃ of chromone ring. Similarly in ^{13}C NMR spectra of a compound **15a**, a peak appears at 191.2 ppm belongs to the carbonyl carbon of benzoyl group, a peak appears at 153.8 ppm belongs to the –CH of chromone ring and a peak appears at the 21.0 ppm belongs to the –CH₃ of chromone ring. In addition, the DEPT 135 spectrum also confirms that the presence of ten aromatic –CH and one aliphatic –CH₃ in the positive phase. Further, the structure of **12b** was confirmed by high resolution mass (HRMS-ESI) spectra of the molecular ion peak $[\text{M}+\text{H}_2\text{O}]^+$ appears at 420.1224 indicate that the confirmation of product formation.

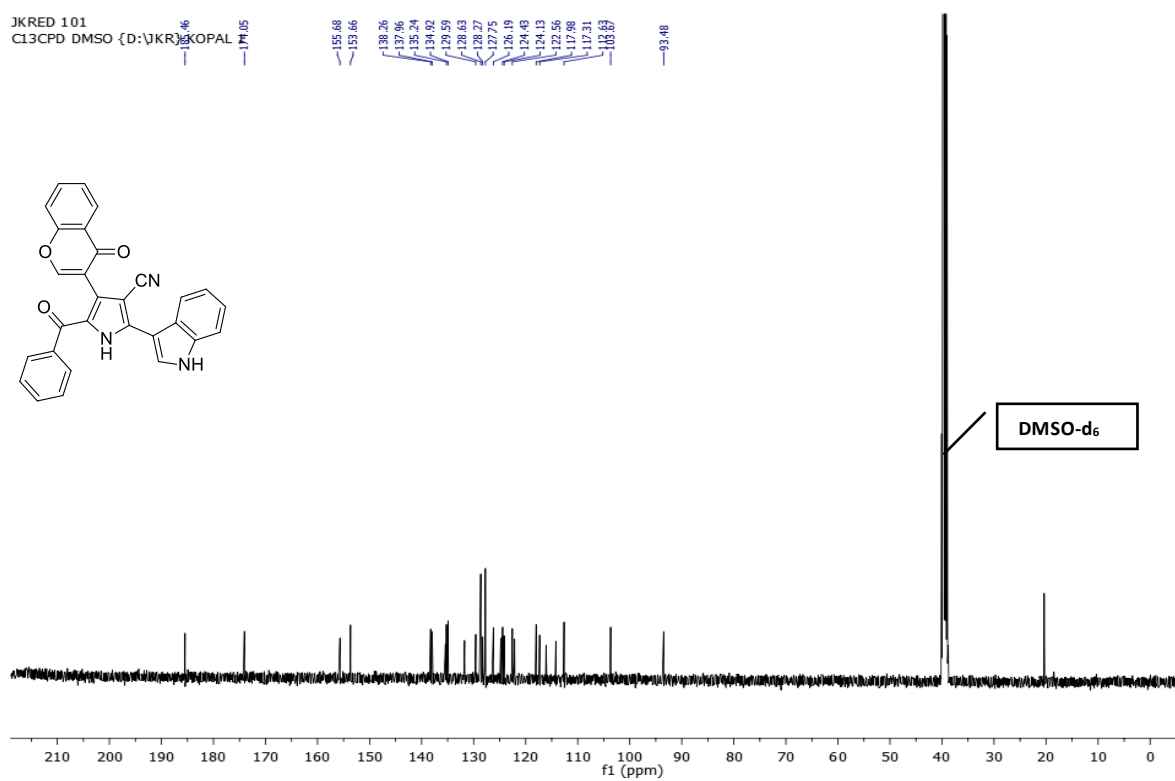


In the ^1H NMR spectra of a compound **18a**, a singlet appears at 12.73 ppm for one proton belongs to the $-\text{NH}$ of the pyrrole ring, a singlet appears at 12.02 ppm for one proton belongs to the $-\text{NH}$ of the indole ring. A peak appears 10.99 ppm for one proton belongs to the $-\text{OH}$ of the benzene ring, a singlet appears at 8.47 ppm for one proton belongs to the $-\text{CH}$ of the pyridine ring, a peak appears at 8.11 ppm as a singlet for one proton belongs to the $-\text{CH}$ of the indole ring, a singlet appears at 2.24 ppm for three protons belongs to the $-\text{CH}_3$ of the benzene ring. Similarly in ^{13}C NMR spectra of a compound **18a**, a peak appears at 196.4 ppm belongs to the carbonyl carbon of the benzoyl group, a peak appears at 157.4 ppm belongs to the $-\text{CH}$ carbon of the pyridine ring and a peak appears at the 19.8 ppm belongs to the $-\text{CH}_3$ of the benzene ring. In addition, the DEPT 135 spectrum also confirms that the presence of eleven aromatic $-\text{CH}$ and one aliphatic $-\text{CH}_3$ in the positive phase. Further, the structure of **18a** was confirmed by high resolution mass (HRMS-ESI) spectra of the molecular ion peak $[\text{M}+\text{H}]^+$ appears at 547.0778 indicate that the confirmation of product formation.

I. ^1H NMR, $^{13}\text{C}\{^1\text{H}\}$ NMR and HRMS (ESI) spectrum

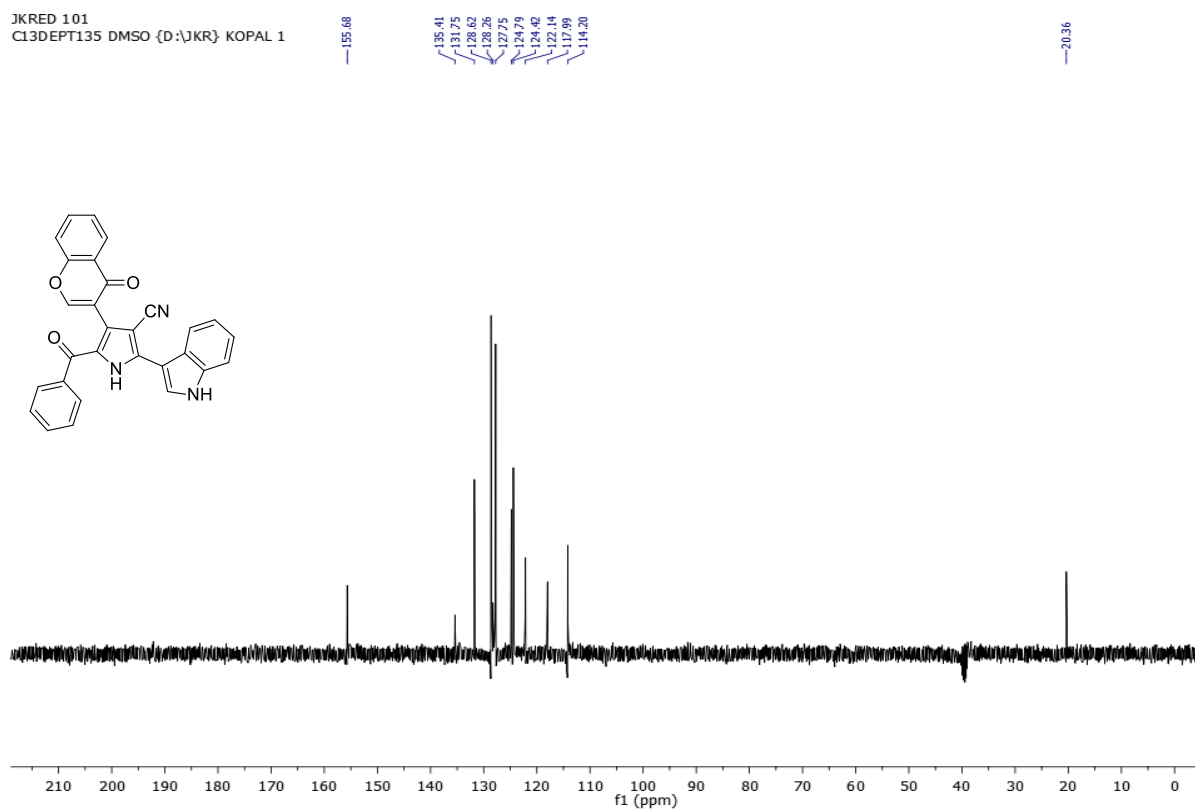


^1H NMR spectrum of **4a** (400 MHz, DMSO- d_6)



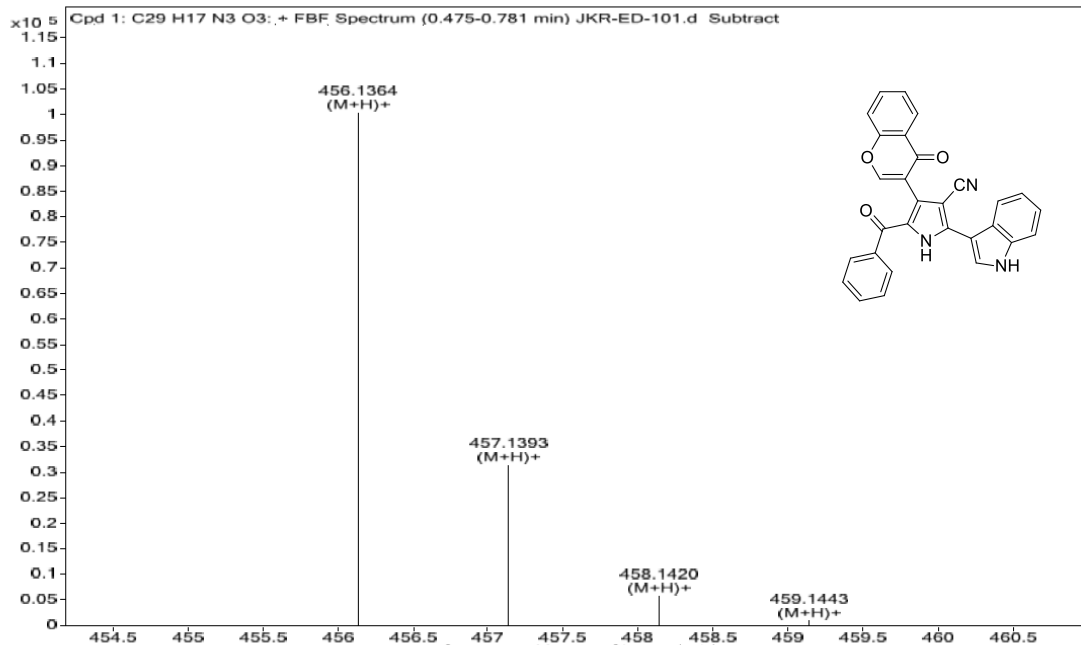
$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **4a** (100 MHz, DMSO- d_6)

JKRED 101
 CL3DEPT135 DMSO {D:\JKR} KOPAL 1

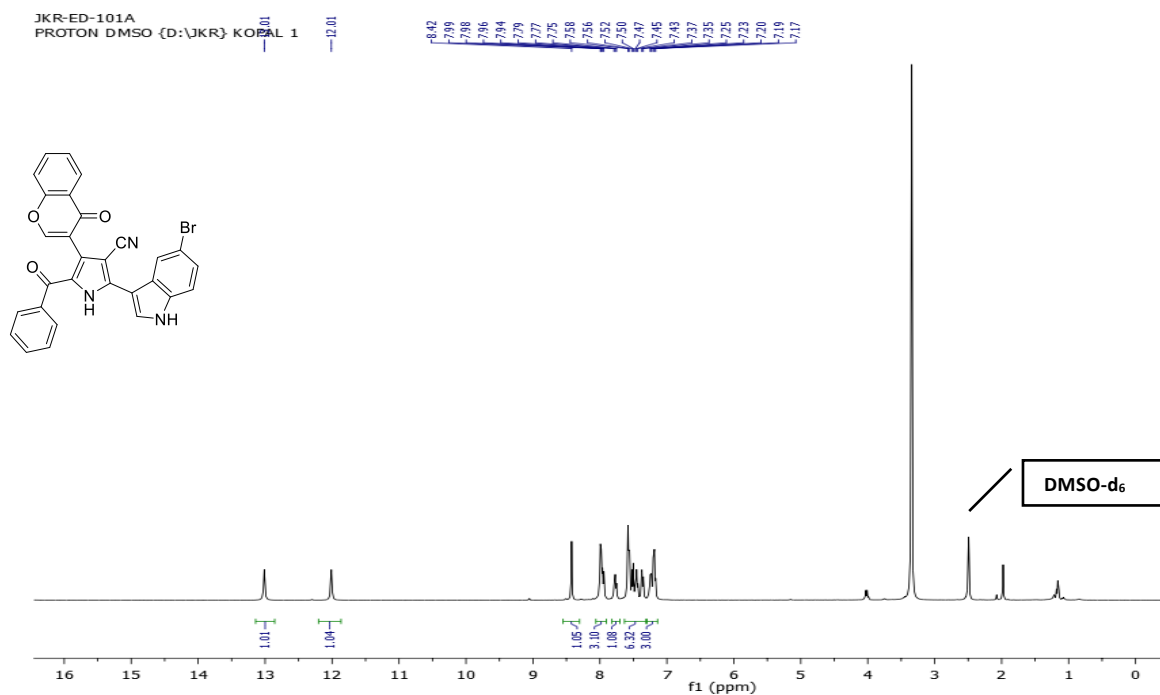


DEPT 135 NMR spectrum of **4a** (100 MHz, DMSO-*d*₆)

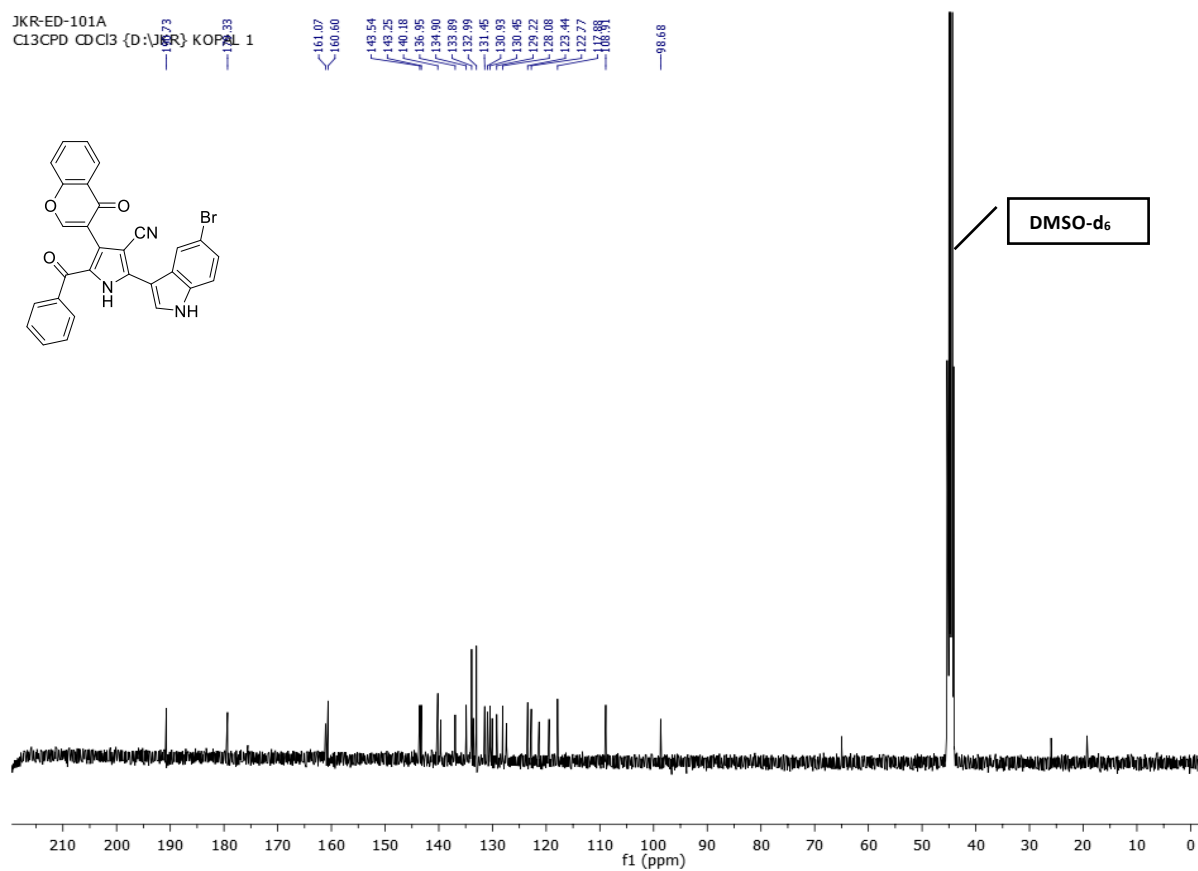
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HRMS (ESI) spectrum of **4a**

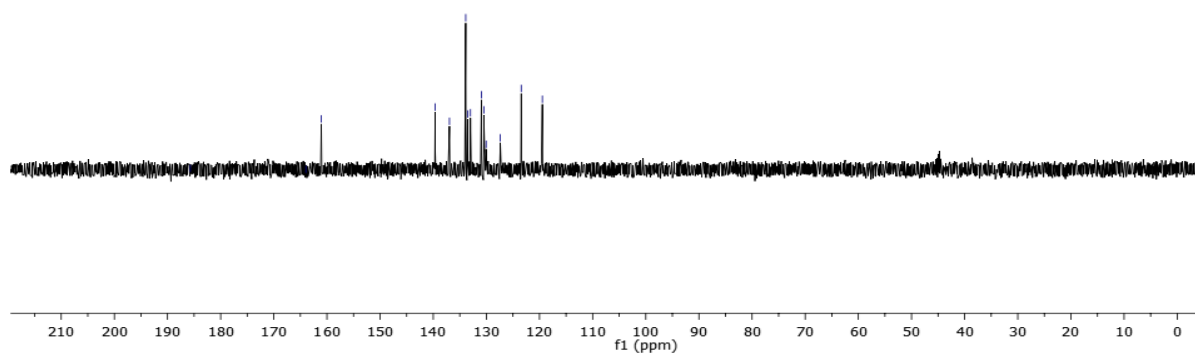
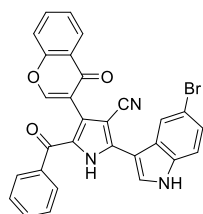


¹H NMR spectrum of **4b** (400 MHz, DMSO-*d*₆)



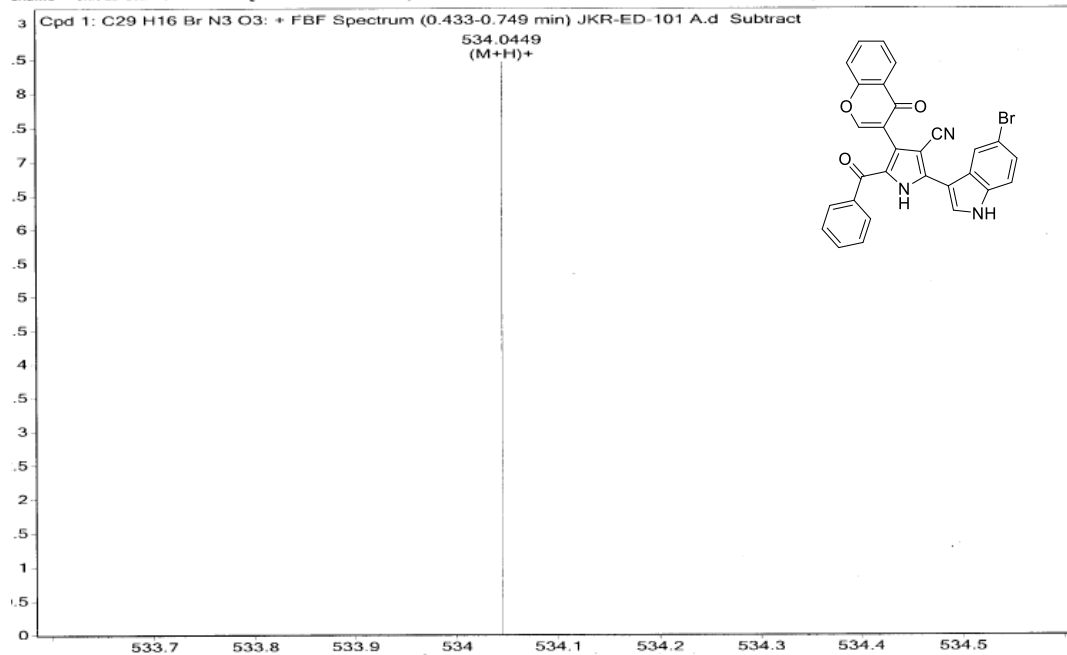
¹³C{¹H} NMR spectrum of **4b** (100 MHz, DMSO-*d*₆)

JKR-ED-101A
 Cl3DEPT135 CDCl3 {D:JKR} KOPAL 1



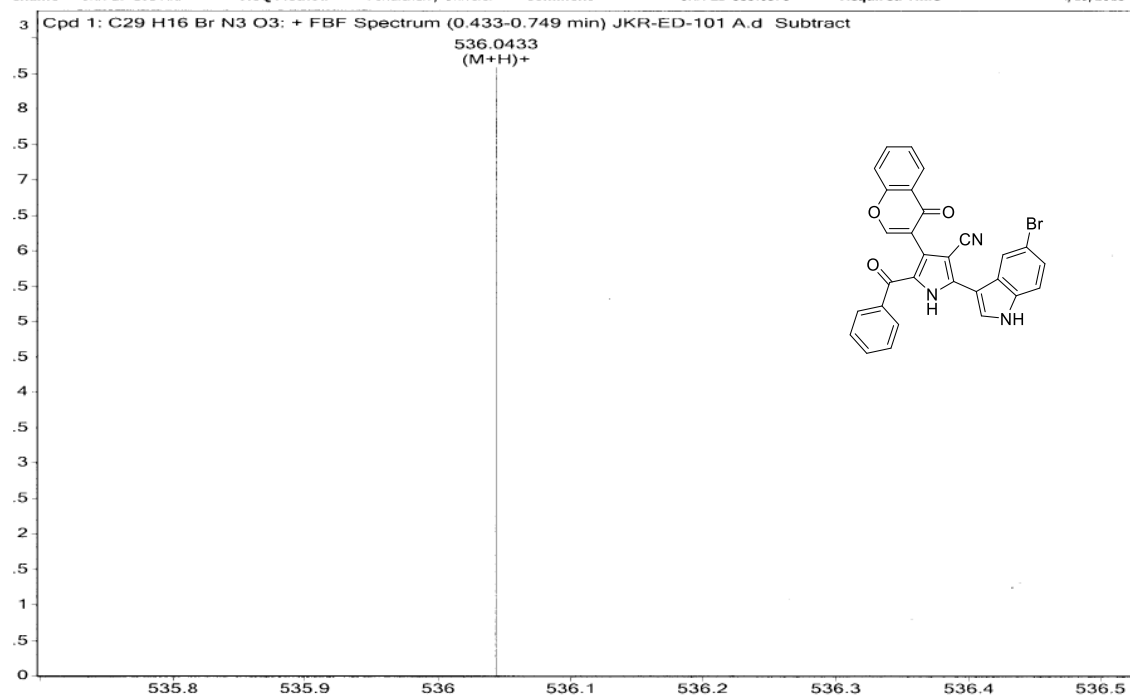
DEPT 135 NMR spectrum of **4b** (100 MHz, DMSO- d_6)

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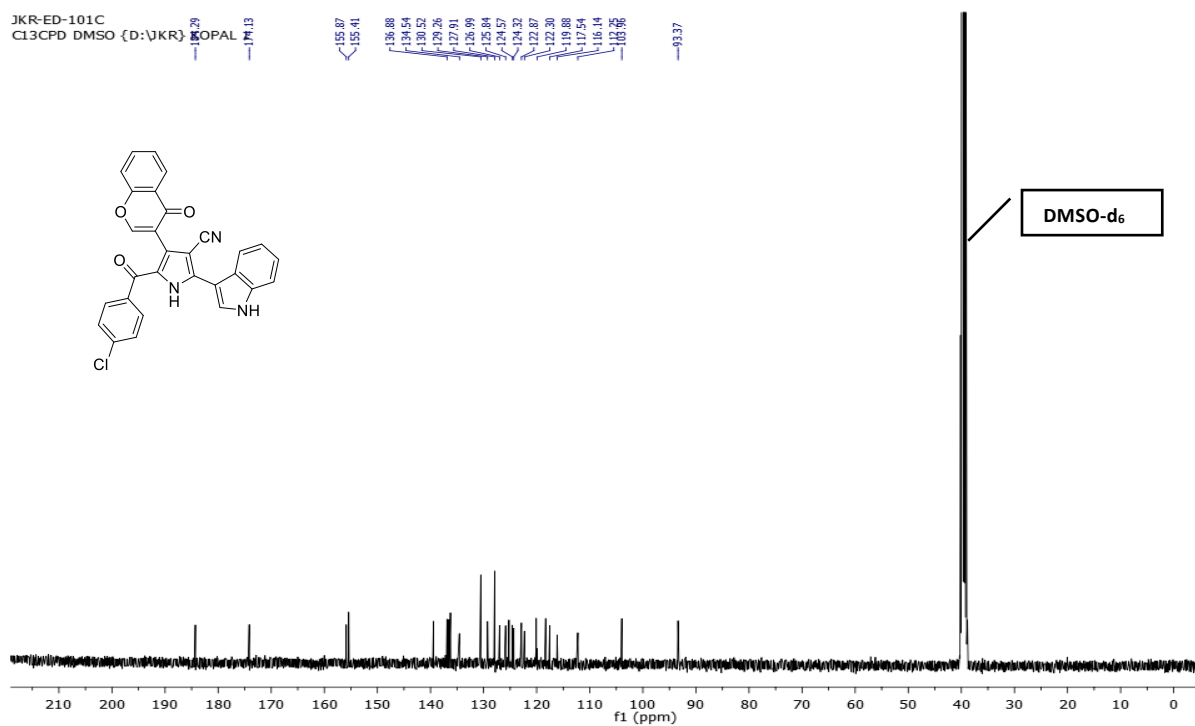
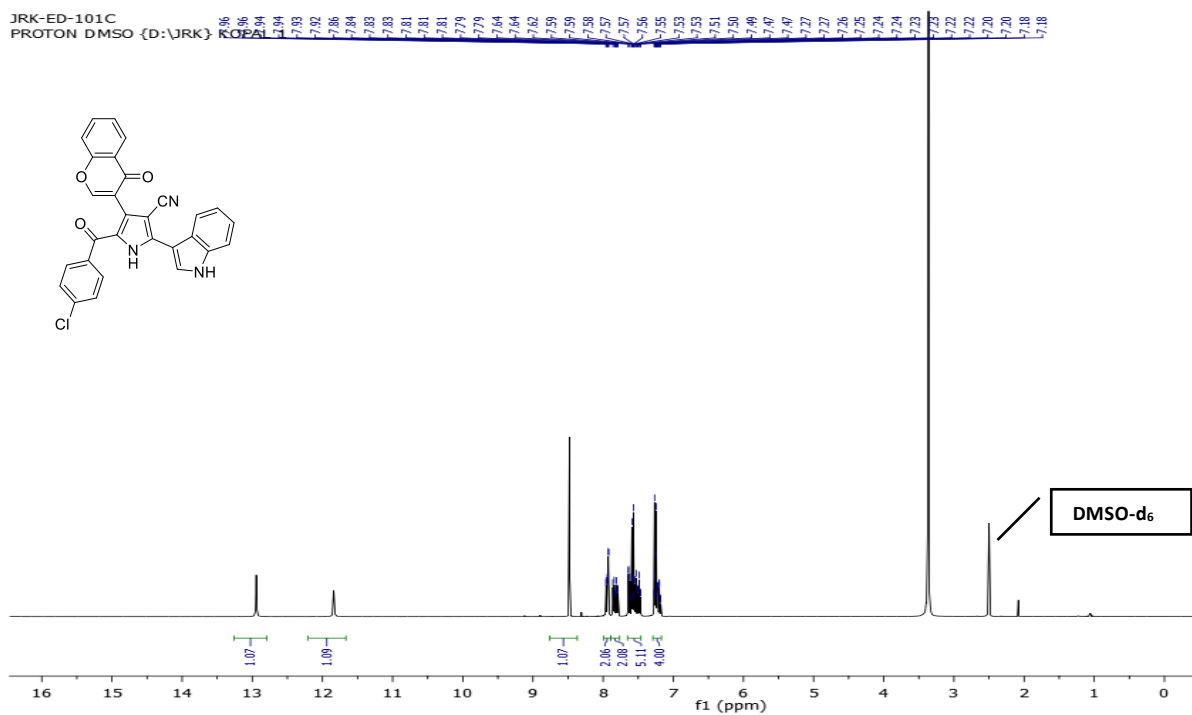


HRMS (ESI) spectrum of **4b** (^{79}Br isotope)

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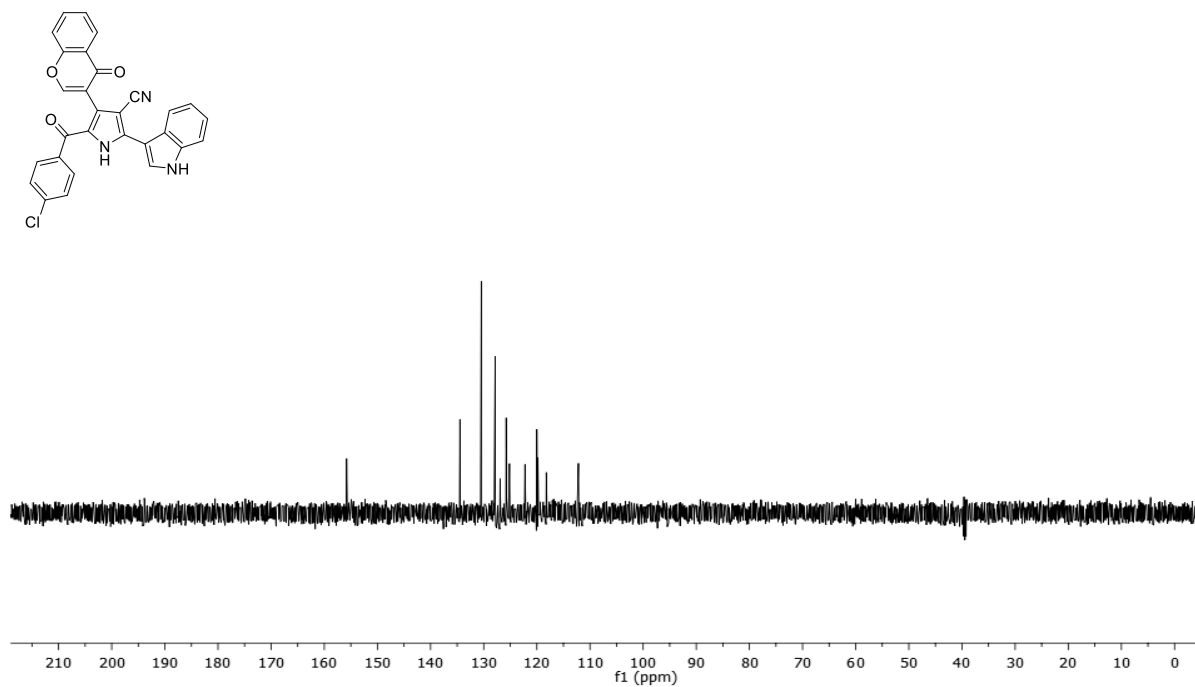


HRMS (ESI) spectrum of **4b** (⁸¹Br isotope)

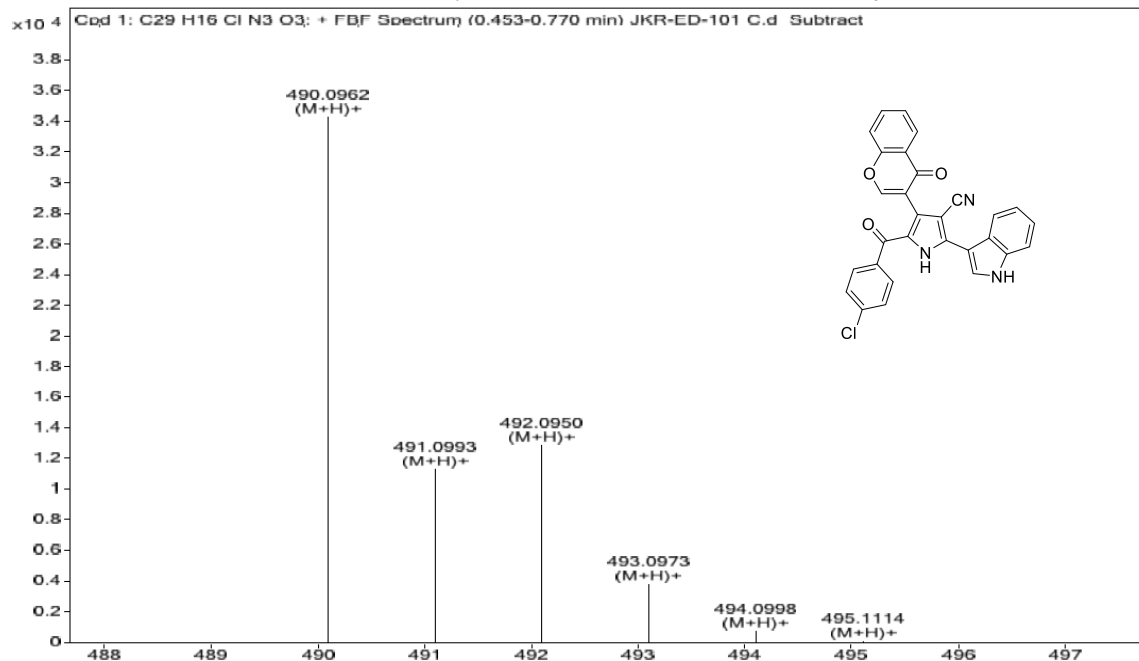


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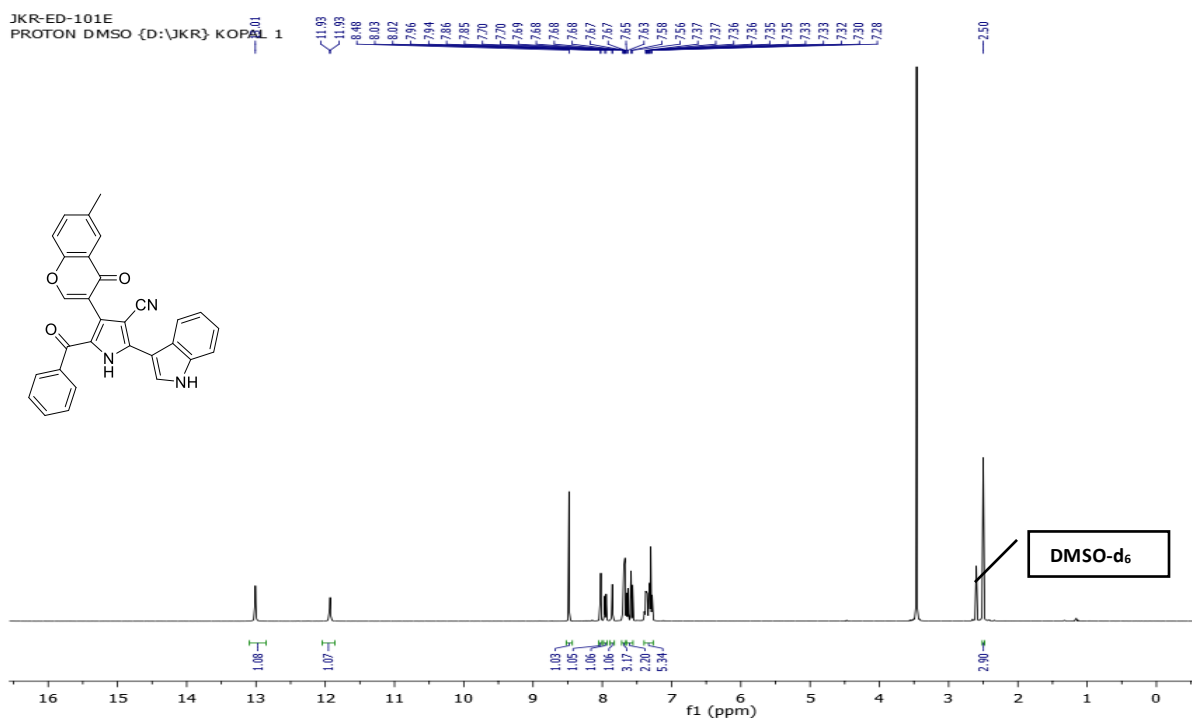
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 112.18



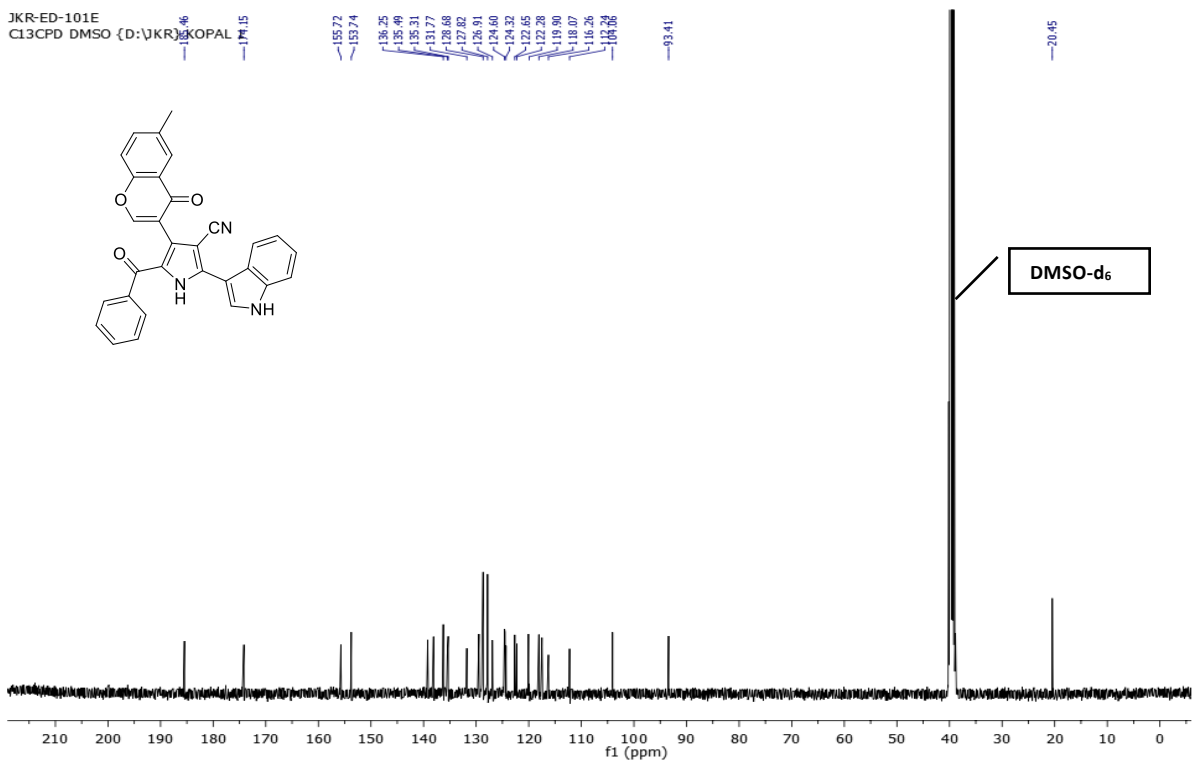
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HRMS (ESI) spectrum of **4c**



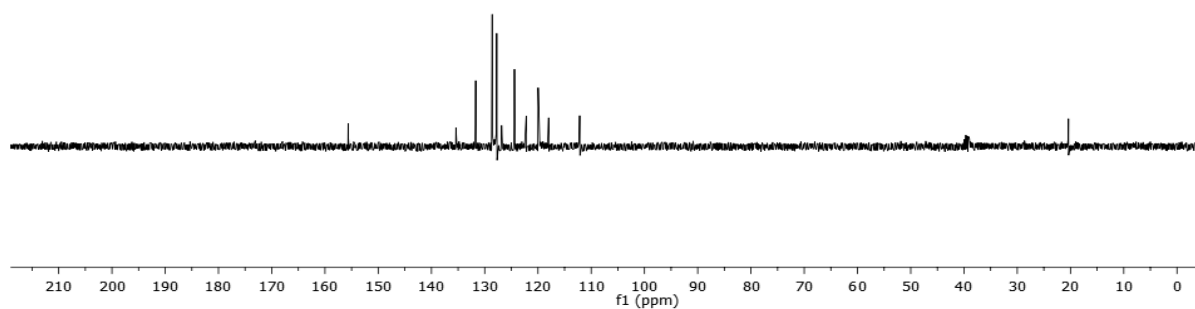
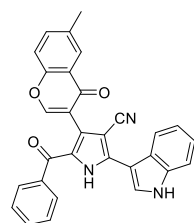
^1H NMR spectrum of **4d** (400 MHz, DMSO- d_6)



$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **4d** (100 MHz, DMSO- d_6)

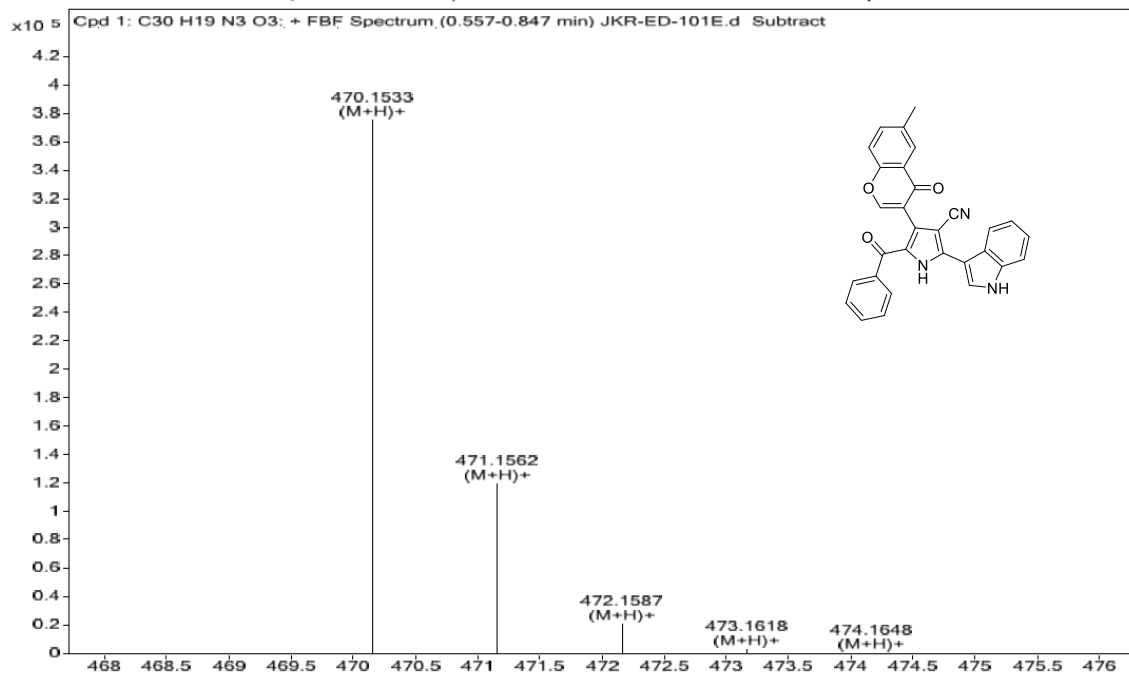
JKR-ED-101E
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20.38

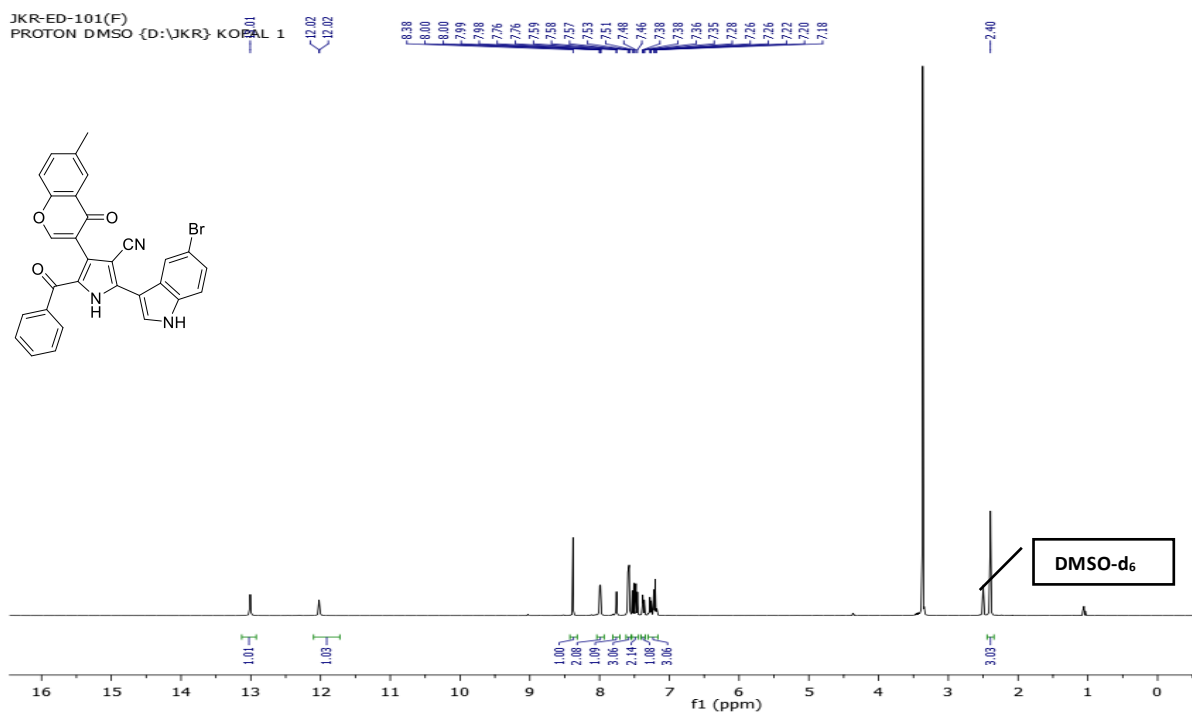


DEPT 135 NMR spectrum of **4d** (100 MHz, DMSO-*d*₆)

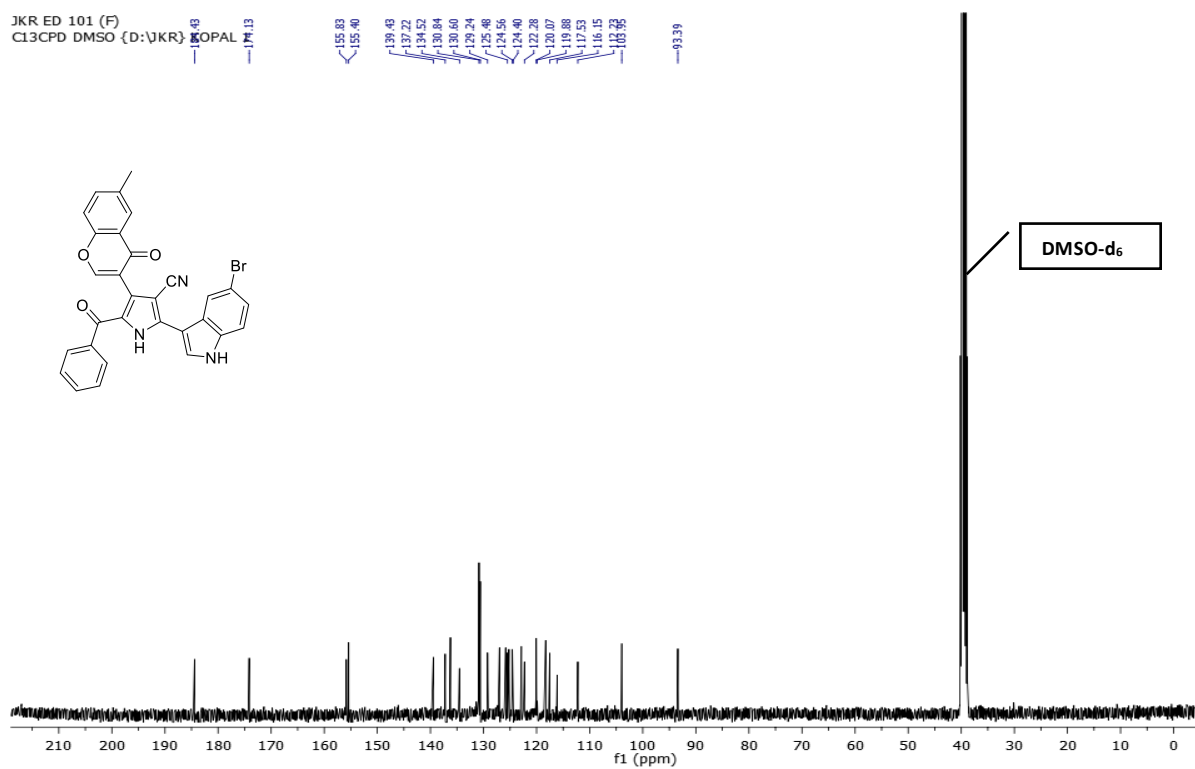
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HRMS (ESI) spectrum of **4d**

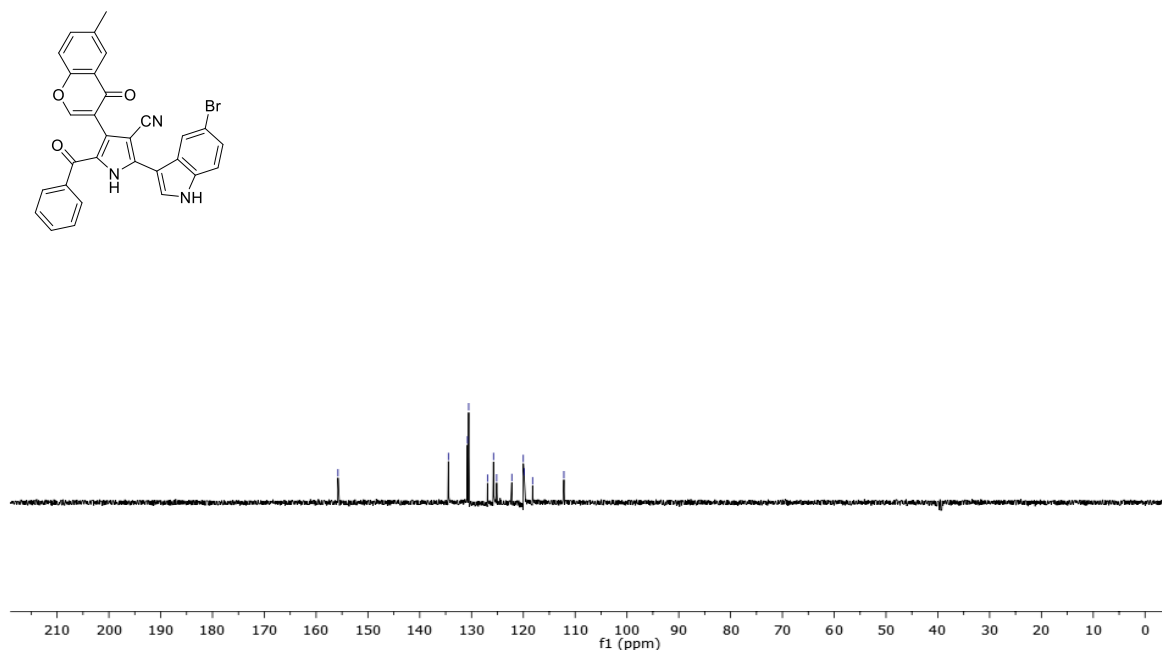


¹H NMR spectrum of **4e** (400 MHz, DMSO-*d*₆)



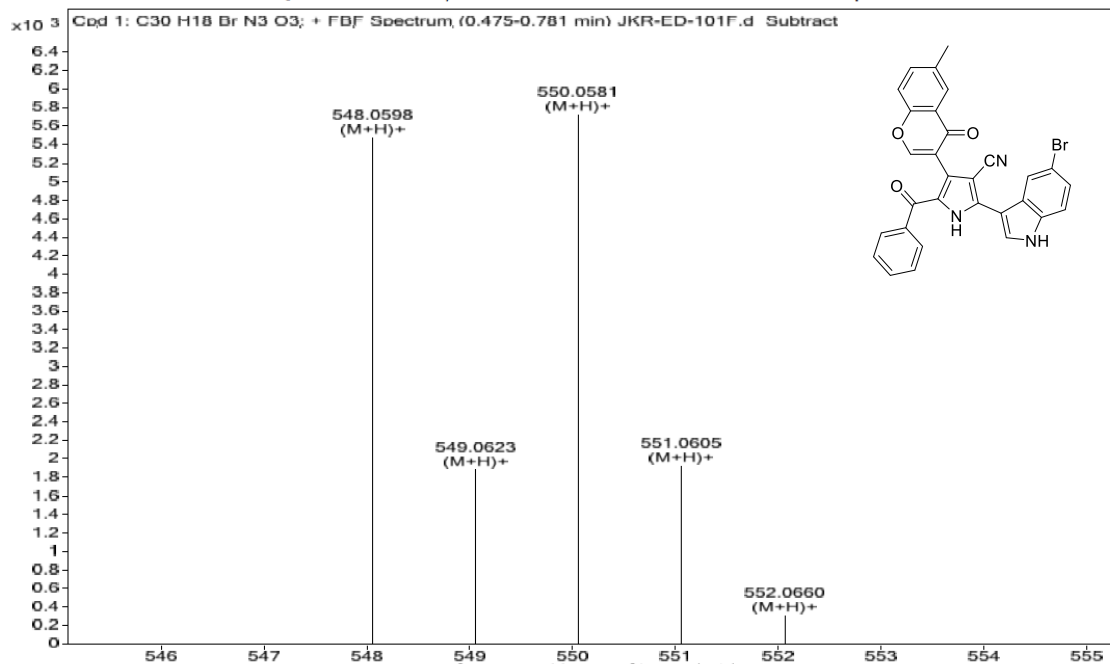
¹³C {¹H} NMR spectrum of **4e** (100 MHz, DMSO-*d*₆)

JKR ED 101 (F)
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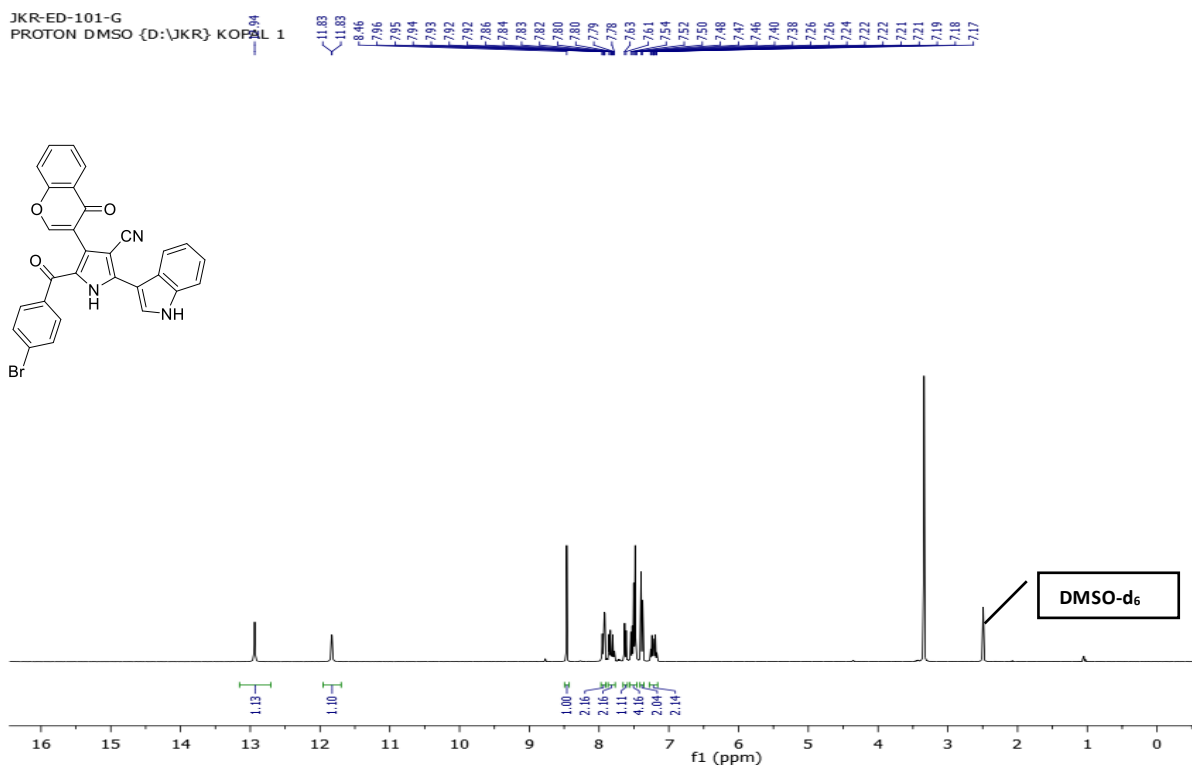


DEPT 135 NMR spectrum of **4e** (100 MHz, DMSO-*d*₆)

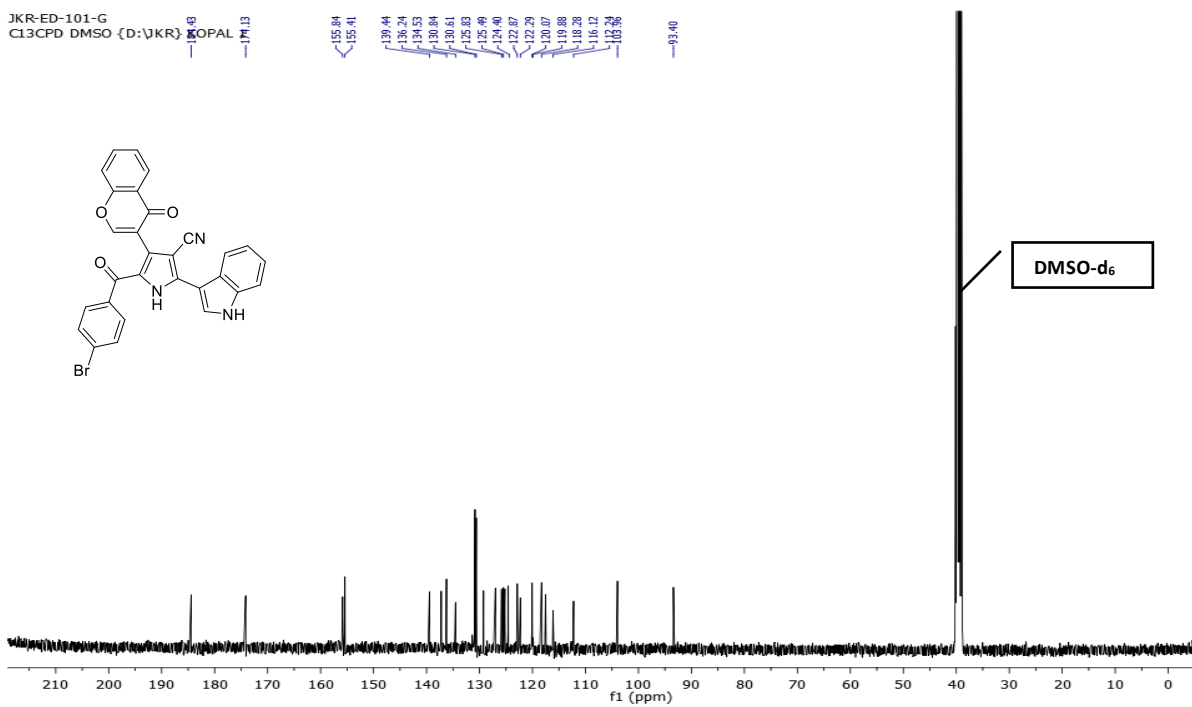
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HRMS (ESI) spectrum of **4e**



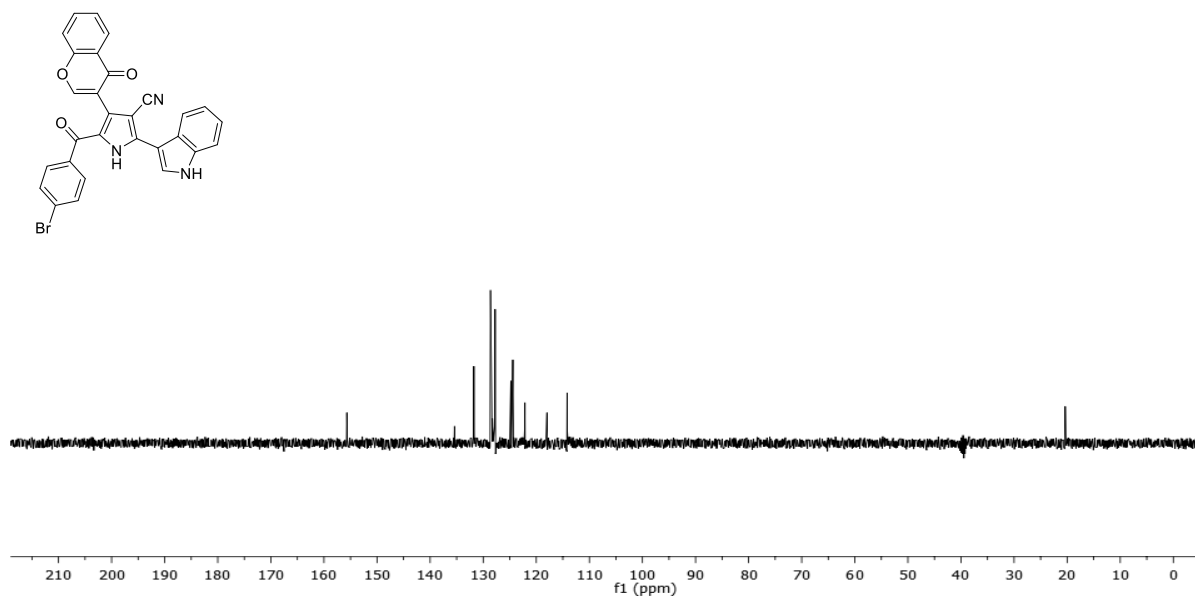
¹H NMR spectrum of **4f** (400 MHz, DMSO-*d*₆)



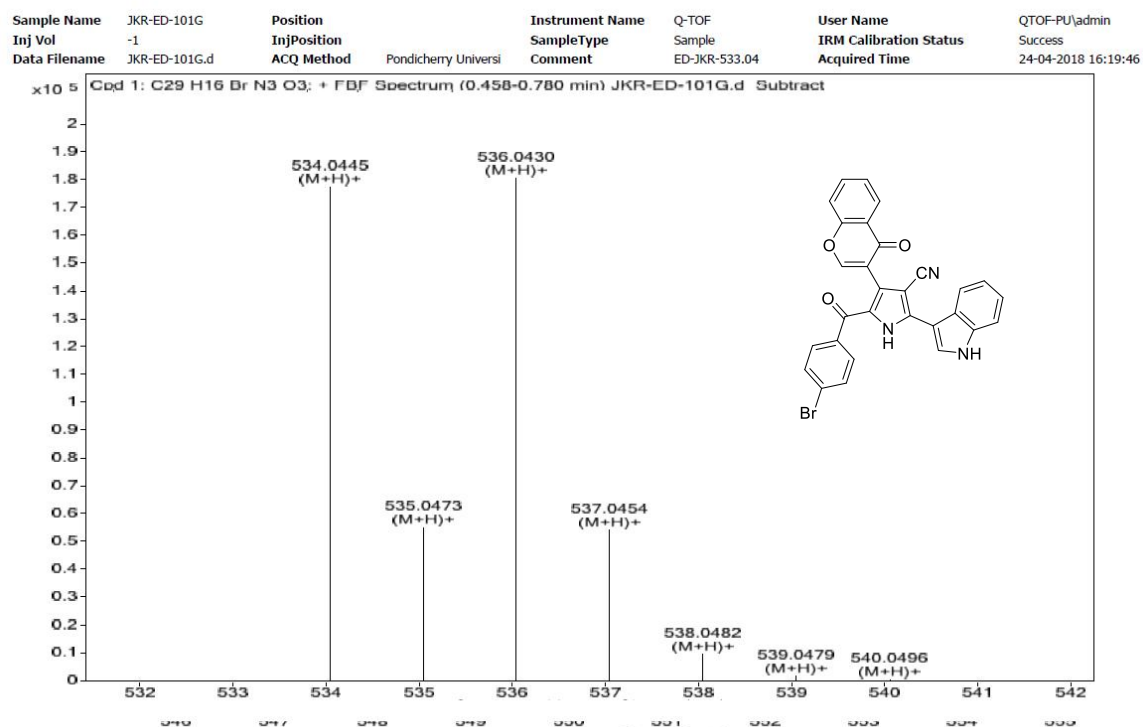
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JKR-ED 101 (G)
 Cl3DEPT135 DMSO {D:\JKR} KOPAL 1

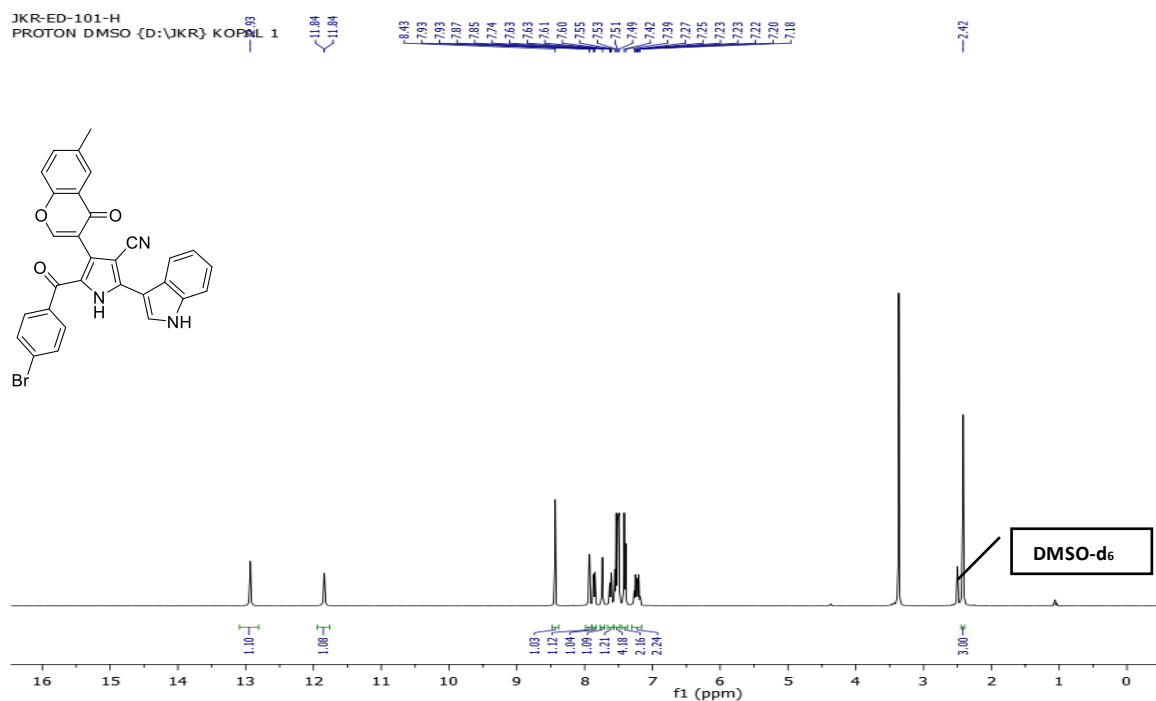
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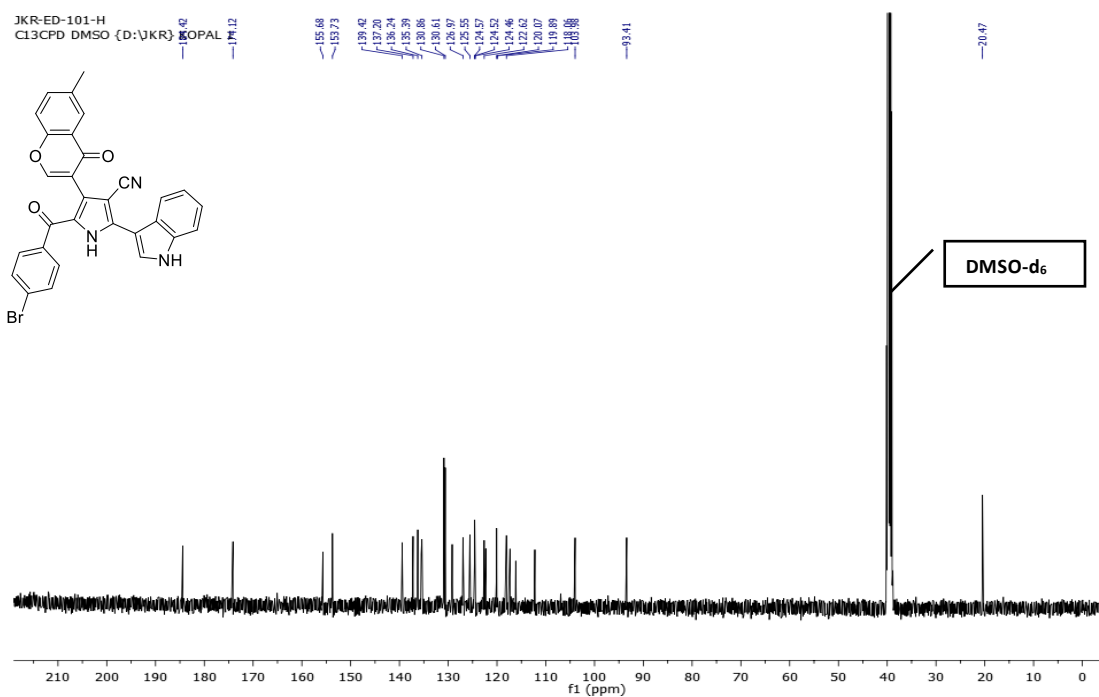
DEPT 135 NMR spectrum of **4f** (100 MHz, DMSO-*d*₆)



HRMS (ESI) spectrum of **4f**



¹H NMR spectrum of **4g** (400 MHz, DMSO-*d*₆)



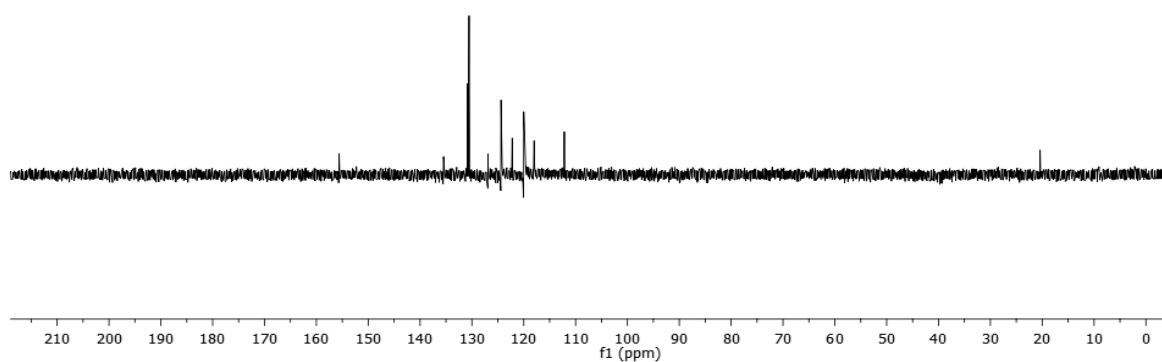
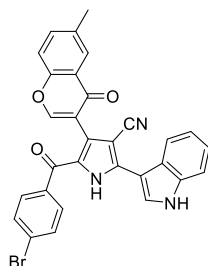
¹³C{¹H} NMR spectrum of **4g** (100 MHz, DMSO-*d*₆)

JKR-ED-101-H
 CL3DEPT135 DMSO {D-}JKR} KOPAL 1

155.61

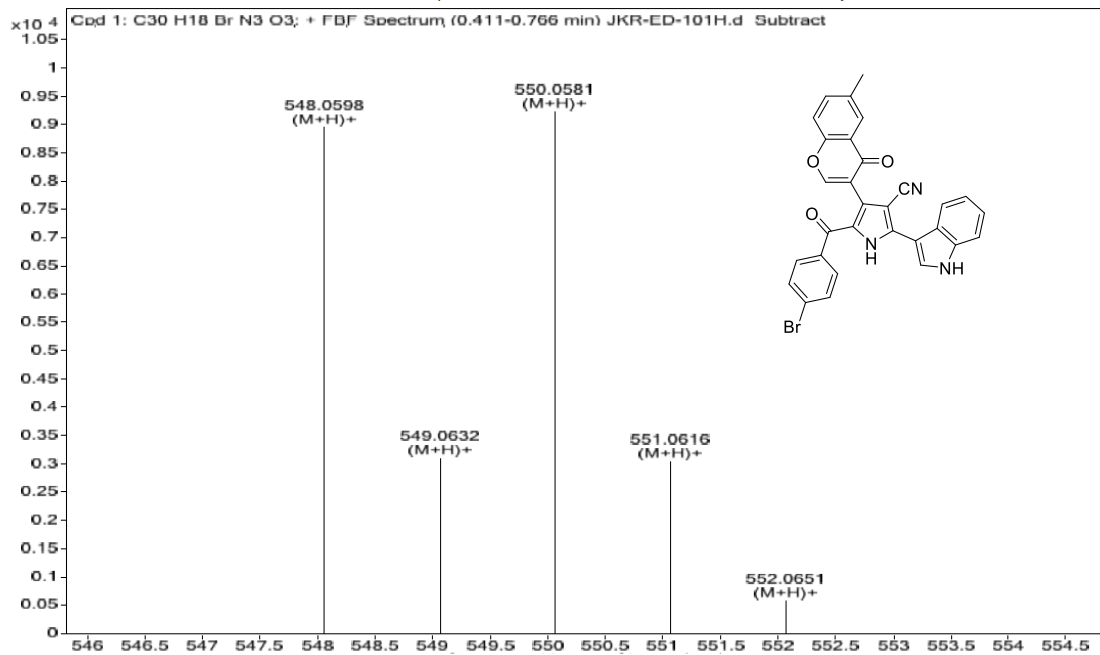
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20.40

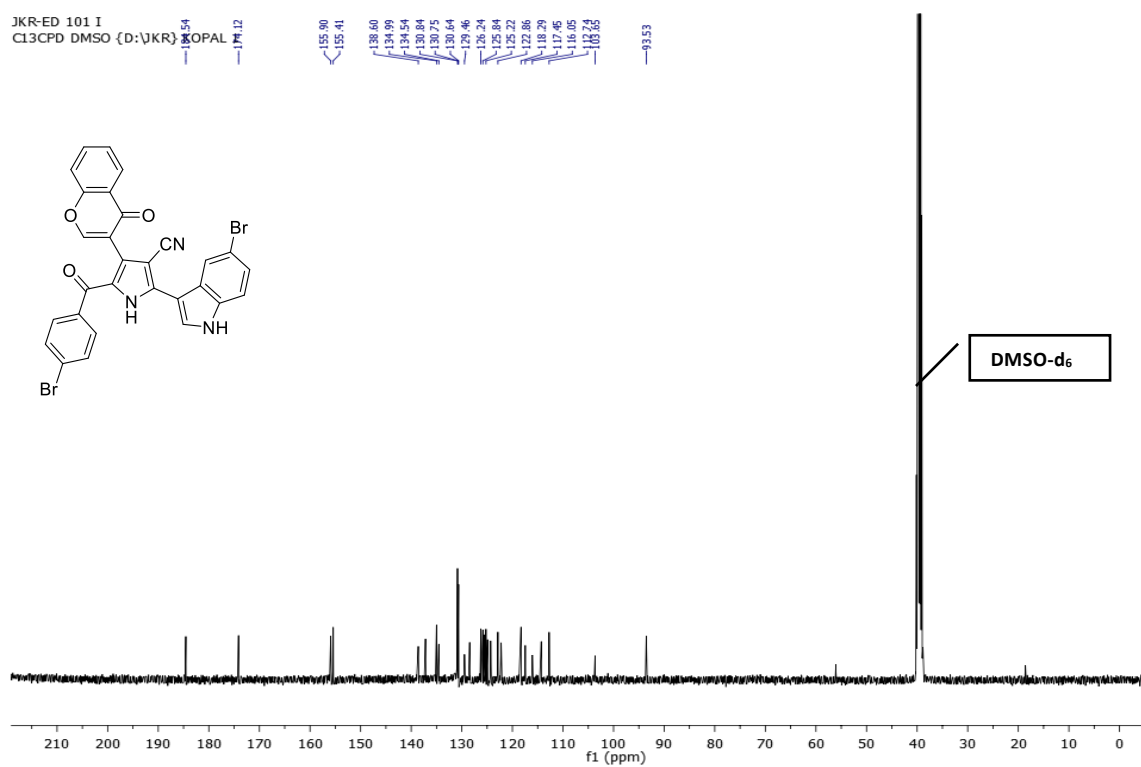
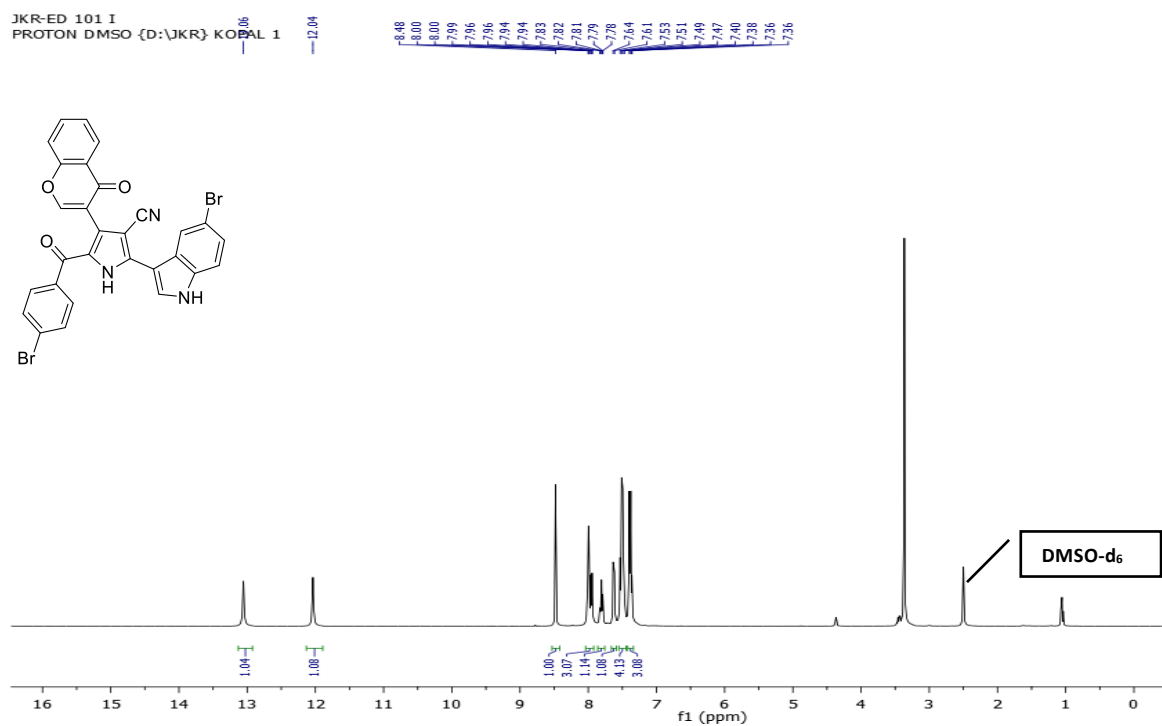


DEPT 135 NMR spectrum of **4g** (100 MHz, DMSO-*d*₆)

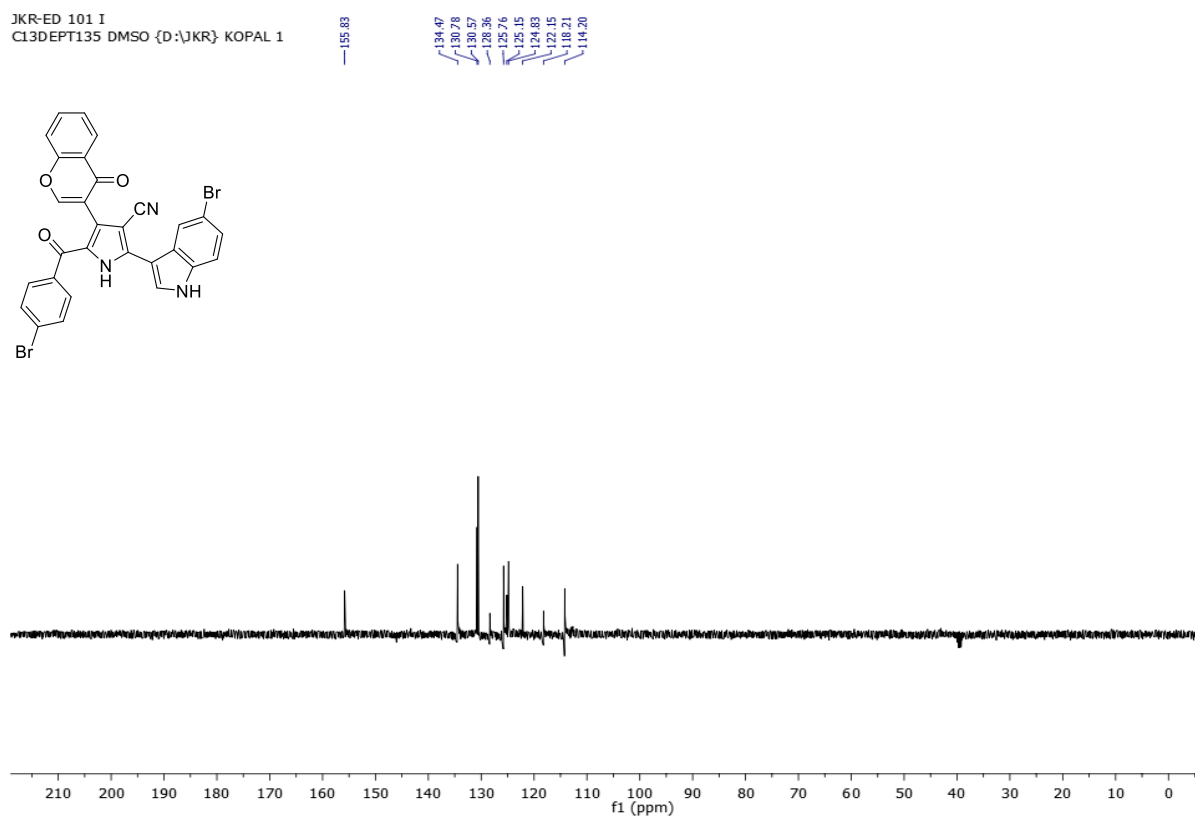
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HRMS (ESI) spectrum of **4g**

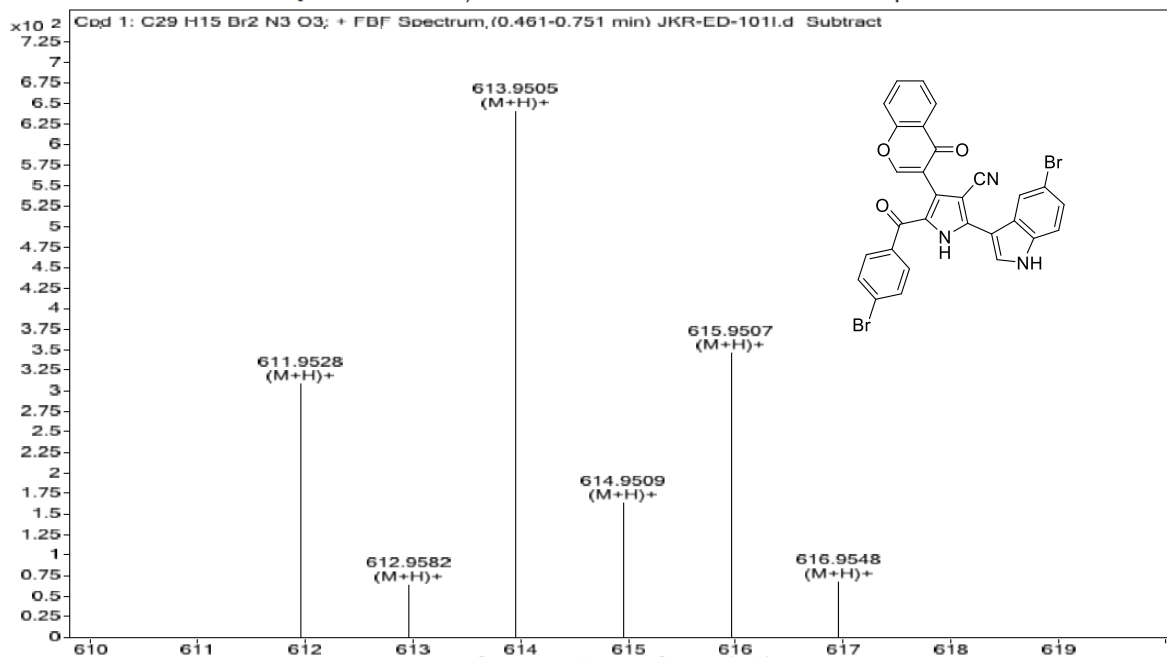


JKR-ED 101 I
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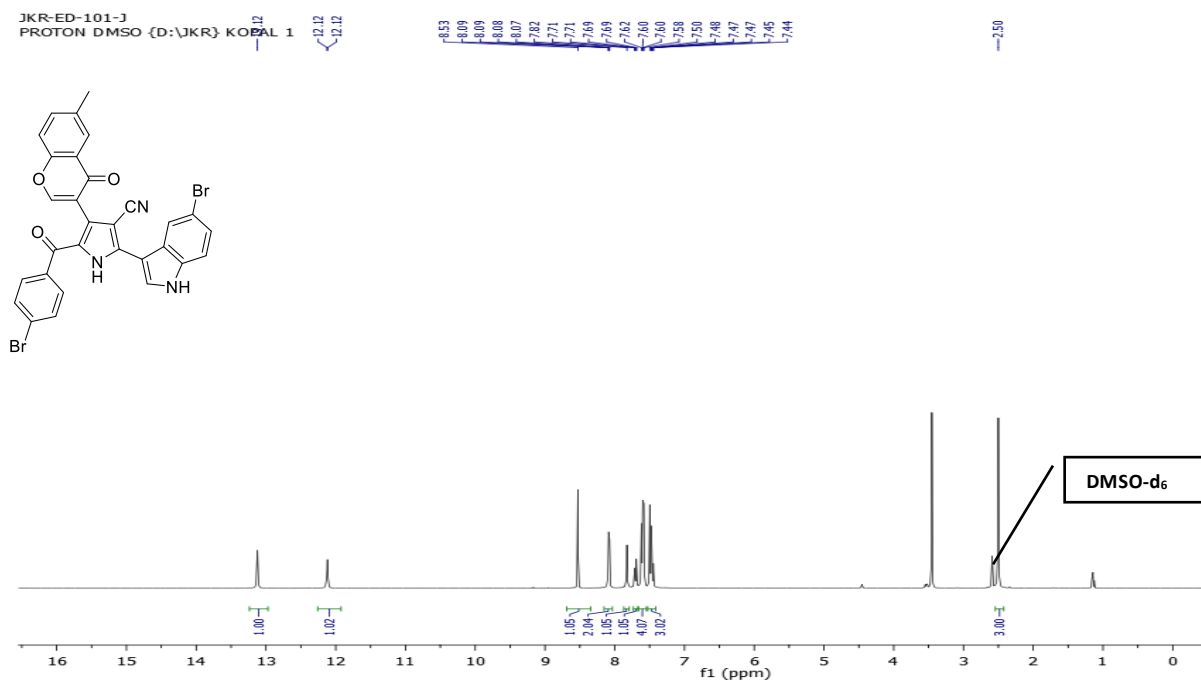


DEPT 135 NMR spectrum of **4h** (100 MHz, DMSO-*d*₆)

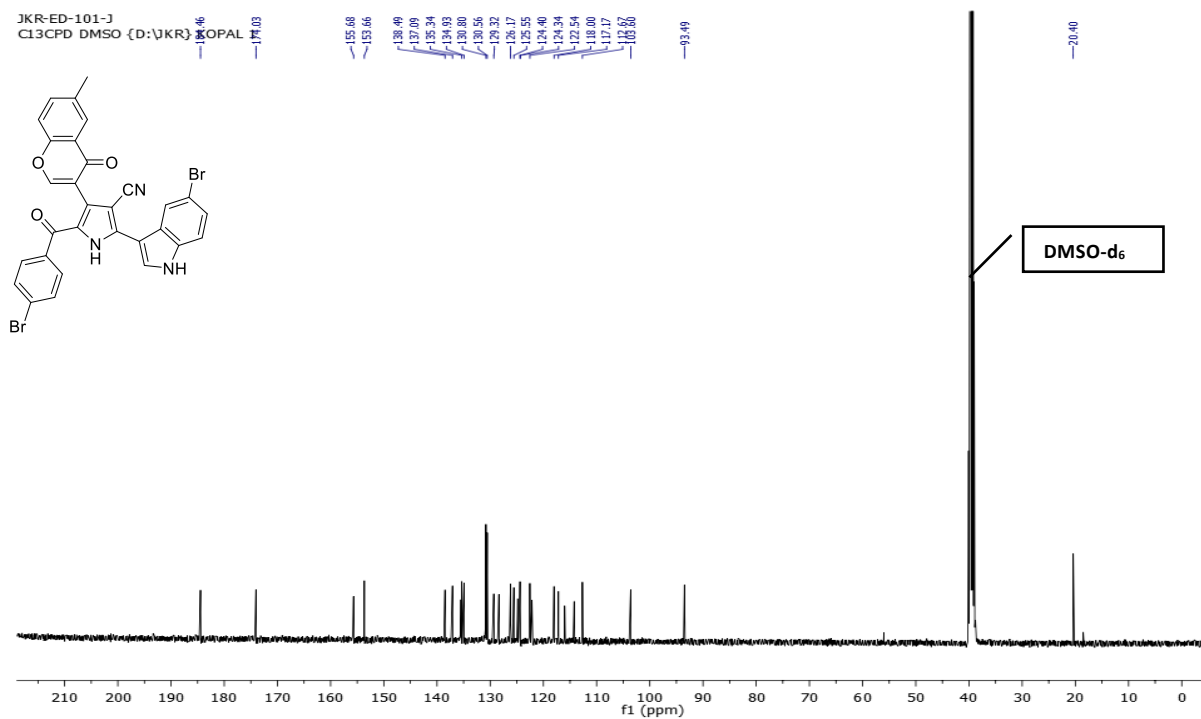
Sample Name	Position	InjPosition	Instrument Name	Q-TOF	User Name	QTOF-PU/admin	
JKR-ED-101I	-1		Sample	Sample	IRM Calibration Status	Success	
Data Filename	JKR-ED-101I.d	ACQ Method	Pondicherry Universi	Comment	JKR-ED-610.95	Acquired Time	25-04-2018 12:24:39



HRMS (ESI) spectrum of **4h**

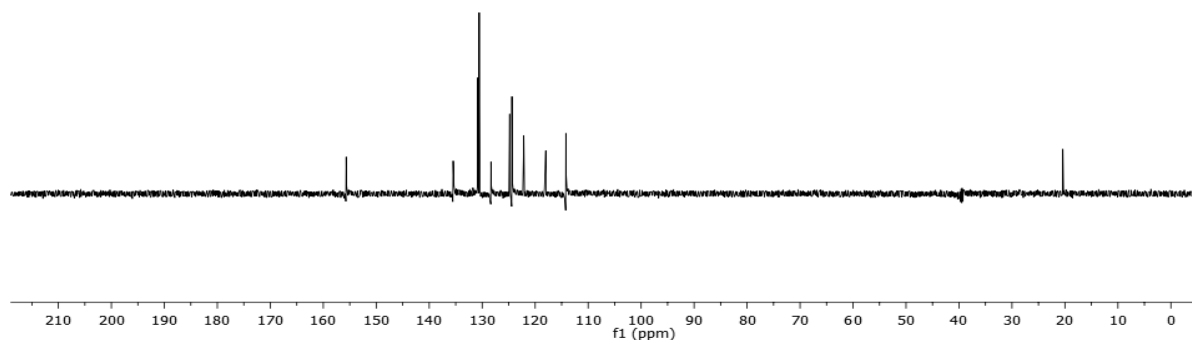
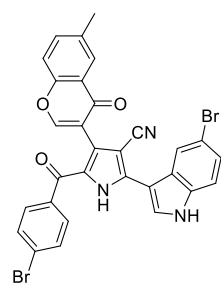


¹H NMR spectrum of **4i** (400 MHz, DMSO-*d*₆)



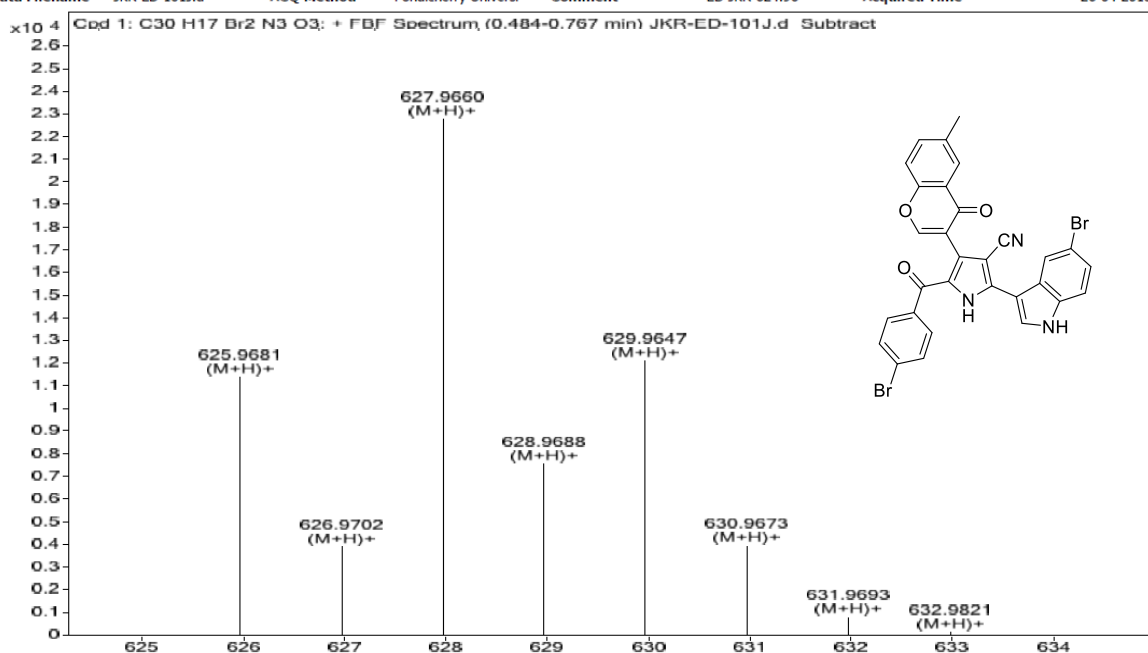
¹³C {¹H} NMR spectrum of **4i** (100 MHz, DMSO-*d*₆)

JKR-ED-101-J
Cl3DEPT135 DMSO {D:\JKR} KOPAL 1



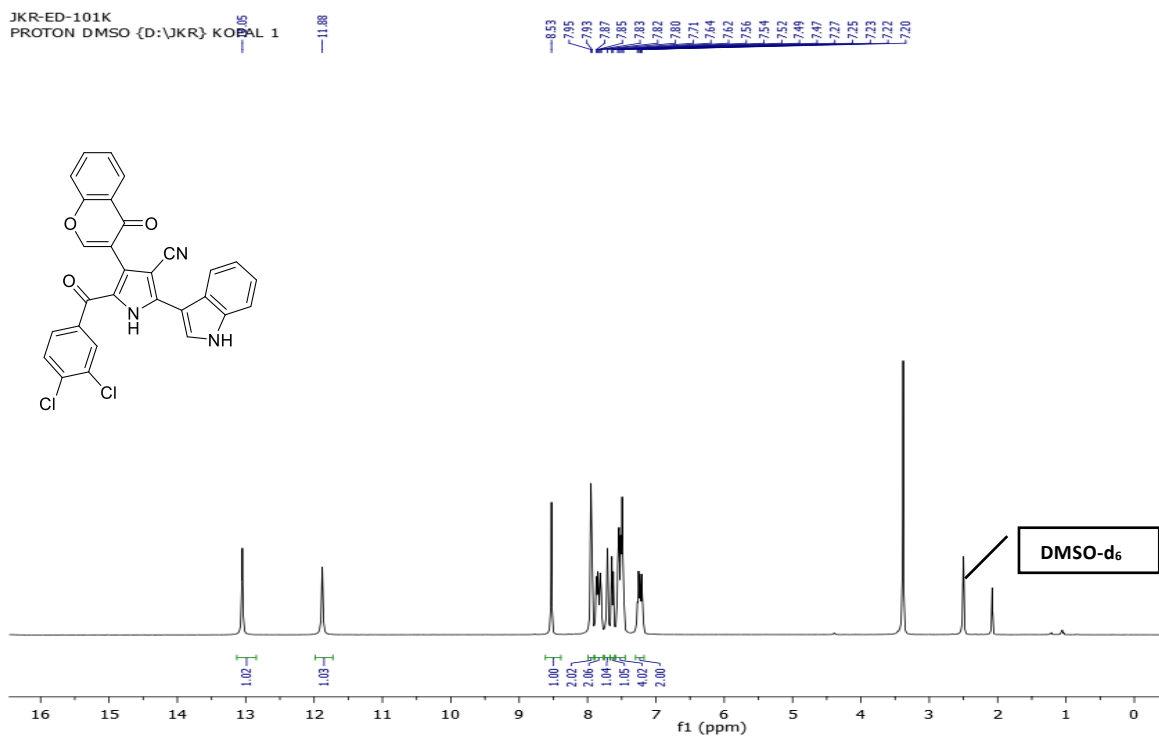
DEPT 135 NMR spectrum of **4i** (100 MHz, DMSO- d_6)

Sample Name	JKR-ED-101J	Position		Instrument Name	Q-TOF	User Name	QTOF-PU\admin
Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	JKR-ED-101J.d	ACQ Method	Pondicherry Universi	Comment	ED-JKR-624.96	Acquired Time	26-04-2018 12:46:44

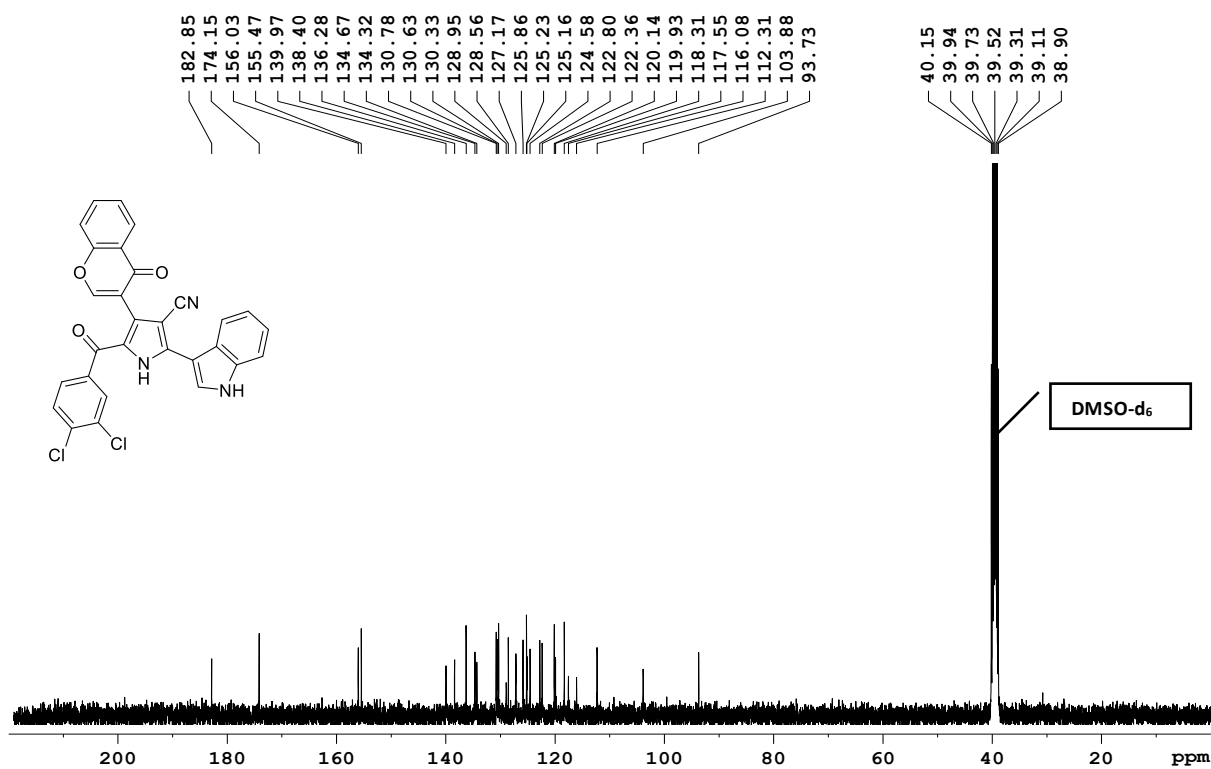


HRMS (ESI) spectrum of **4i**

JKR-ED-101K
PROTON DMSO (D:\JKR) KOPAL 1



¹H NMR spectrum of **4j** (400 MHz, DMSO-*d*₆)

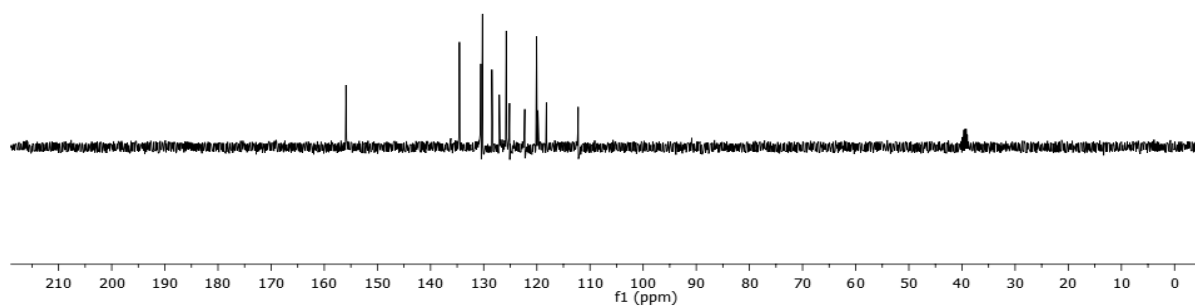
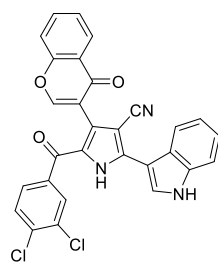


¹³C{¹H} NMR spectrum of **4j** (100 MHz, DMSO-*d*₆)

JKR-ED-101K
C13DEPT135 DMSO {D:\JKR} KOPAL 1

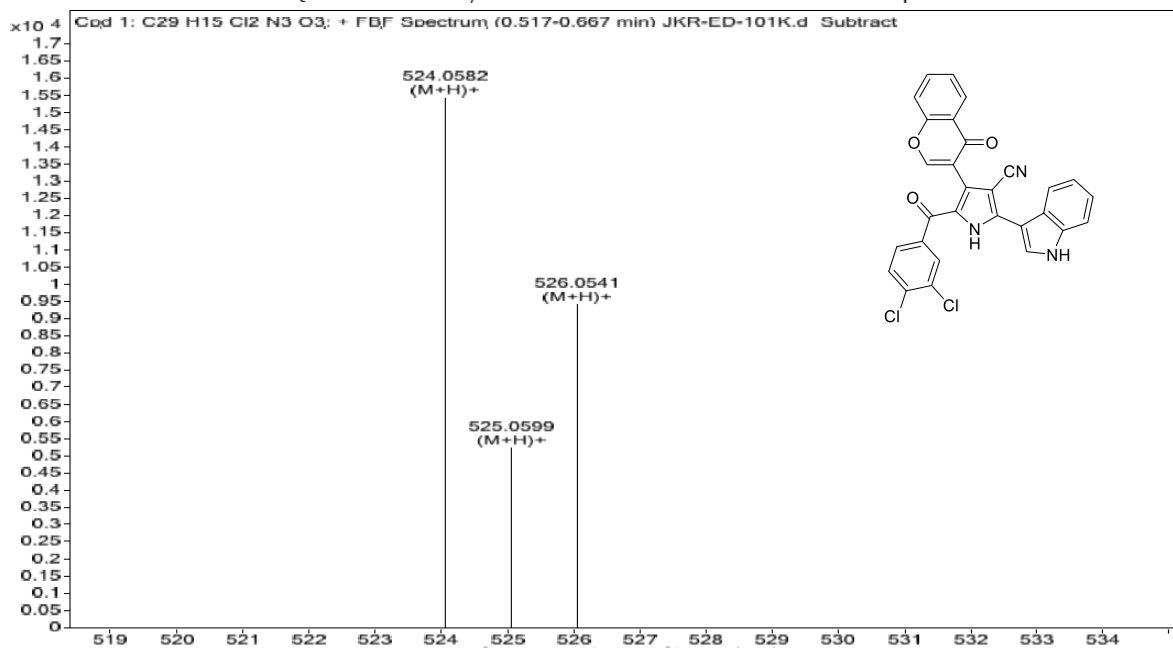
155.92

134.57
130.54
130.23
128.46
127.06
125.76
125.14
122.27
120.04
119.83
118.21
112.22



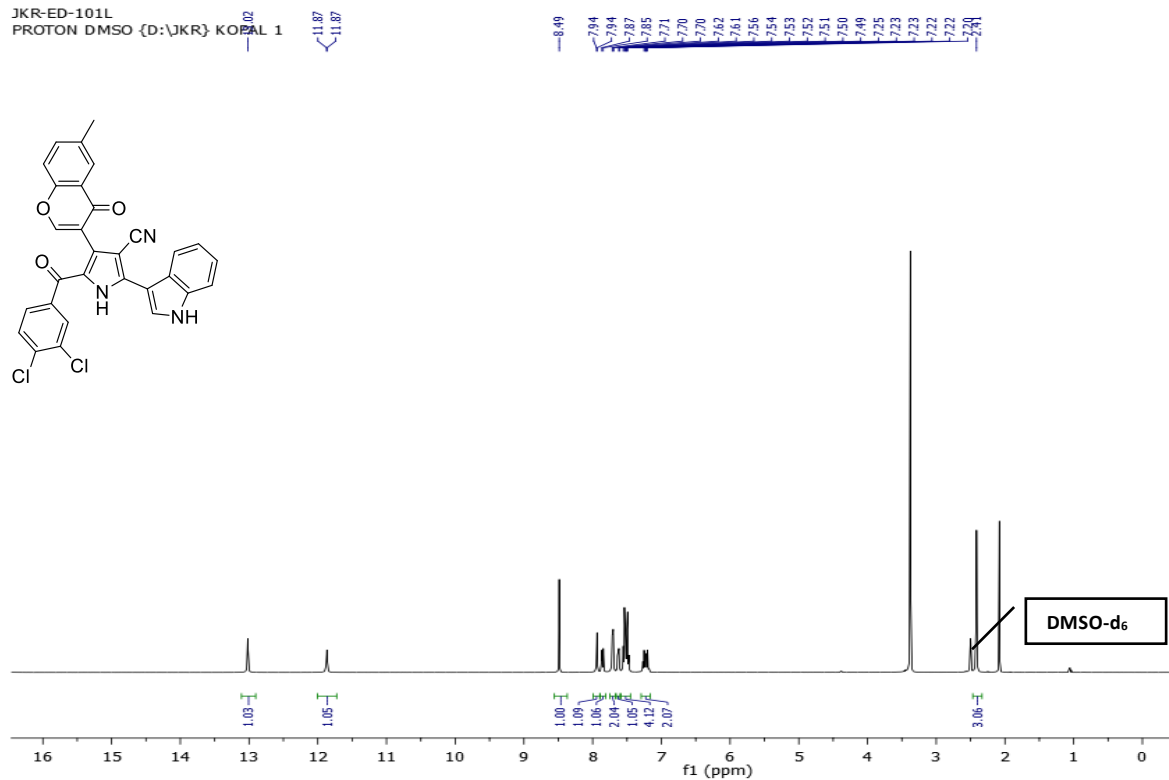
DEPT 135 NMR spectrum of **4j** (100 MHz, DMSO- d_6)

Sample Name	JKR-ED-101K	Position		Instrument Name	Q-TOF	User Name	QTOF-PU\admin
Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	JKR-ED-101K.d	ACQ Method	Pondicherry Universi	Comment	ED-JKR-523.05	Acquired Time	26-04-2018 12:43:00

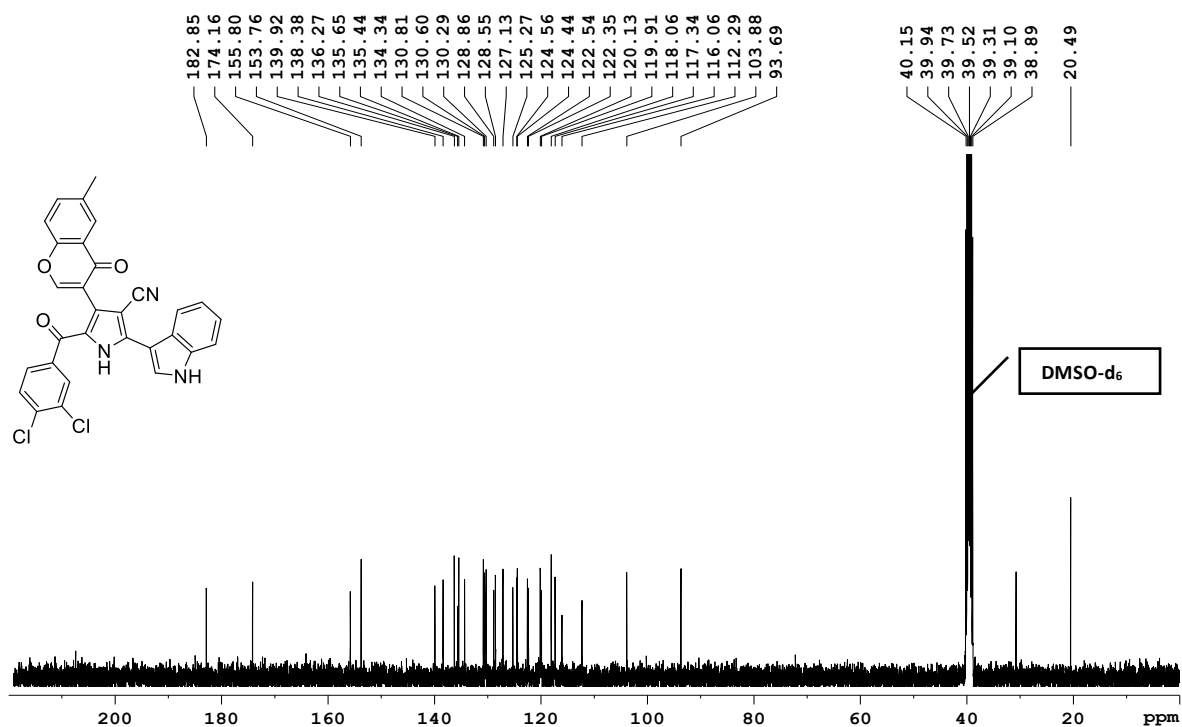


HRMS (ESI) spectrum of **4j**

JKR-ED-101L
PROTON DMSO {D:\JKR\KOPAL 1



¹H NMR spectrum of **4k** (400 MHz, DMSO-*d*₆)



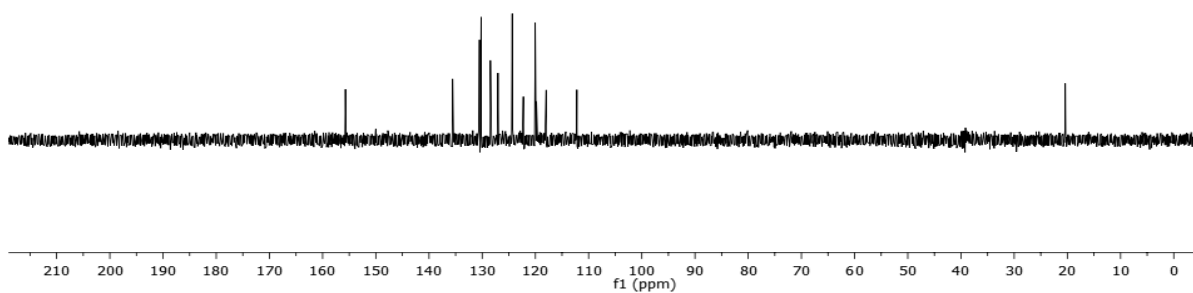
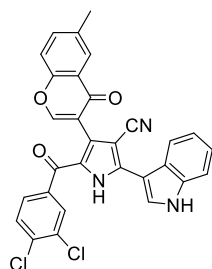
¹³C{¹H} NMR spectrum of **4k** (100 MHz, DMSO-*d*₆)

JKR-ED-101L
C13DEPT135 DMSO {D:\JKR} KOPAL 1

155.71

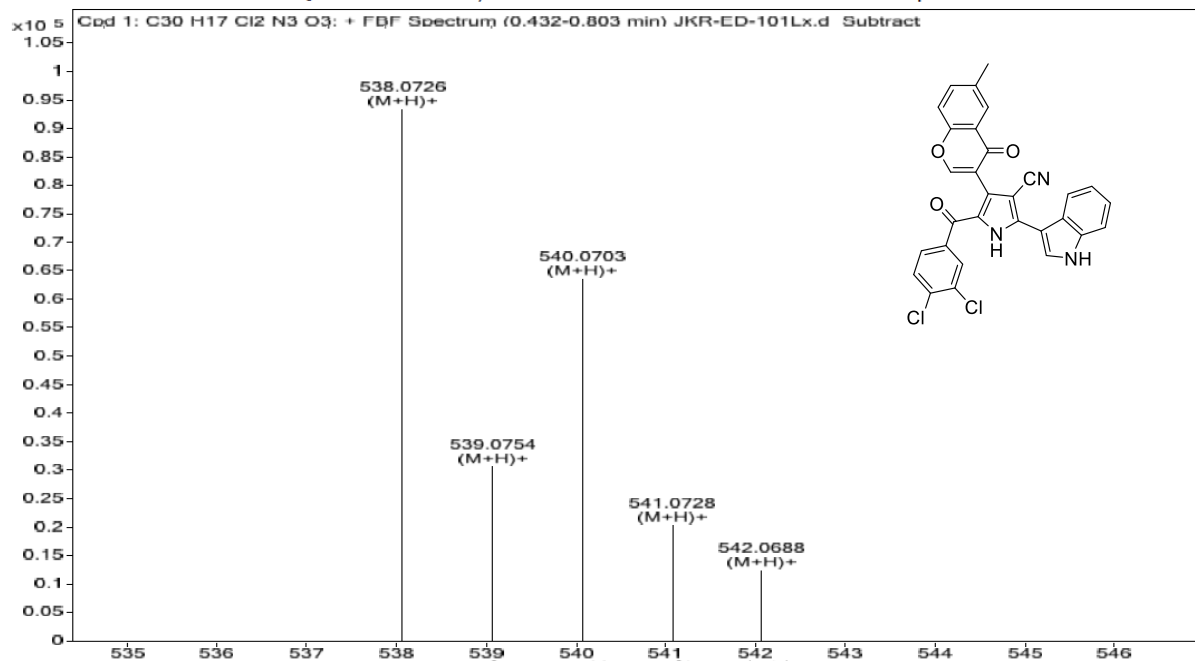
135.56
130.52
130.21
128.46
127.04
124.36
122.26
120.03
119.82
117.88
112.21

20.40

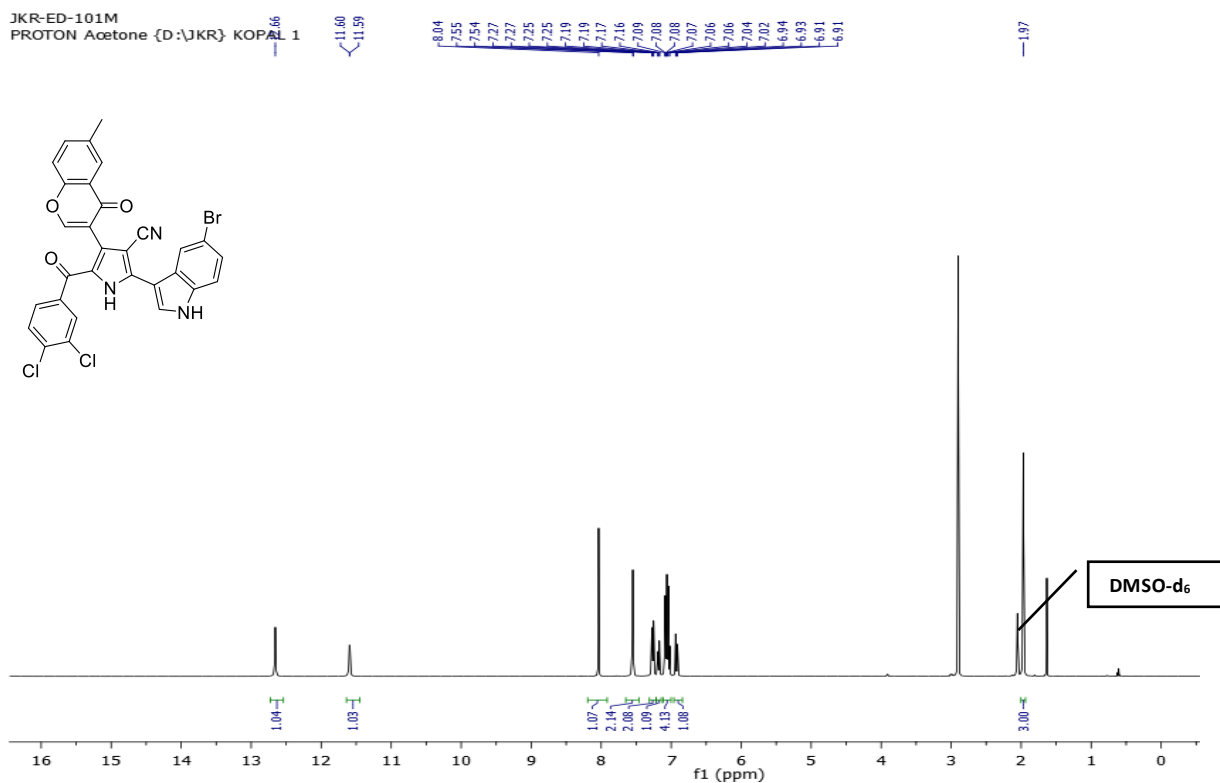


DEPT 135 NMR spectrum of **4k** (100 MHz, DMSO-*d*₆)

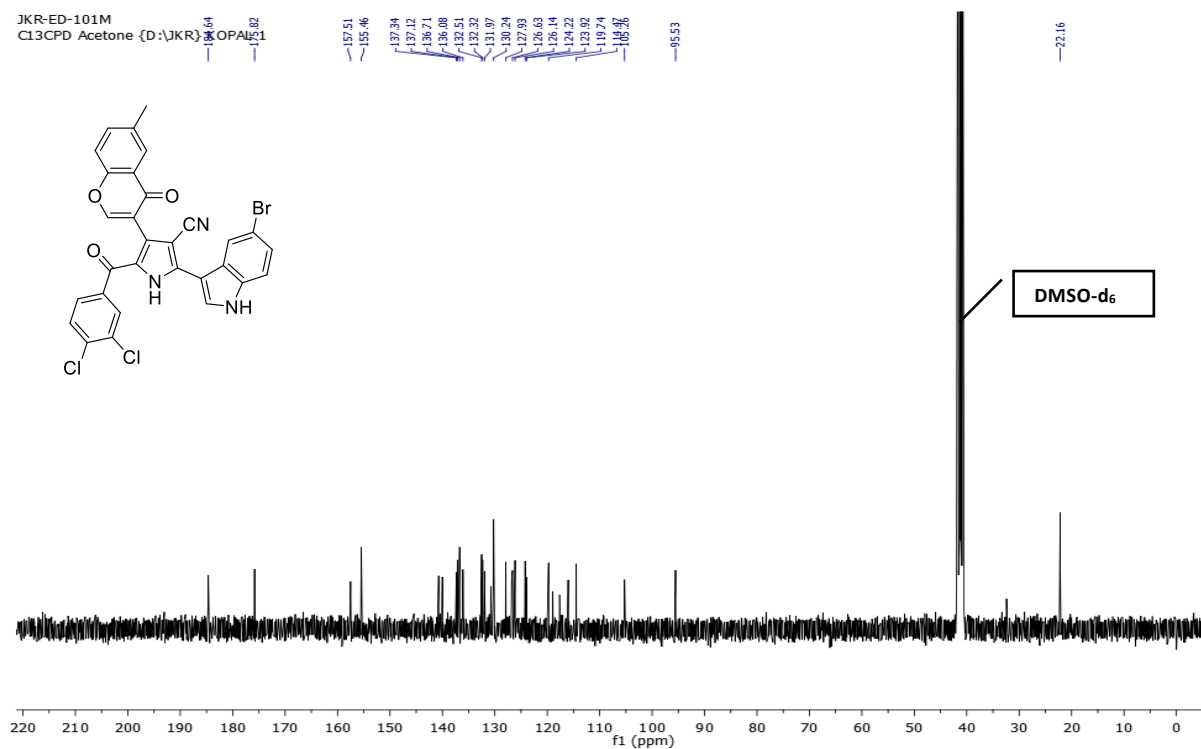
Sample Name	JKR-ED-101L	Position		Instrument Name	Q-TOF	User Name	QTOF-PU\admin
Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	JKR-ED-101Lx.d	ACQ Method	Pondicherry Universi	Comment	ED-JKR-537.06	Acquired Time	02-05-2018 14:52:52



HRMS (ESI) spectrum of **4k**

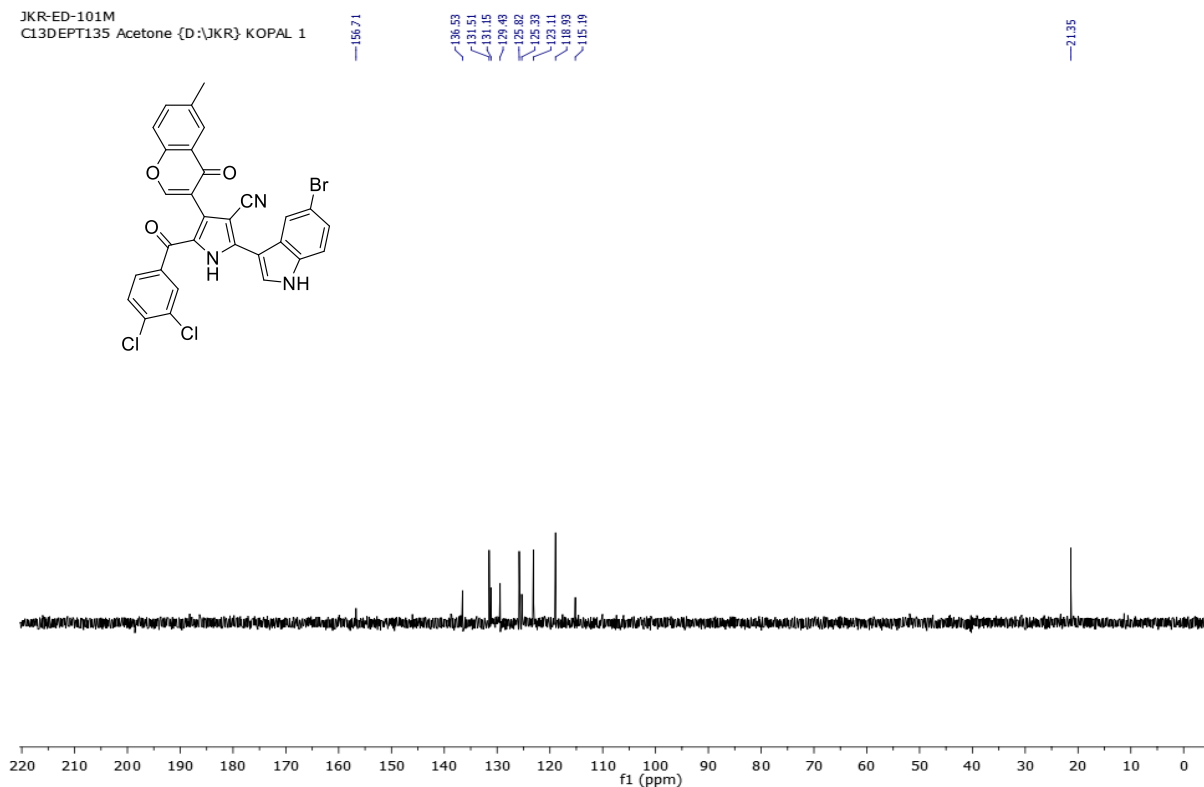


^1H NMR spectrum of **4I** (400 MHz, DMSO- d_6)



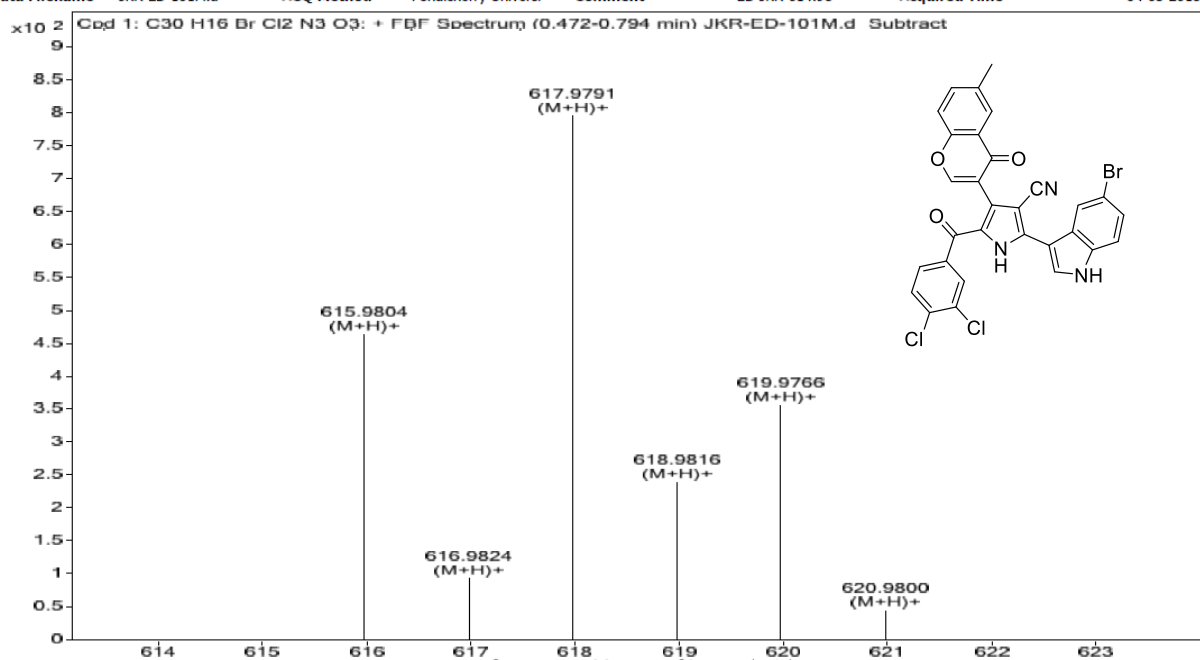
$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **4I** (100 MHz, DMSO- d_6)

JKR-ED-101M
Cl3DEPT135 Acetone {D:\JKR} KOPAL 1



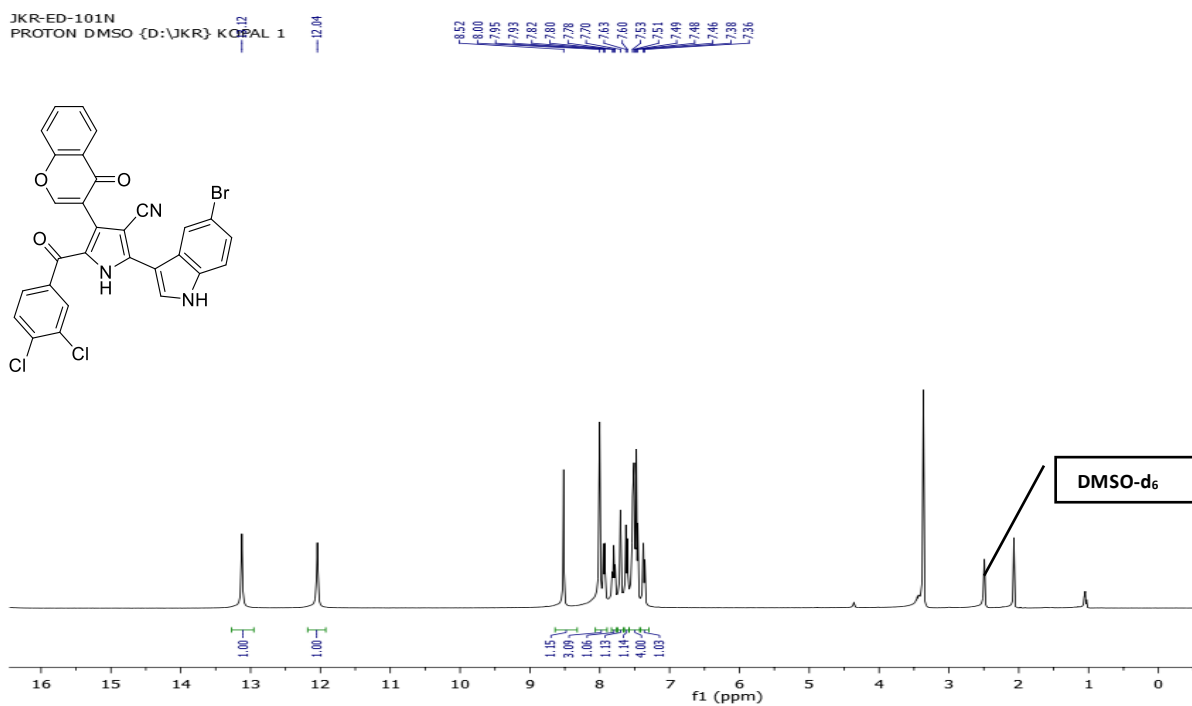
DEPT 135 NMR spectrum of **4l** (100 MHz, DMSO- d_6)

Sample Name	JKR-ED-101M	Position	Instrument Name	Q-TOF	User Name	QTOF-PU\admin
Inj Vol	-1	InjPosition	SampleType	Sample	IRM Calibration Status	Success
Data Filename	JKR-ED-101M.d	ACQ Method	Comment	ED-JKR-614.98	Acquired Time	04-05-2018 11:54:36



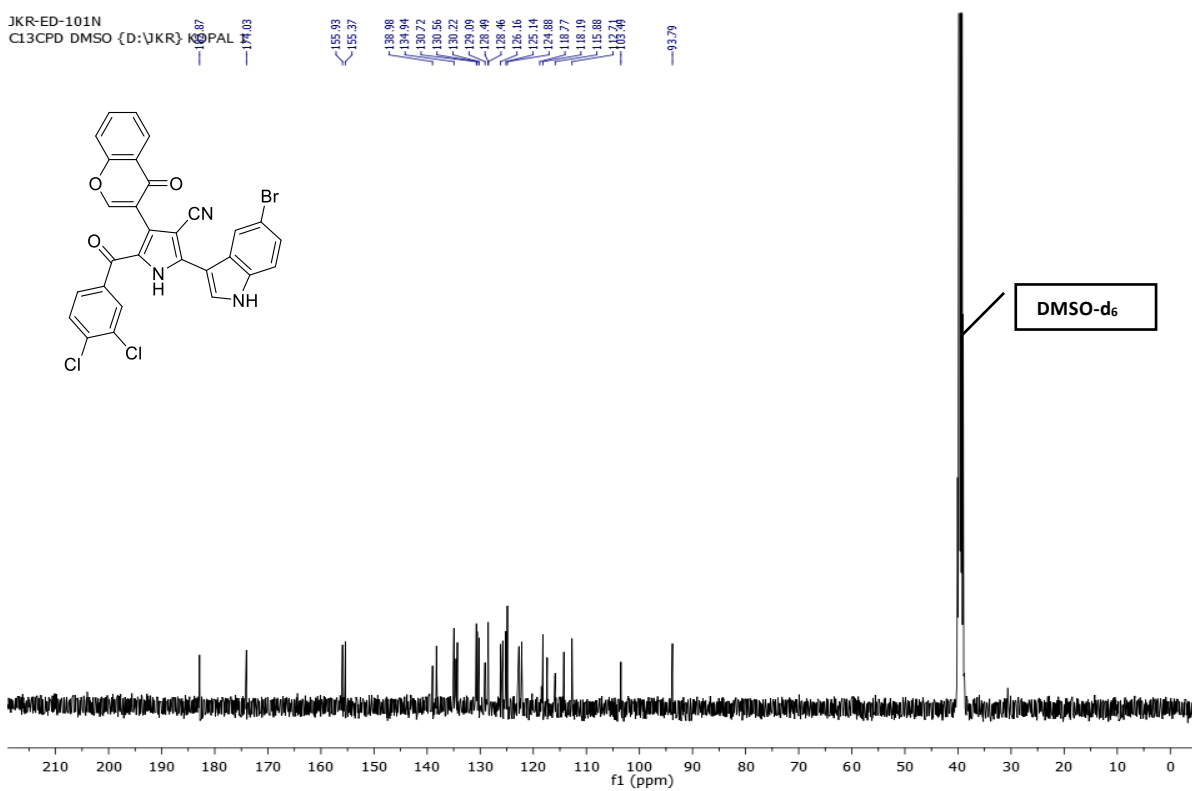
HRMS (ESI) spectrum of **4l**

JKR-ED-101N
PROTON DMSO {D:\JKR} KOPAL 1



¹H NMR spectrum of **4m** (400 MHz, DMSO-*d*₆)

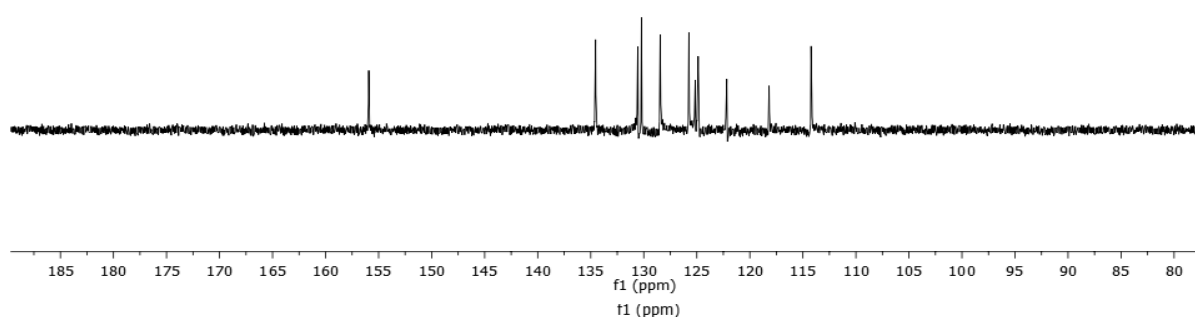
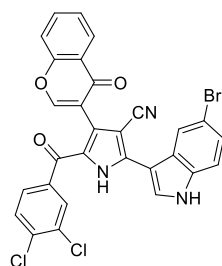
JKR-ED-101N
C13CPD DMSO {D:\JKR} KOPAL 1



¹³C {¹H} NMR spectrum of **4m** (100 MHz, DMSO-*d*₆)

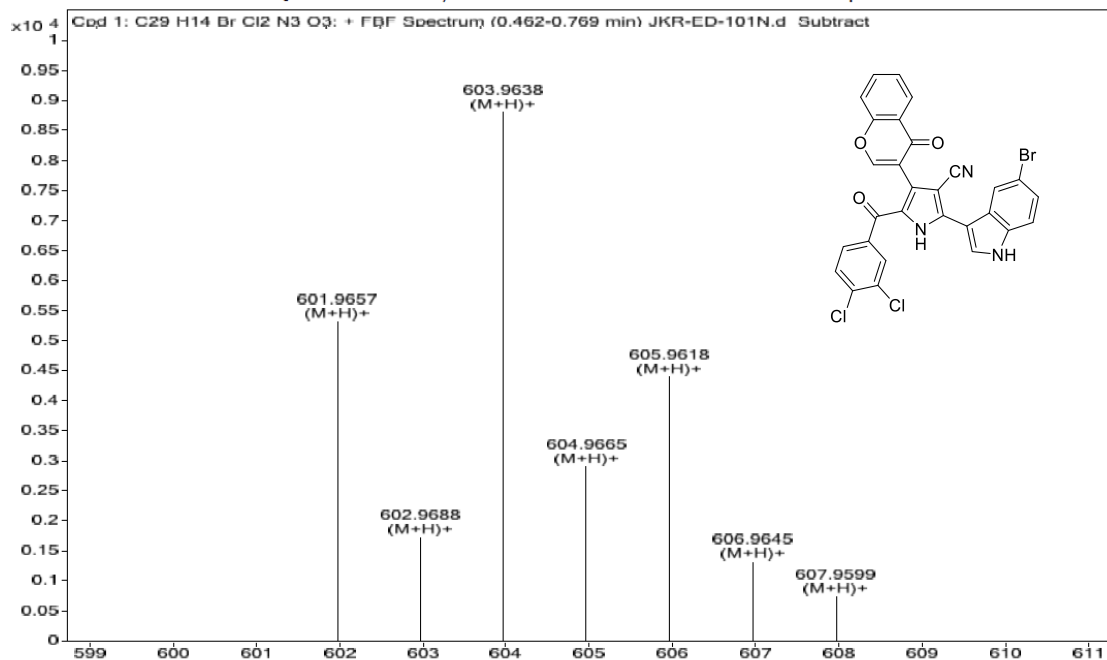
JKR-ED-101N
 CL3DEPT135 DMSO {D:\JKR} KOPAL 1

155.93 134.54 130.56 130.22 128.46 125.75 125.15 124.87 122.17 118.18 114.23

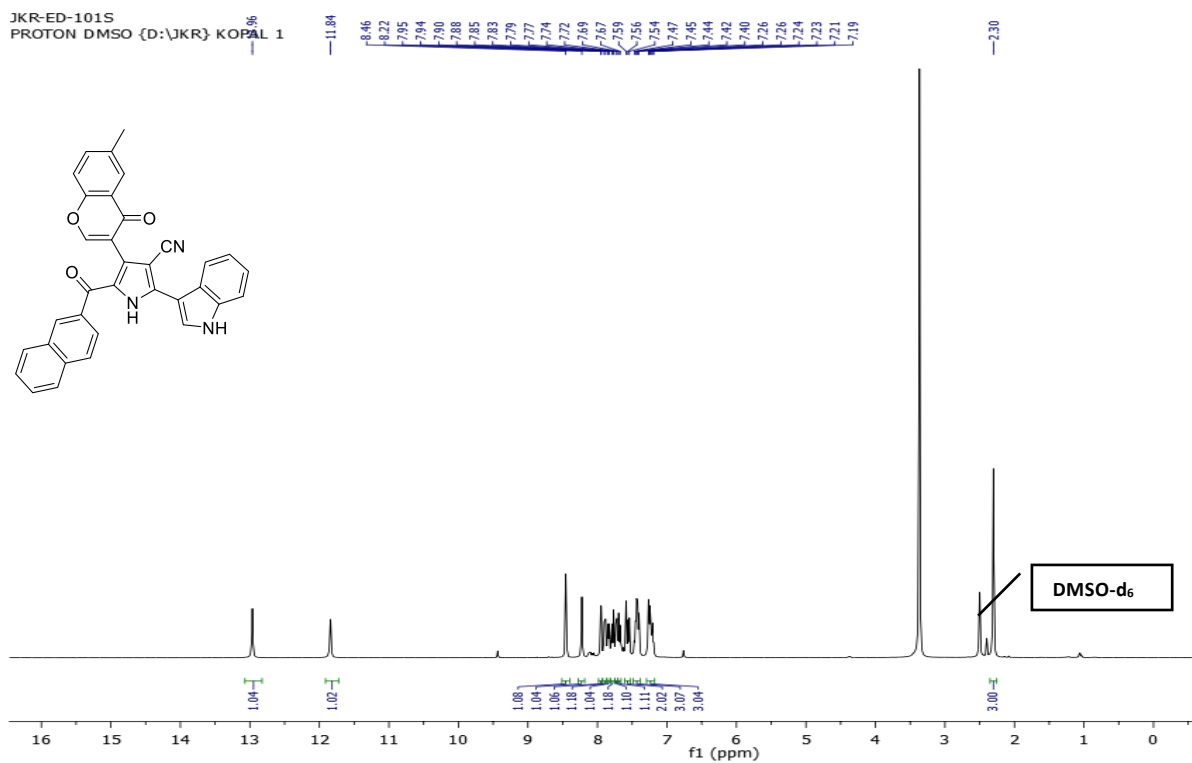


DEPT 135 NMR spectrum of **4m** (100 MHz, DMSO-*d*₆)

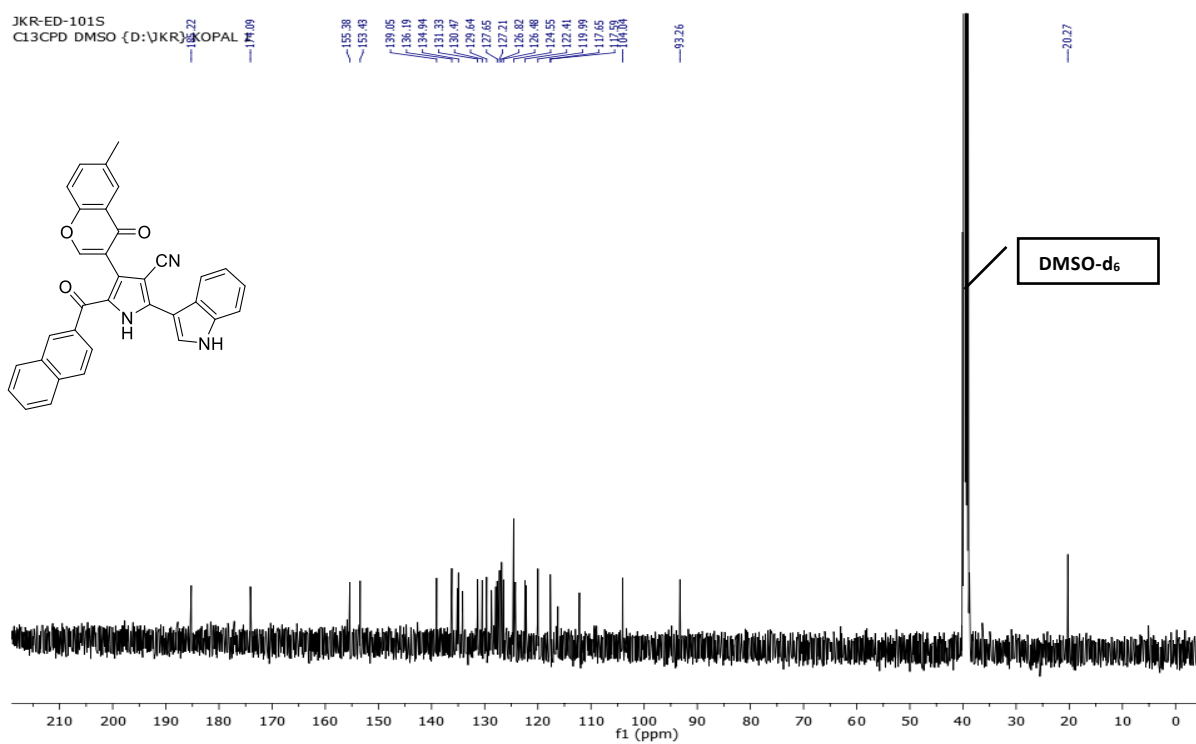
Sample Name	JKR-ED-101N	Position	Instrument Name	Q-TOF	User Name	QTOF-PU\admin
Inj Vol	-1	InjPosition	SampleType	Sample	IRM Calibration Status	Success
Data Filename	JKR-ED-101N.d	ACQ Method	Comment	ED-JKR-600.96	Acquired Time	02-05-2018 14:56:27



HRMS (ESI) spectrum of **4m**



¹H NMR spectrum of **4n** (400 MHz, DMSO-*d*₆)

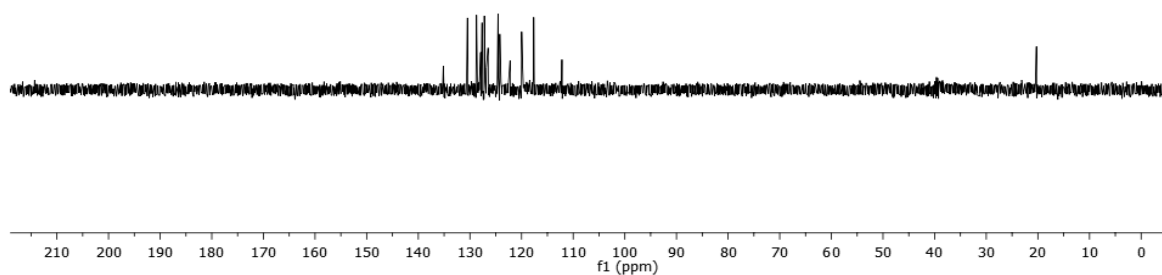
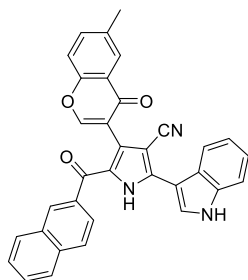


¹³C{¹H} NMR spectrum of **4n** (100 MHz, DMSO-*d*₆)

JKR-ED-101S
Cl3DEPT135 DMSO {D-JKR} KOPAL 1

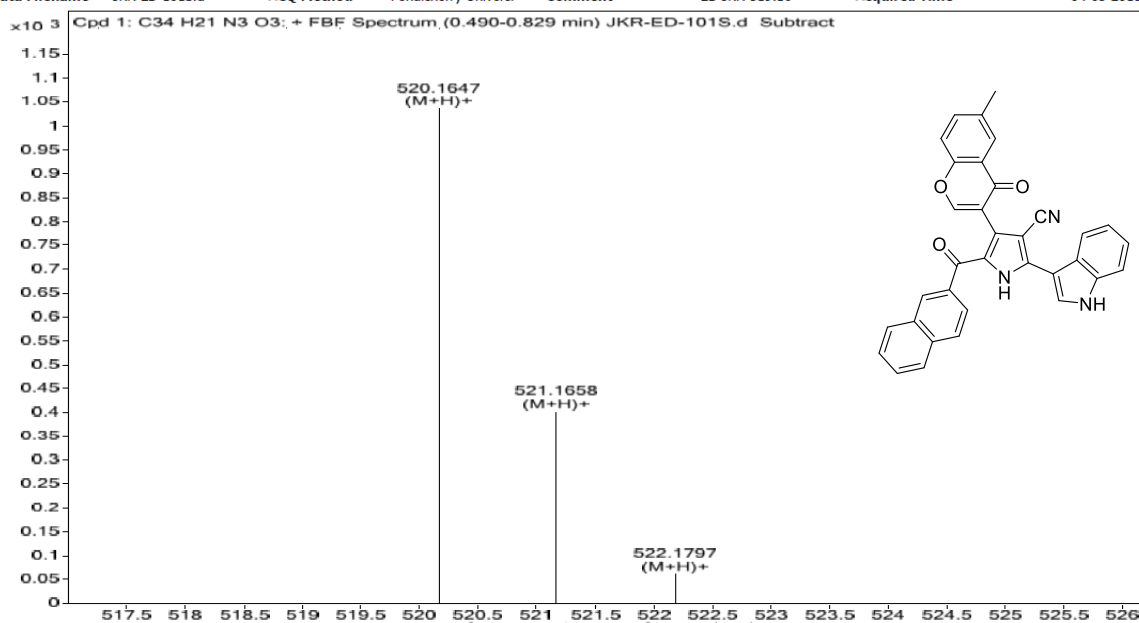
135.15
130.47
128.72
127.92
127.66
127.21
126.81
126.48
124.55
124.21
122.22
119.88
119.83
117.65
112.18

20.27

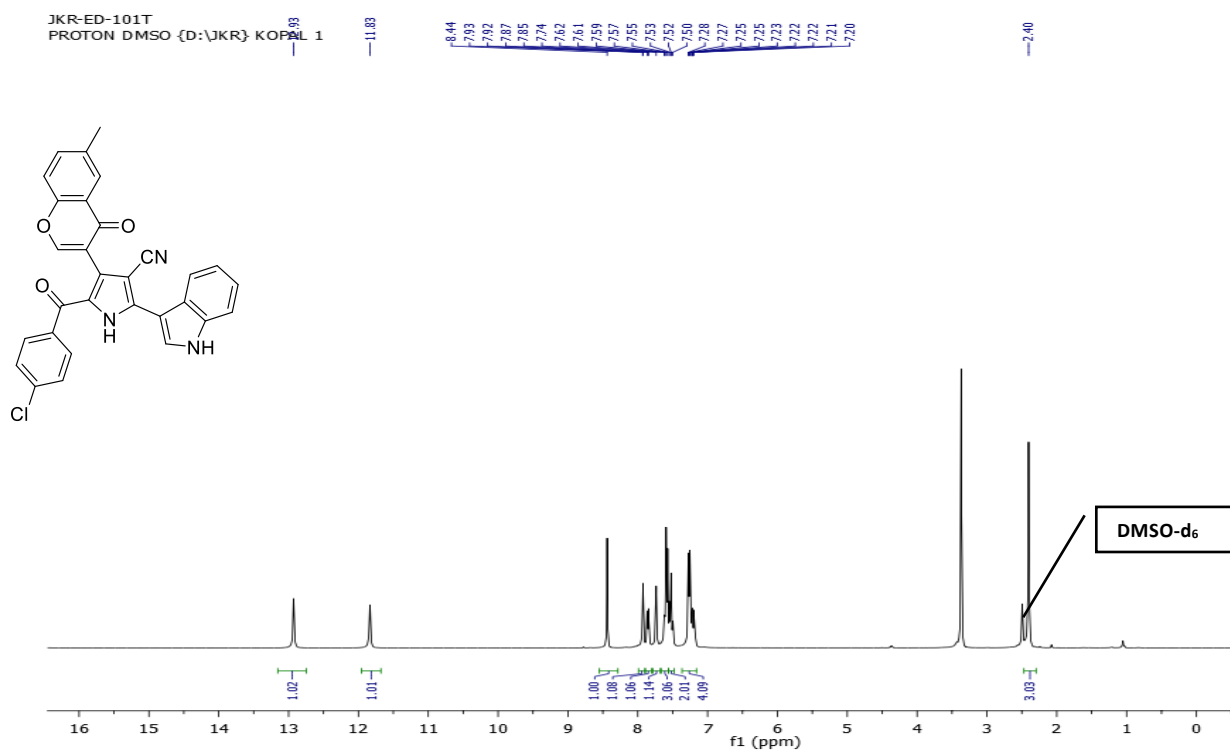


DEPT 135 NMR spectrum of **4n** (100 MHz, DMSO-*d*₆)

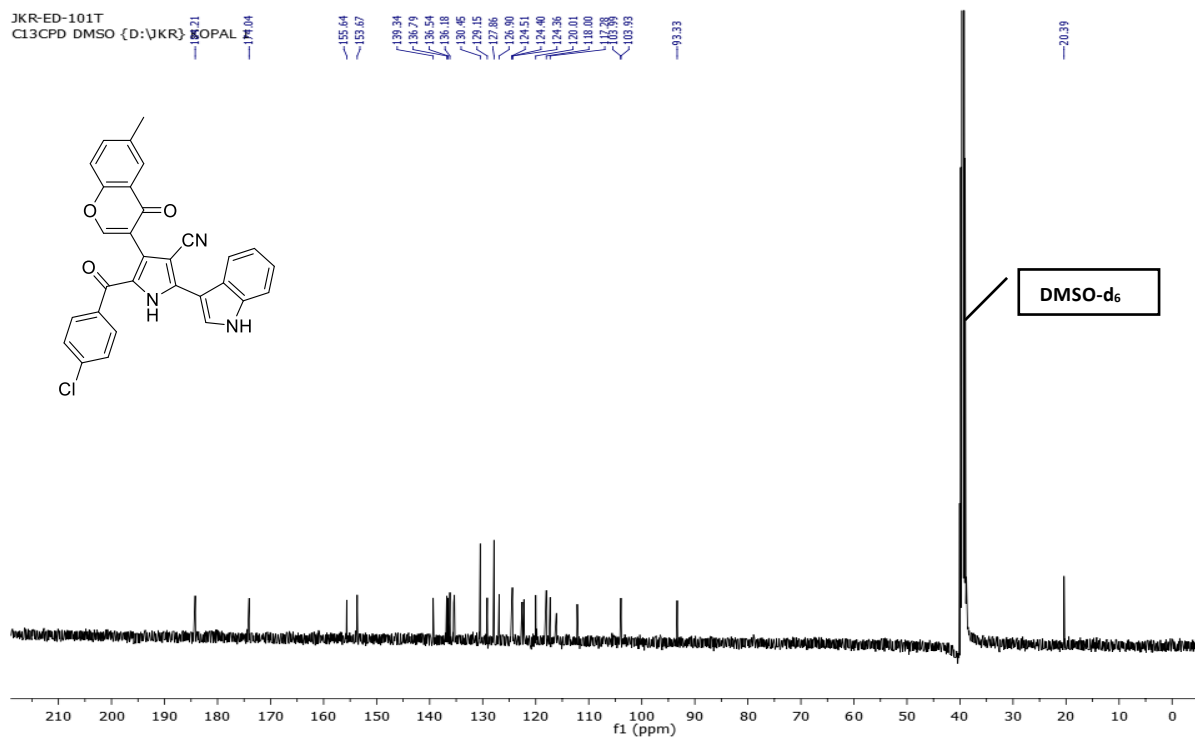
Sample Name	JKR-ED-101S	Position		Instrument Name	Q-TOF	User Name	QTOF-PU/admin
Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	JKR-ED-101S.d	ACQ Method	Pondicherry Universi	Comment	ED-JKR-519.16	Acquired Time	04-05-2018 11:50:03



HRMS (ESI) spectrum of **4n**

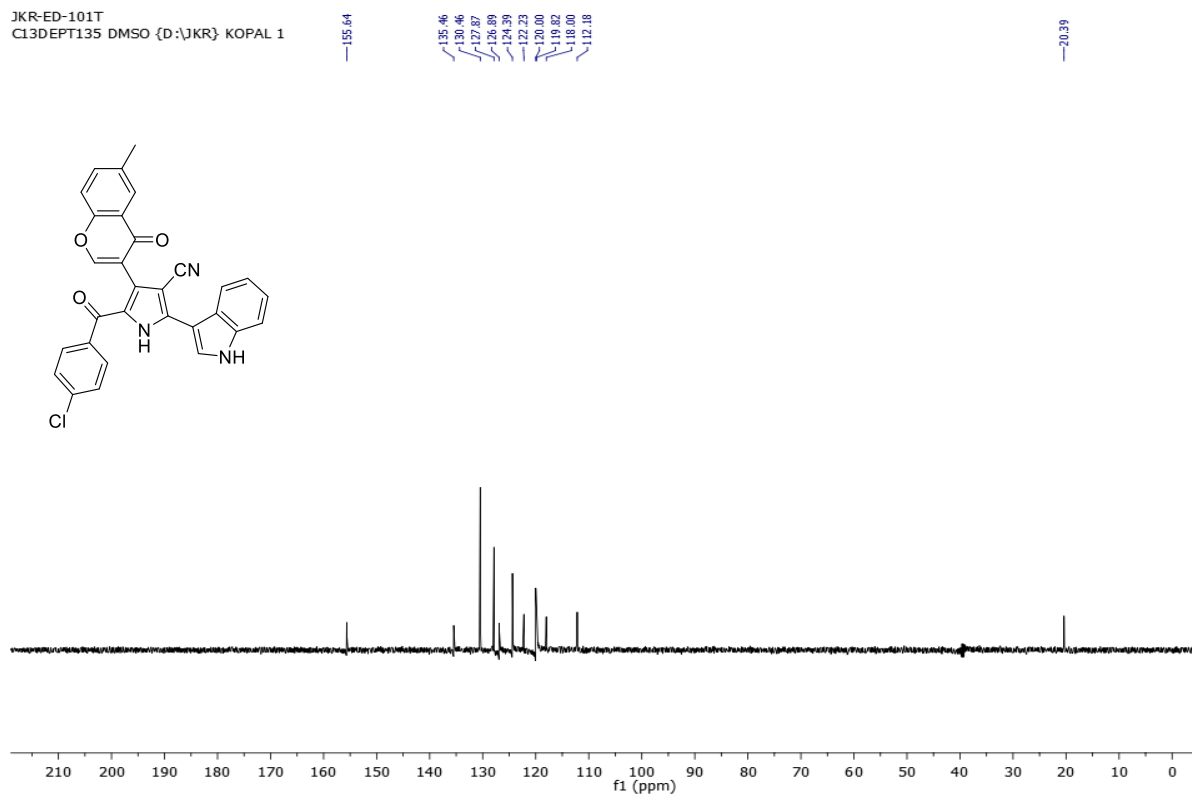


^1H NMR spectrum of **4o** (400 MHz, DMSO- d_6)



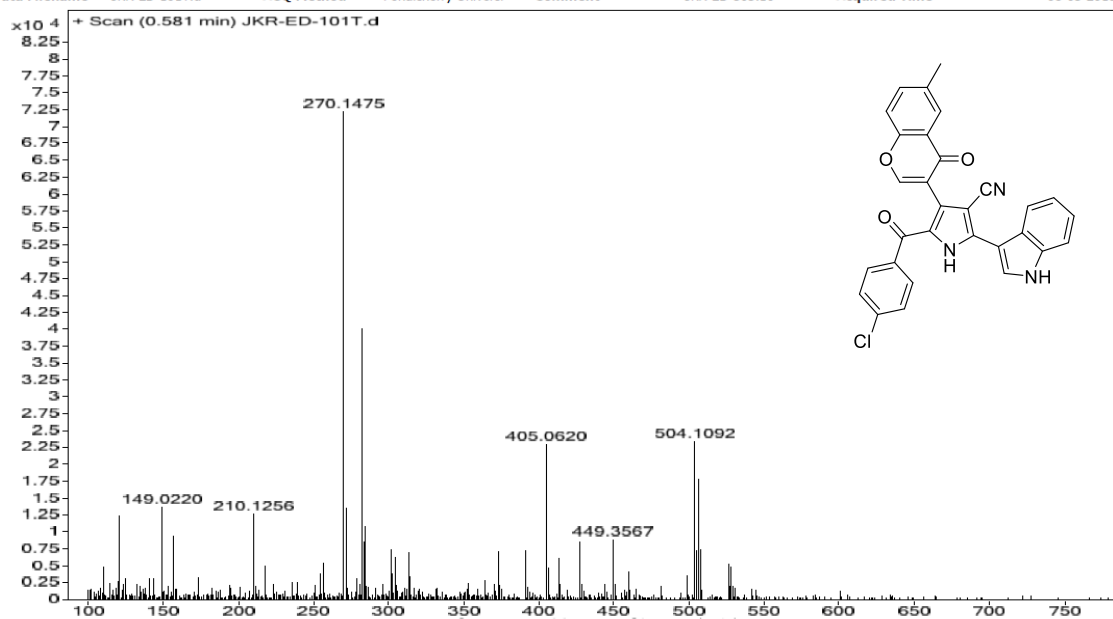
$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **4o** (100 MHz, DMSO- d_6)

JKR-ED-101T
C13DEPT135 DMSO {D:\JKR} KOPAL 1

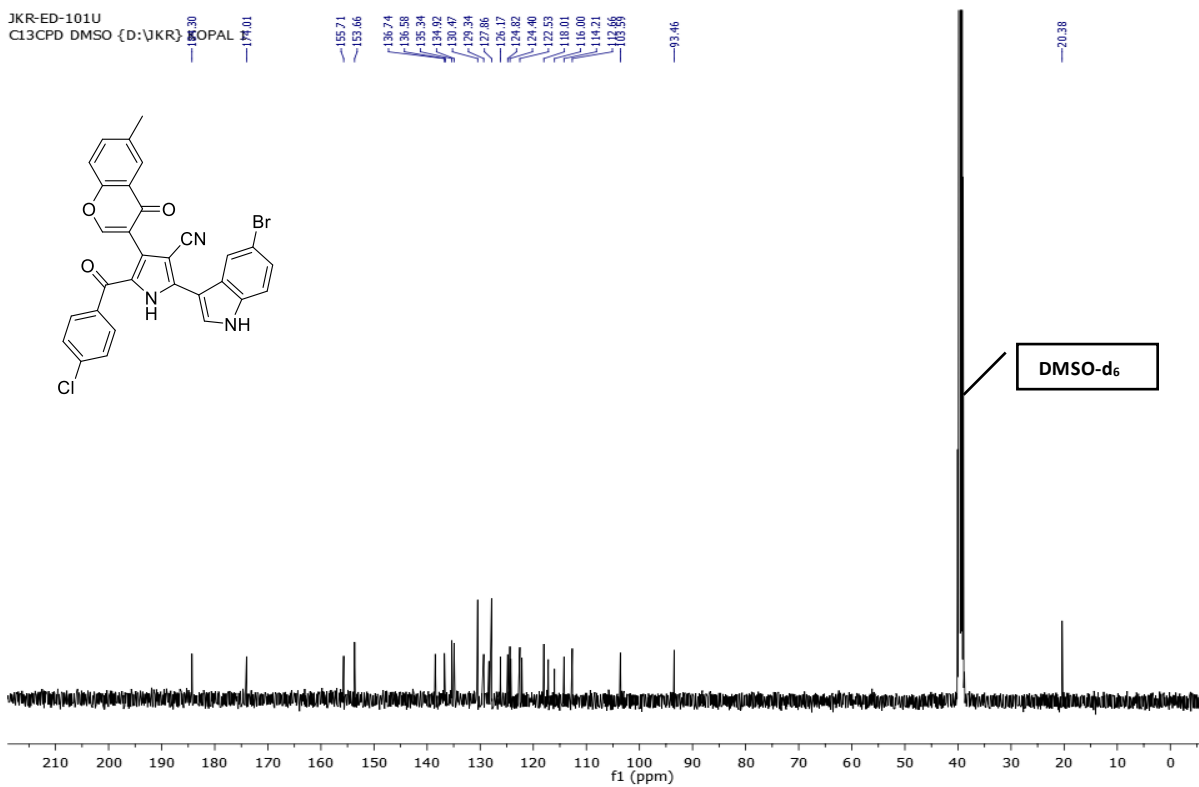
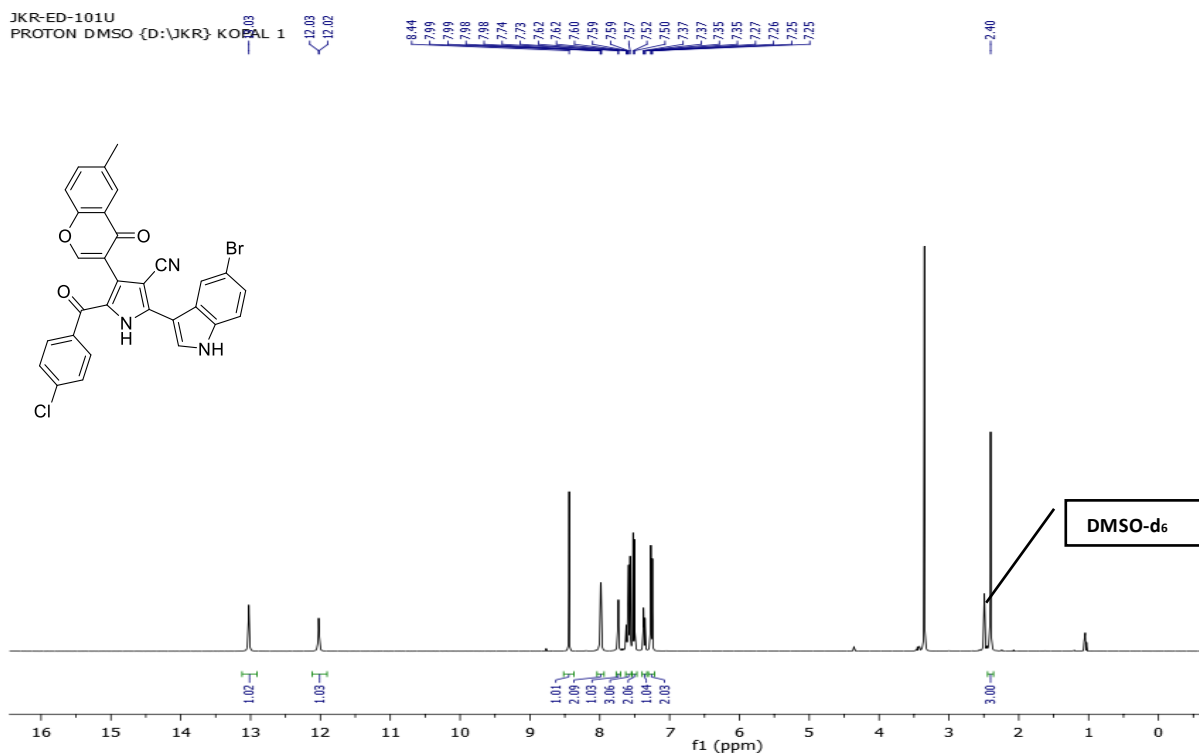


DEPT 135 NMR spectrum of **4o** (100 MHz, DMSO-*d*₆)

Sample Name	JKR-ED-101T	Position	Instrument Name	Q-TOF	User Name	QTOF-PU\admin
Inj Vol	-1	InjPosition	Sample	Sample	IRM Calibration Status	Success
Data Filename	JKR-ED-101T.d	ACQ Method	Comment	JKR-ED-503.10	Acquired Time	08-05-2018 15:14:14



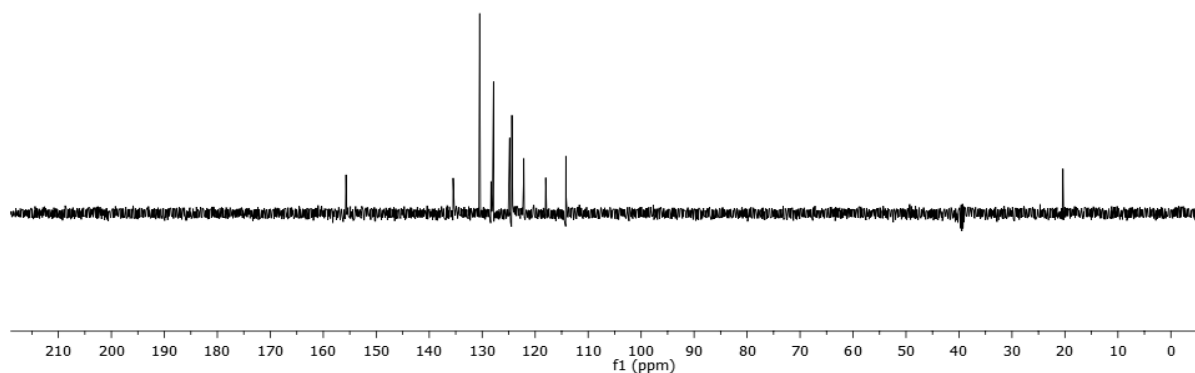
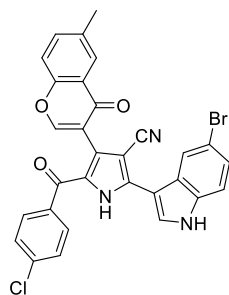
HRMS (ESI) spectrum of **4o**



JKR-ED-101U
CL3DEPT135 DMSO {D:\JKR} KOPAL 1

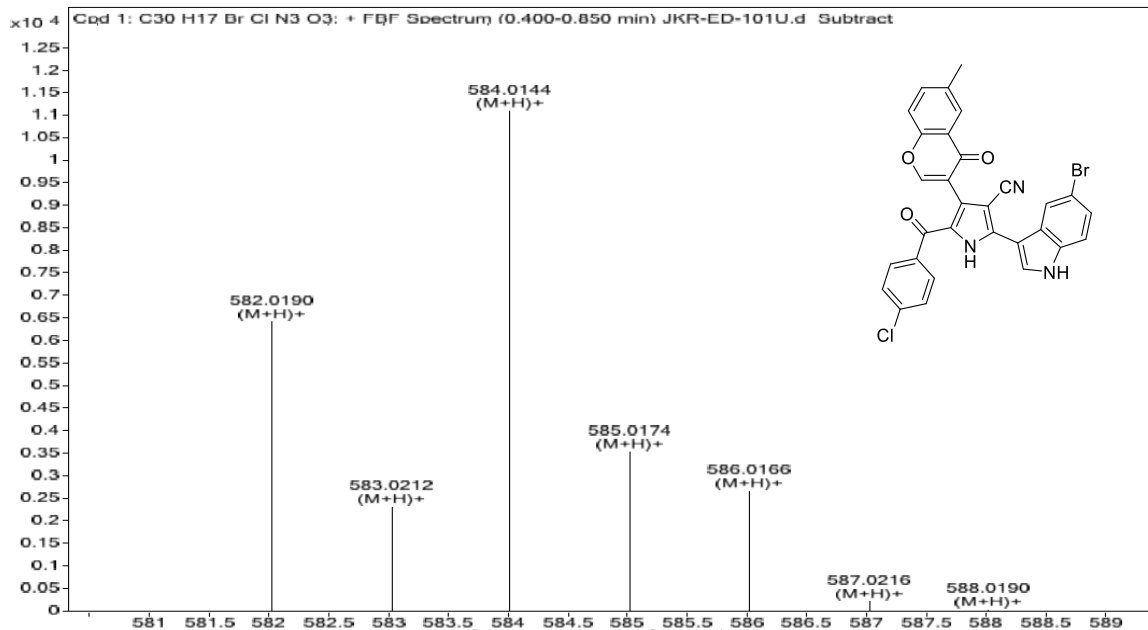
155.71

135.48
130.47
128.34
127.86
124.82
124.40
122.15
118.01
114.21

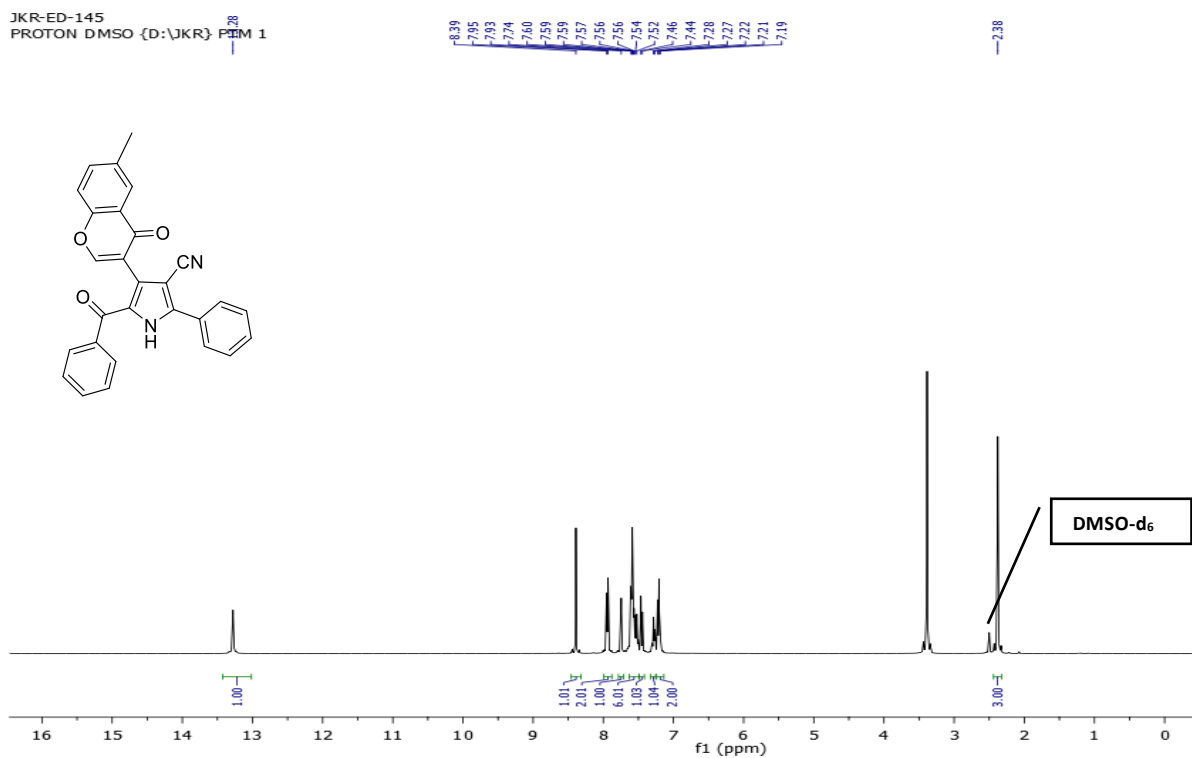


DEPT 135 NMR spectrum of **4p** (100 MHz, DMSO- d_6)

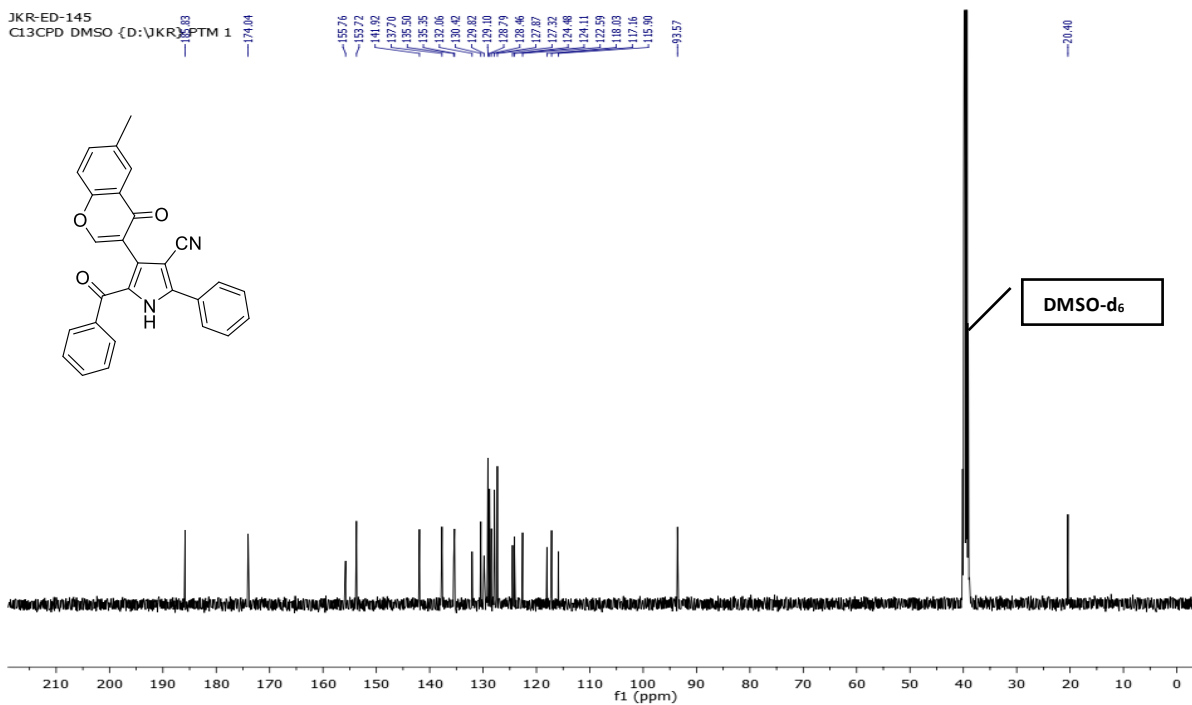
Sample Name	JKR-ED-101U	Position		Instrument Name	Q-TOF	User Name	QTOF-PU/admin
Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	JKR-ED-101U.d	ACQ Method	Pondicherry Universi	Comment	JKR-ED-581.01	Acquired Time	08-05-2018 15:03:07



HRMS (ESI) spectrum of **4p**

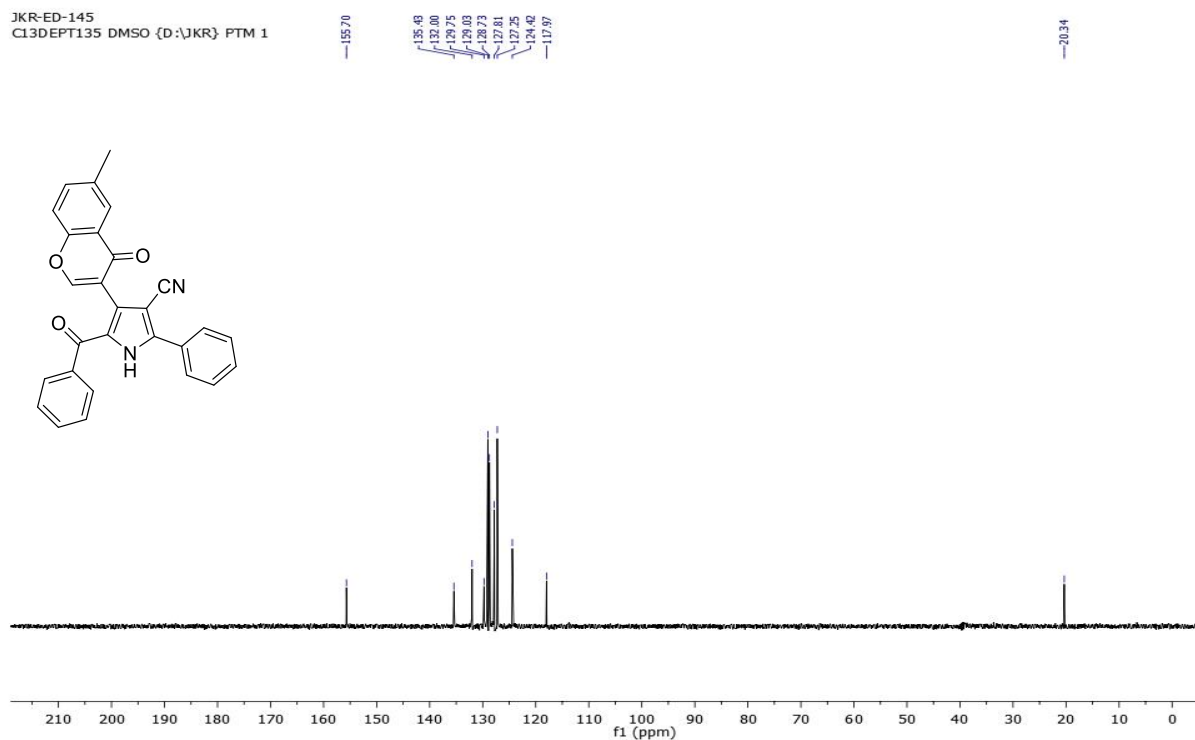


¹H NMR spectrum of **4q** (400 MHz, DMSO-*d*₆)



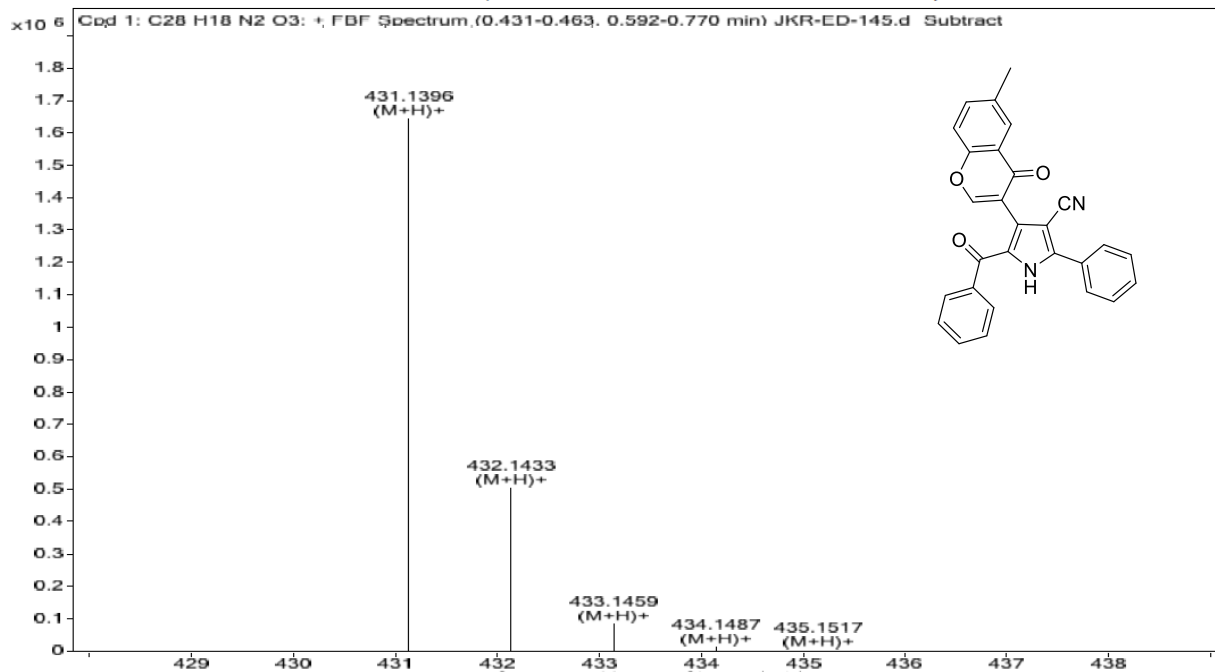
¹³C {¹H} NMR spectrum of **4q** (100 MHz, DMSO-*d*₆)

JKR-ED-145
C13DEPT135 DMSO {D:\JKR} PTM 1

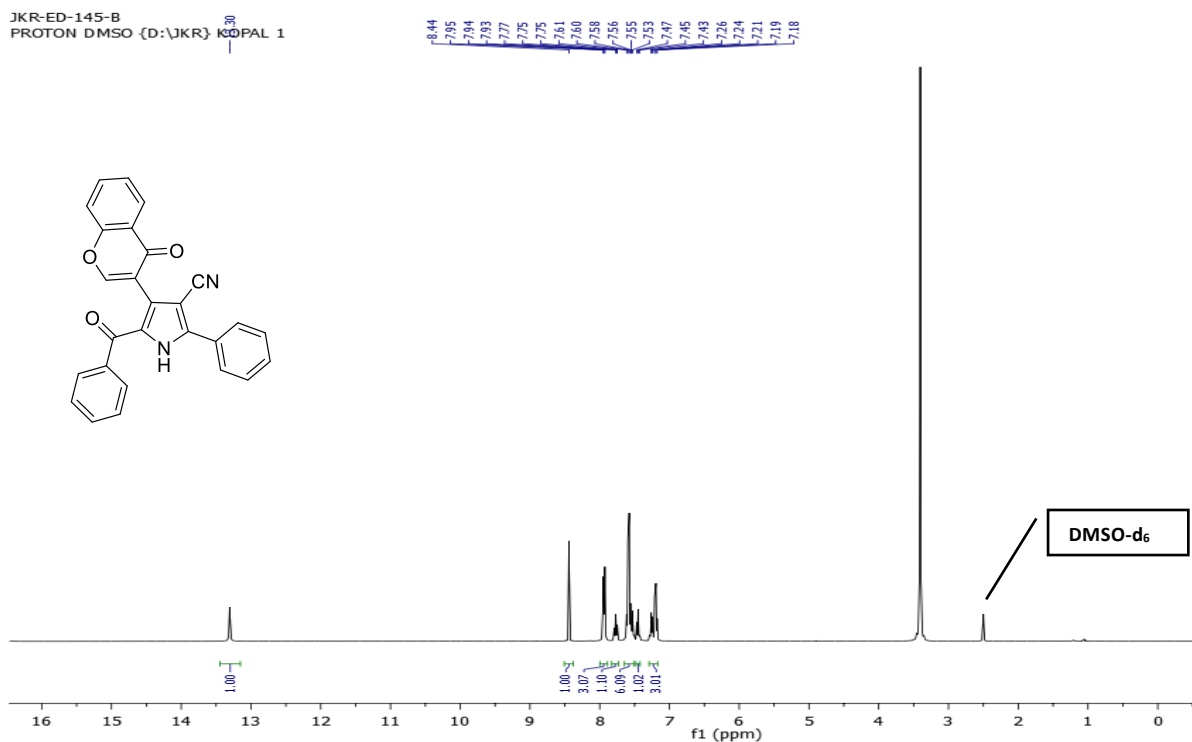


DEPT 135 NMR spectrum of **4q** (100 MHz, DMSO-*d*₆)

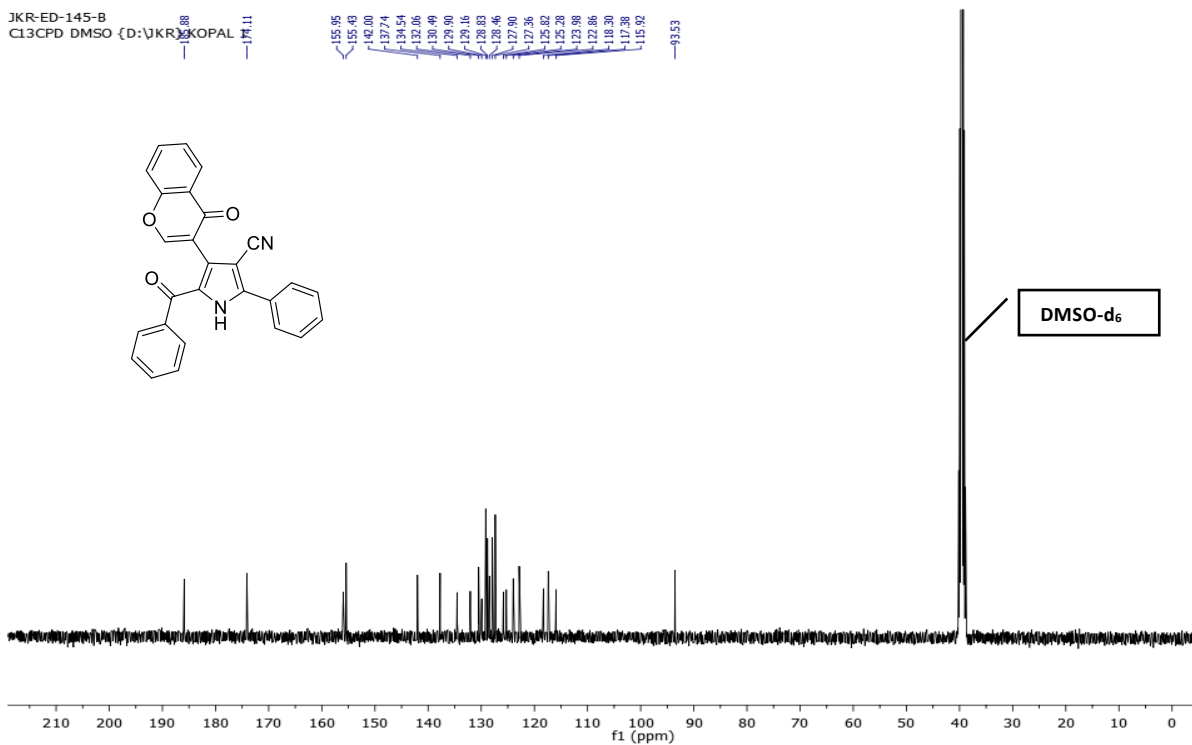
Sample Name	JKR-ED-145	Position		Instrument Name	Q-TOF	User Name	QTOF-PU\admin
Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	JKR-ED-145.d	ACQ Method	Pondicherry Universi	Comment	ED-JKR-430.1317	Acquired Time	14-08-2018 12:33:06



HRMS (ESI) spectrum of **4q**

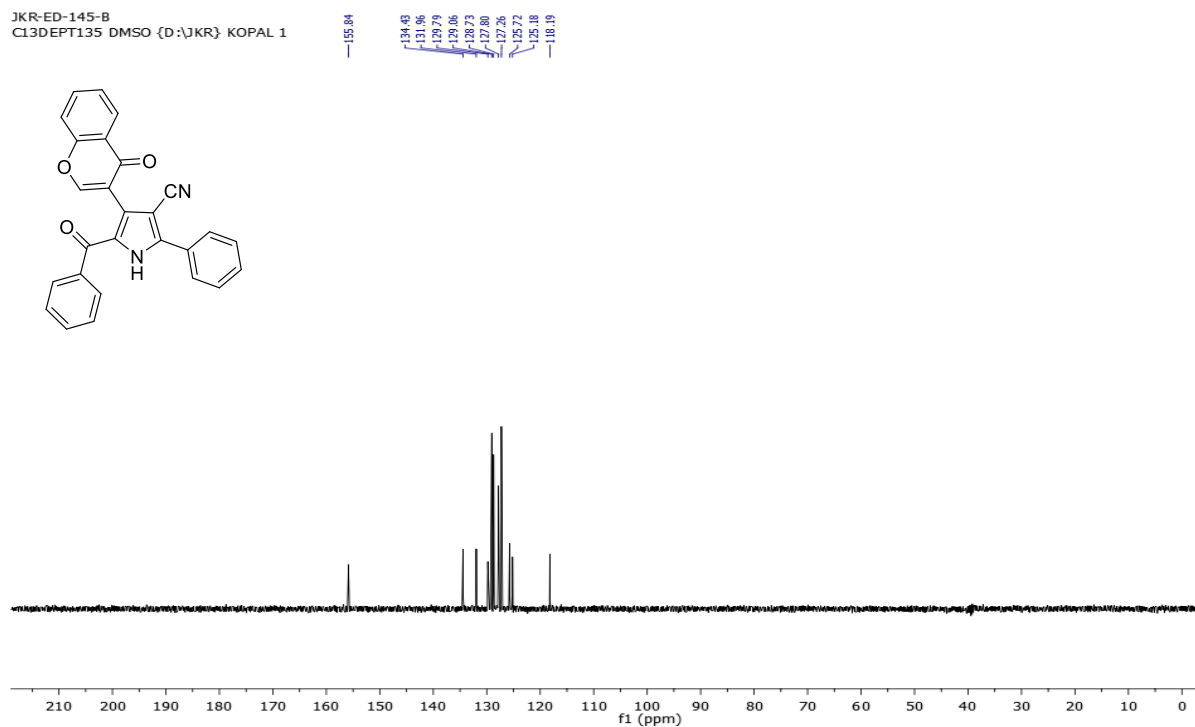


¹H NMR spectrum of **4r** (400 MHz, DMSO-*d*₆)



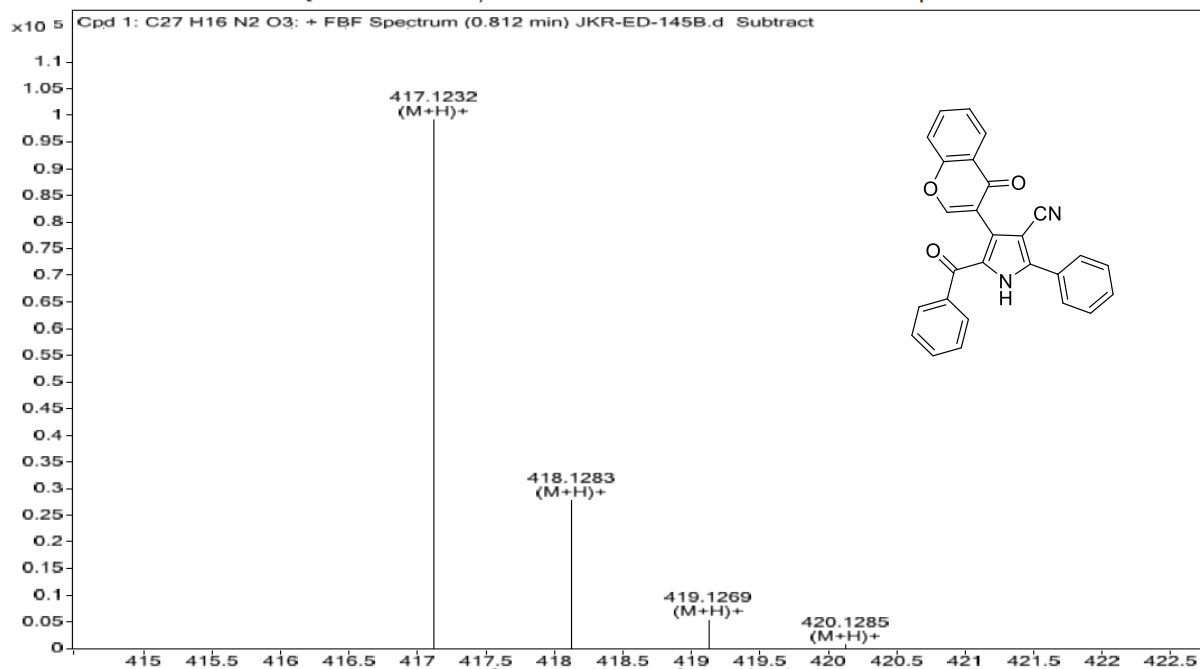
¹³C{¹H} NMR spectrum of **4r** (100 MHz, DMSO-*d*₆)

JKR-ED-145-B
C13DEPT135 DMSO (D-;JKR) KOPAL 1

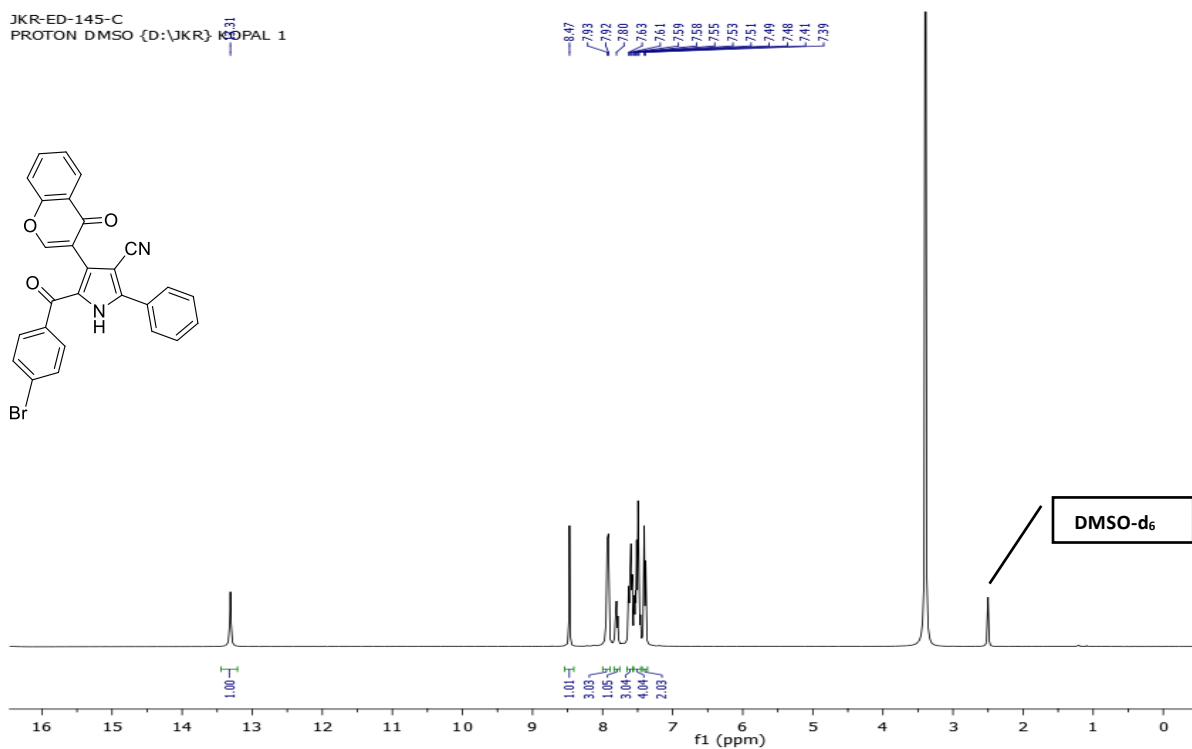


DEPT 135 NMR spectrum of **4r** (100 MHz, DMSO- d_6)

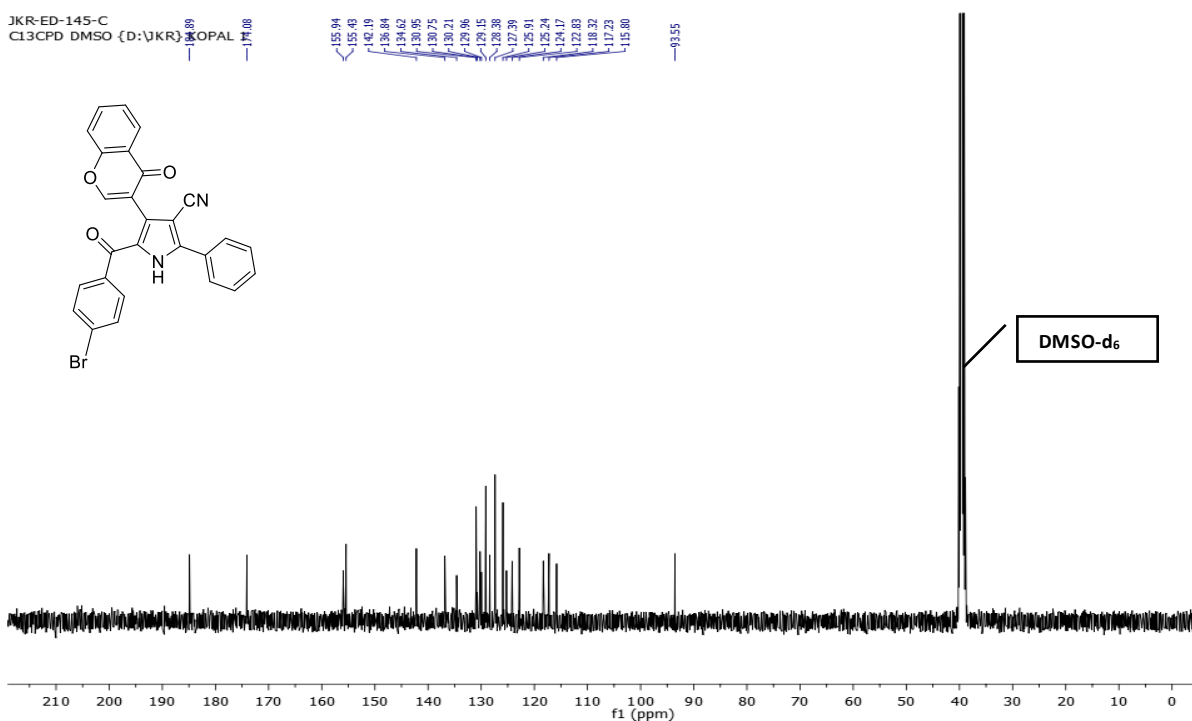
Sample Name	Position	Instrument Name	User Name
JKR-ED-145B	-1	Q-TOF	QTOF-PU\admin
Inj Vol	JKR-ED-145B.d	Sample	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time
	Pondicherry Universi	ED-JKR-416.1161	Success
			10-09-2018 12:43:22



HRMS (ESI) spectrum of **4r**

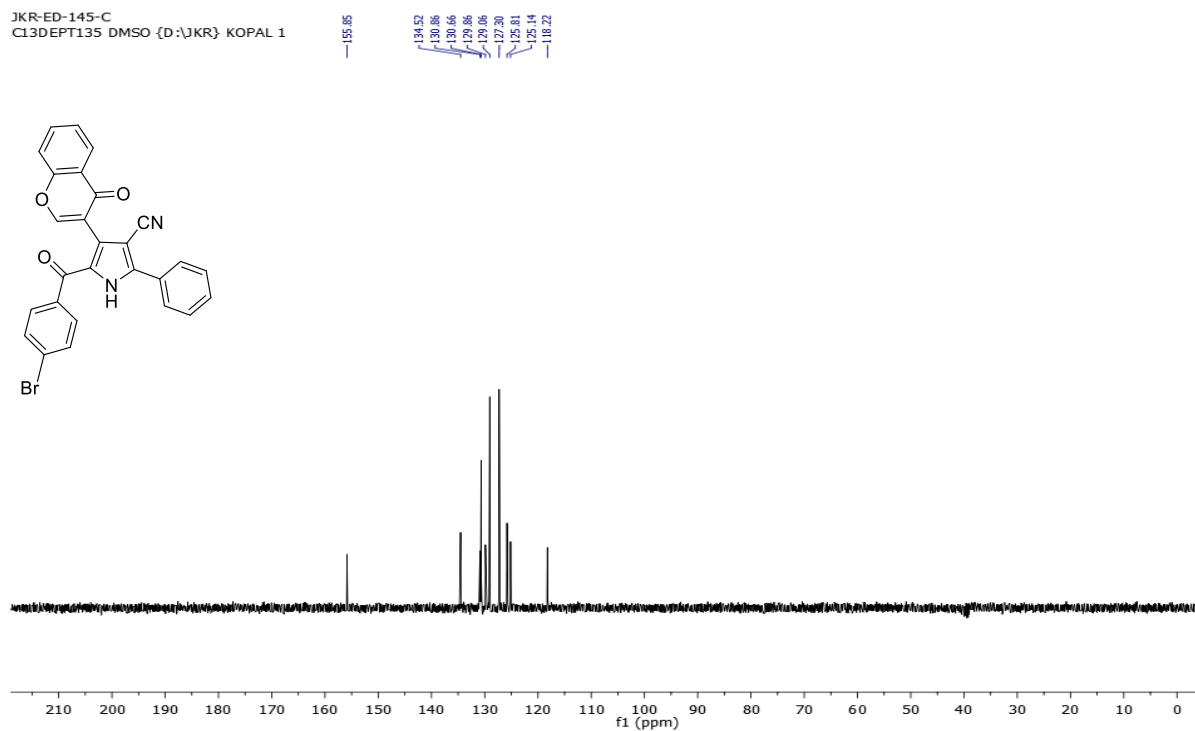


¹H NMR spectrum of **4s** (400 MHz, DMSO-*d*₆)



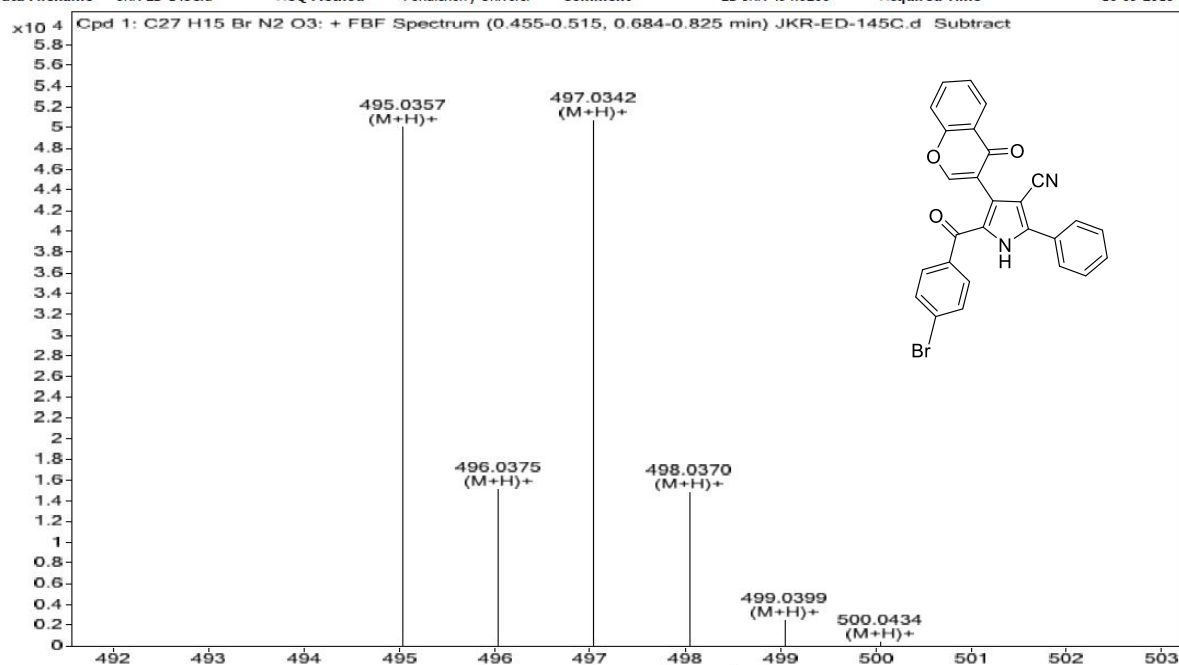
¹³C{¹H} NMR spectrum of **4s** (100 MHz, DMSO-*d*₆)

JKR-ED-145-C
C13DEPT135 DMSO (D:\JKR) KOPAL 1

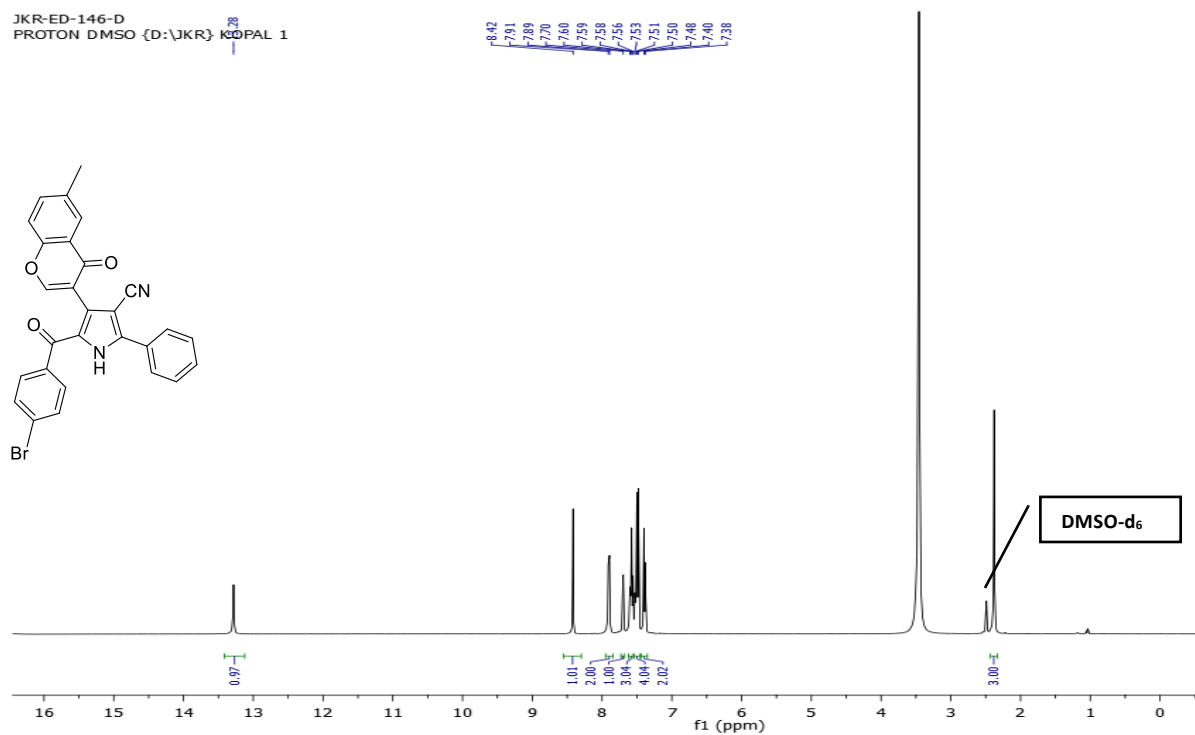


DEPT 135 NMR spectrum of **4s** (100 MHz, DMSO-*d*₆)

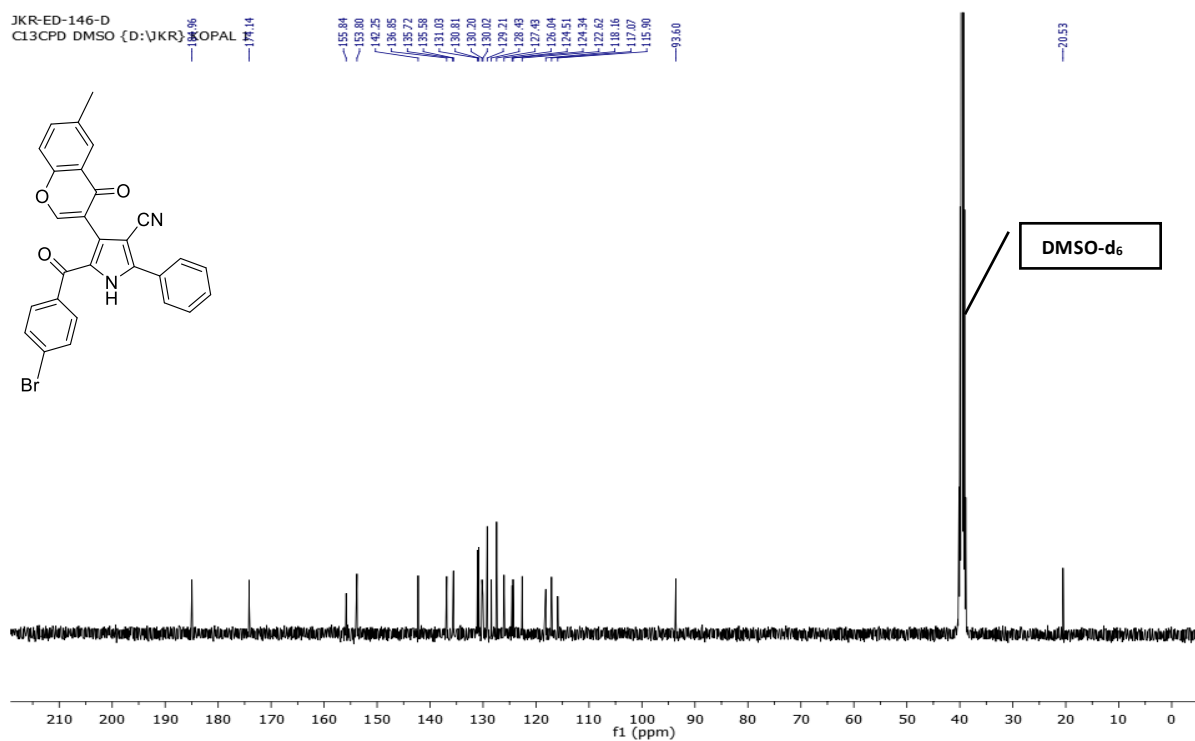
Sample Name	JKR-ED-145C	Position		Instrument Name	Q-TOF	User Name	QTOF-PU/admin
Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	JKR-ED-145C.d	ACQ Method	Pondicherry Universi	Comment	ED-JKR-494.0266	Acquired Time	10-09-2018 12:36:56



HRMS (ESI) spectrum of **4s**

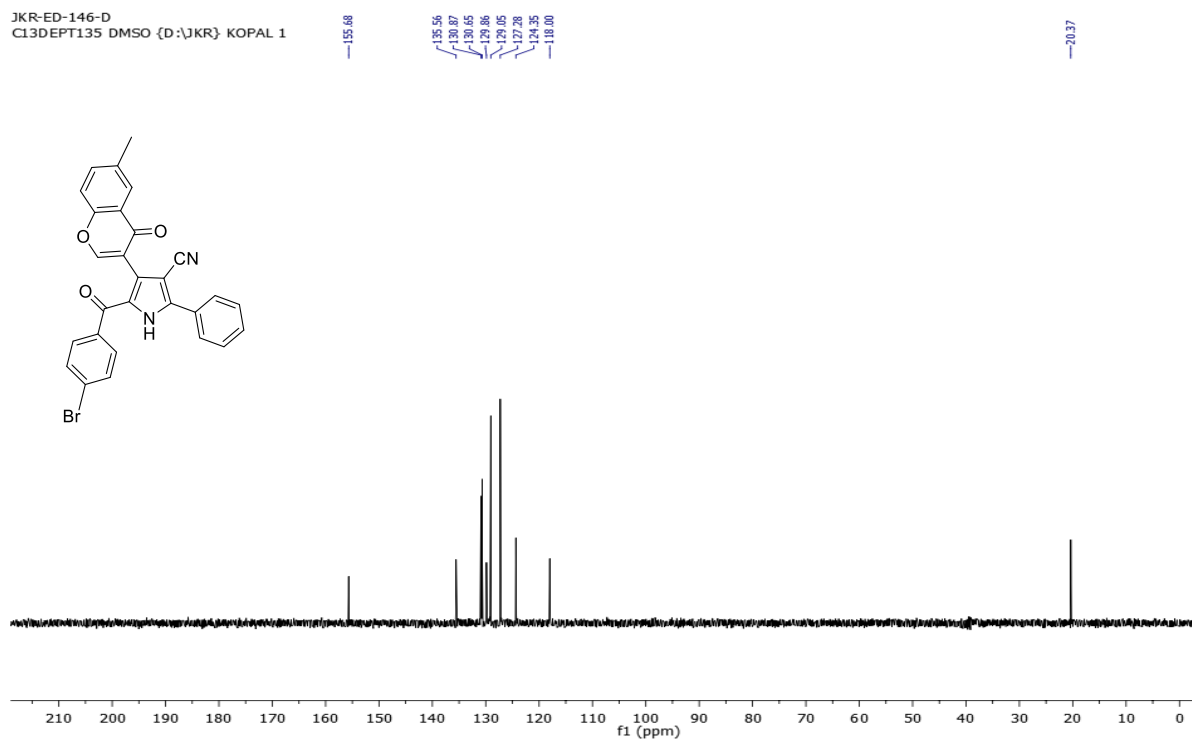


^1H NMR spectrum of **4t** (400 MHz, DMSO- d_6)

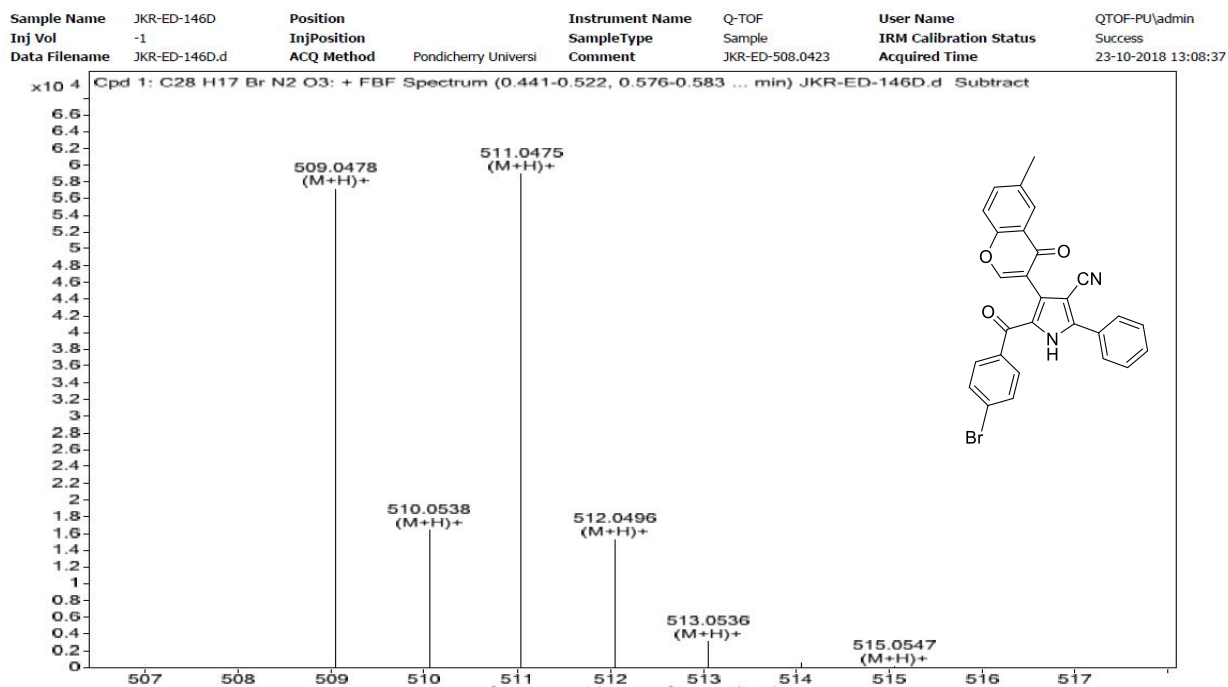


$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **4t** (100 MHz, DMSO- d_6)

JKR-ED-146-D
C13DEPT135 DMSO {D:\JKR\ KOPAL 1

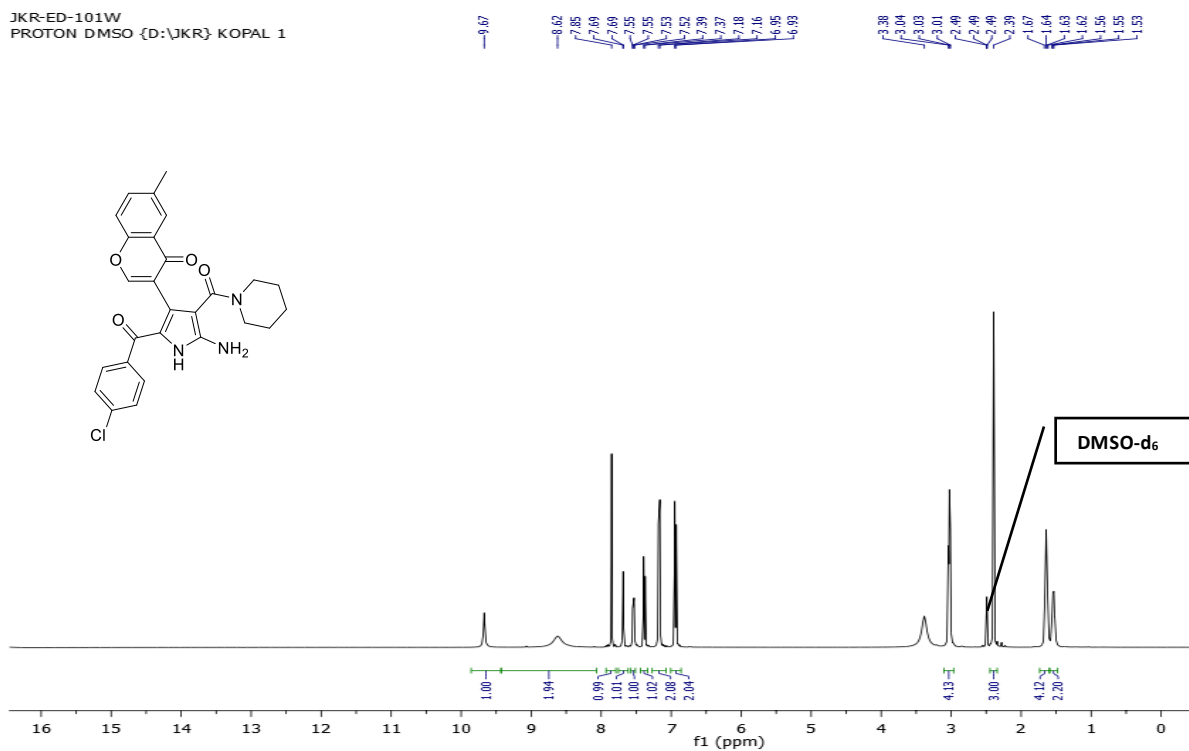


DEPT 135 NMR spectrum of **4t** (100 MHz, DMSO-*d*₆)

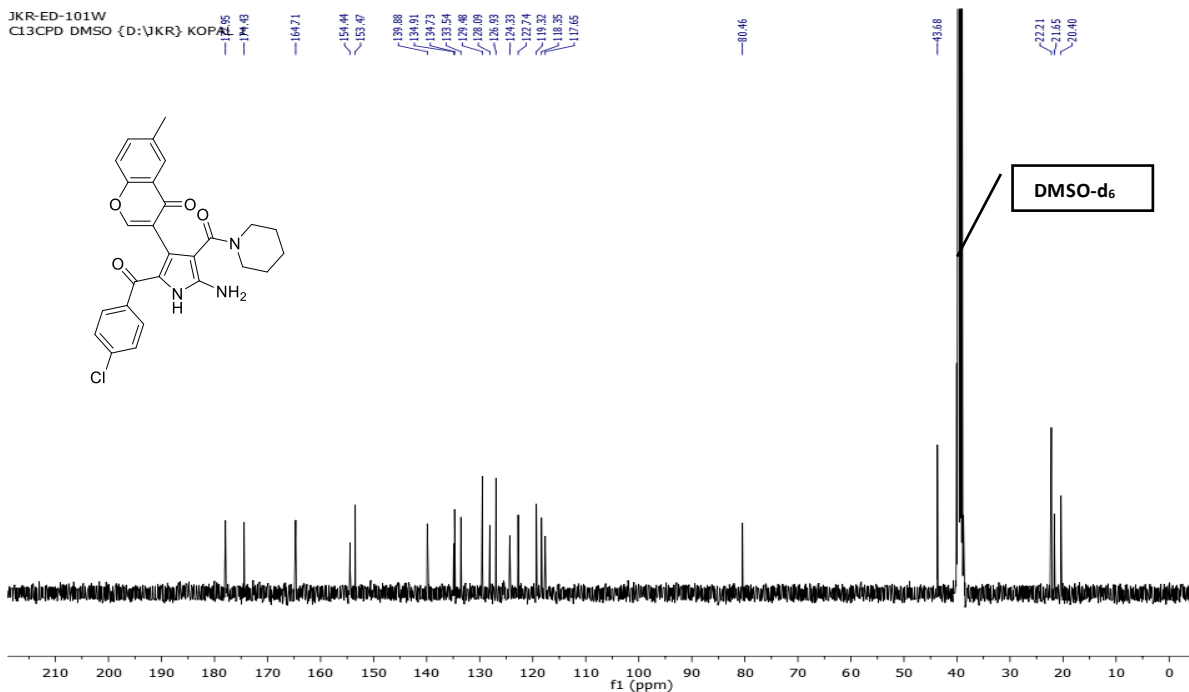


HRMS (ESI) spectrum of **4t**

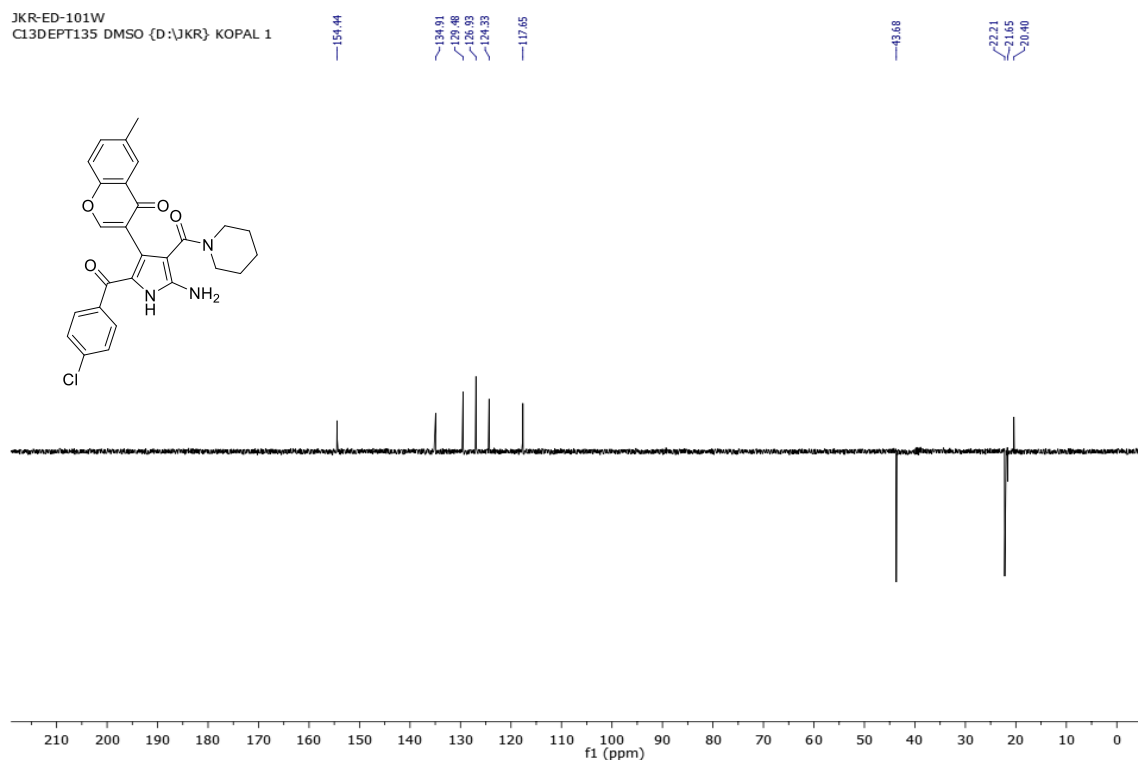
JKR-ED-101W
PROTON DMSO {D:\JKR} KOPAL 1



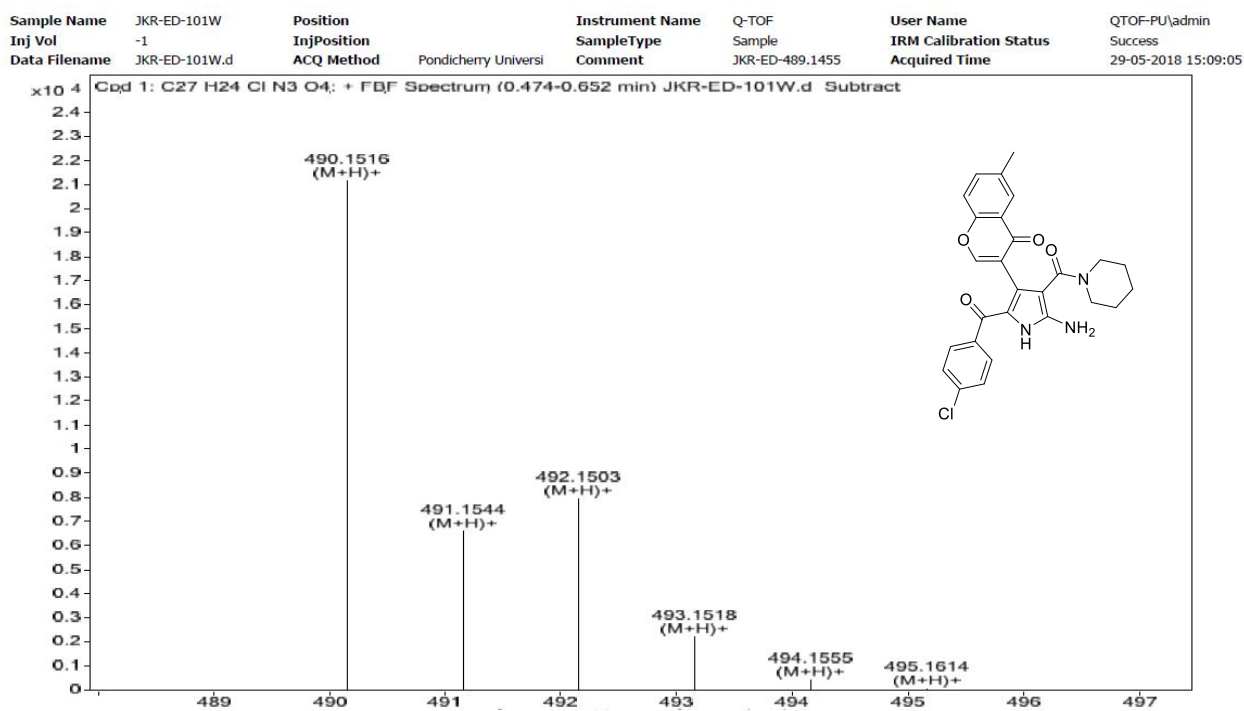
¹H NMR spectrum of **8a** (400 MHz, DMSO-*d*₆)



¹³C{¹H} NMR spectrum of **8a** (100 MHz, DMSO-*d*₆)

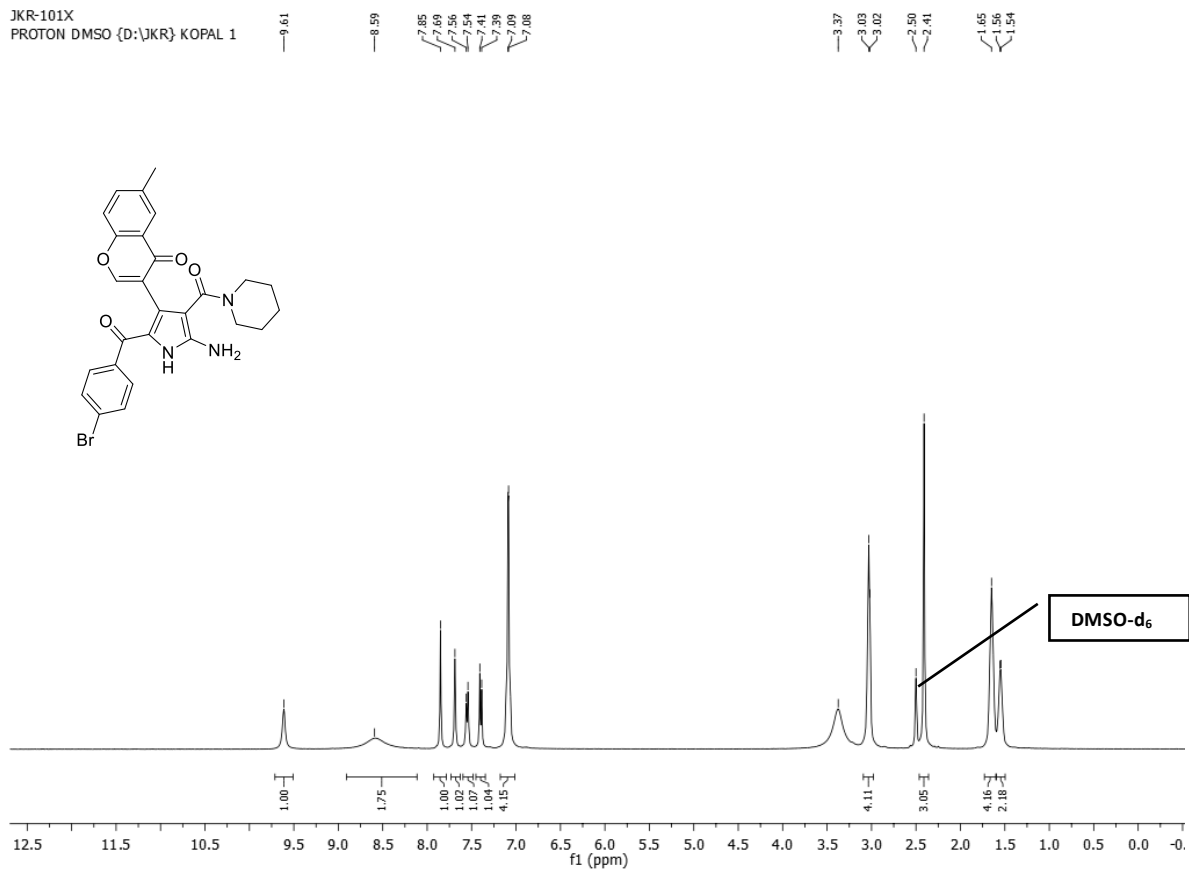


DEPT 135 NMR spectrum of **8a** (100 MHz, DMSO- d_6)

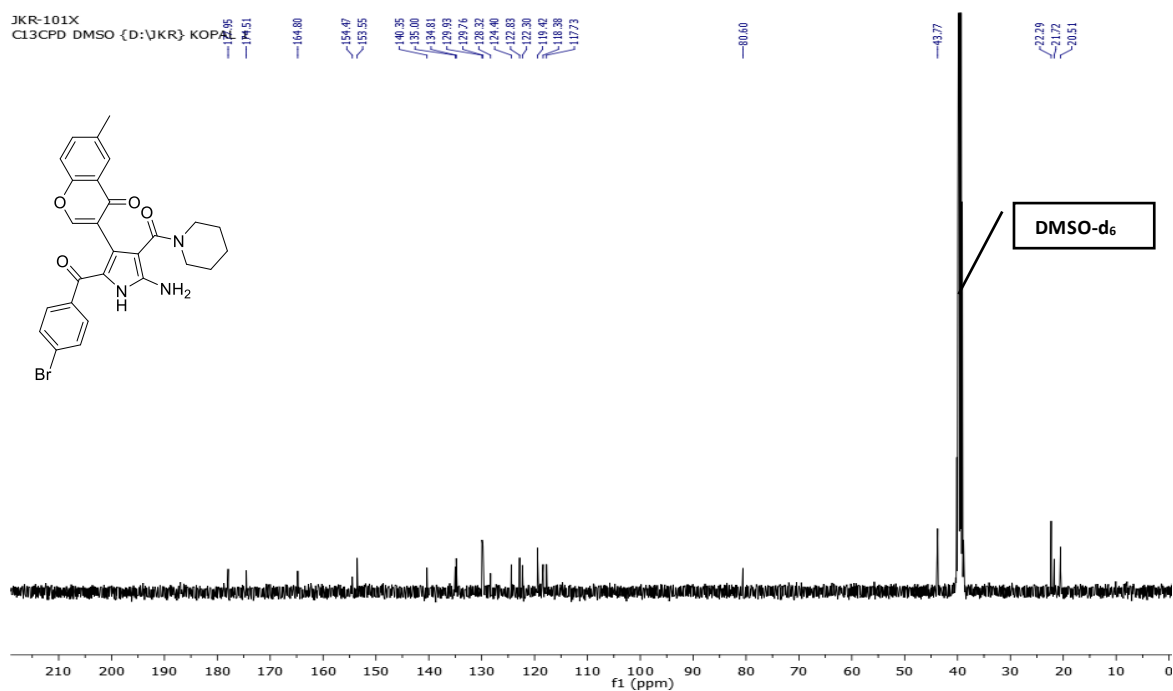


HRMS (ESI) spectrum of **8a**

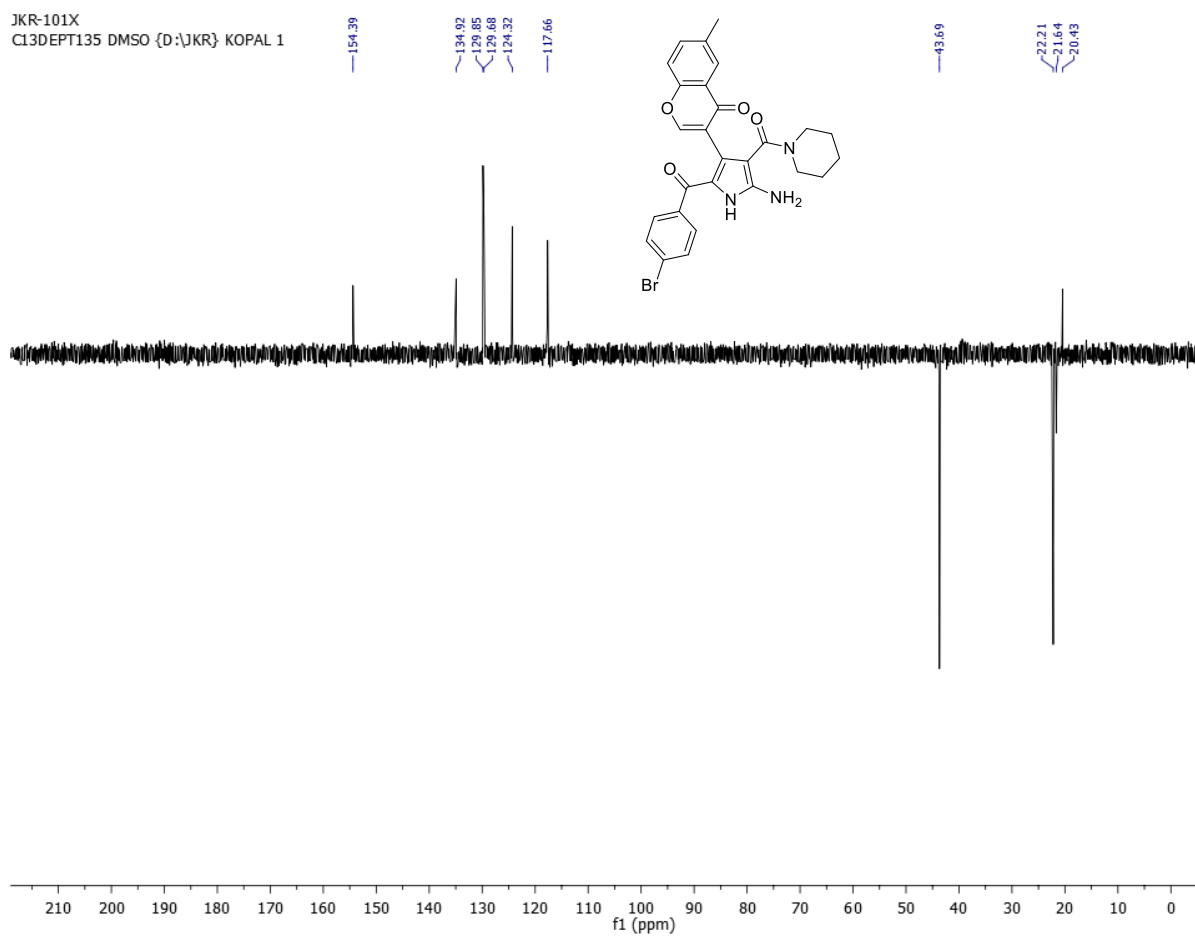
JKR-101X
PROTON DMSO {D:\JKR} KOPAL 1



¹H NMR spectrum of **8b** (400 MHz, DMSO-d₆)

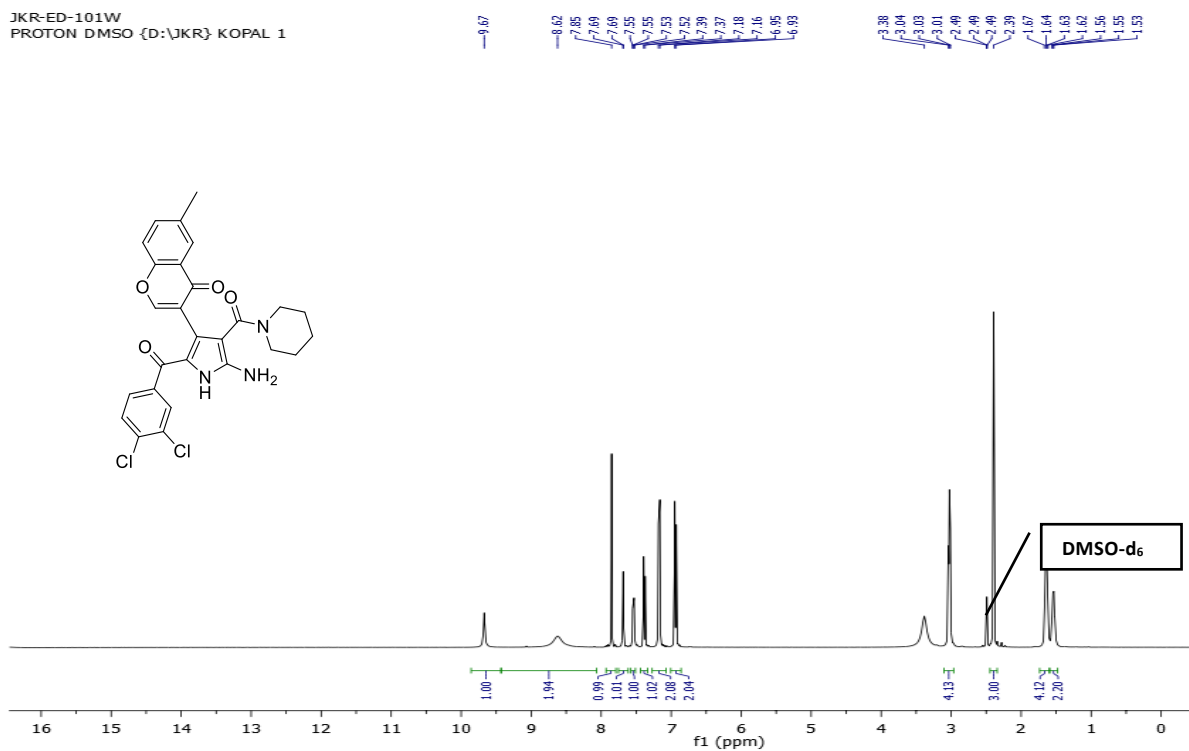


¹³C{¹H} NMR spectrum of **8b** (100 MHz, DMSO-d₆)



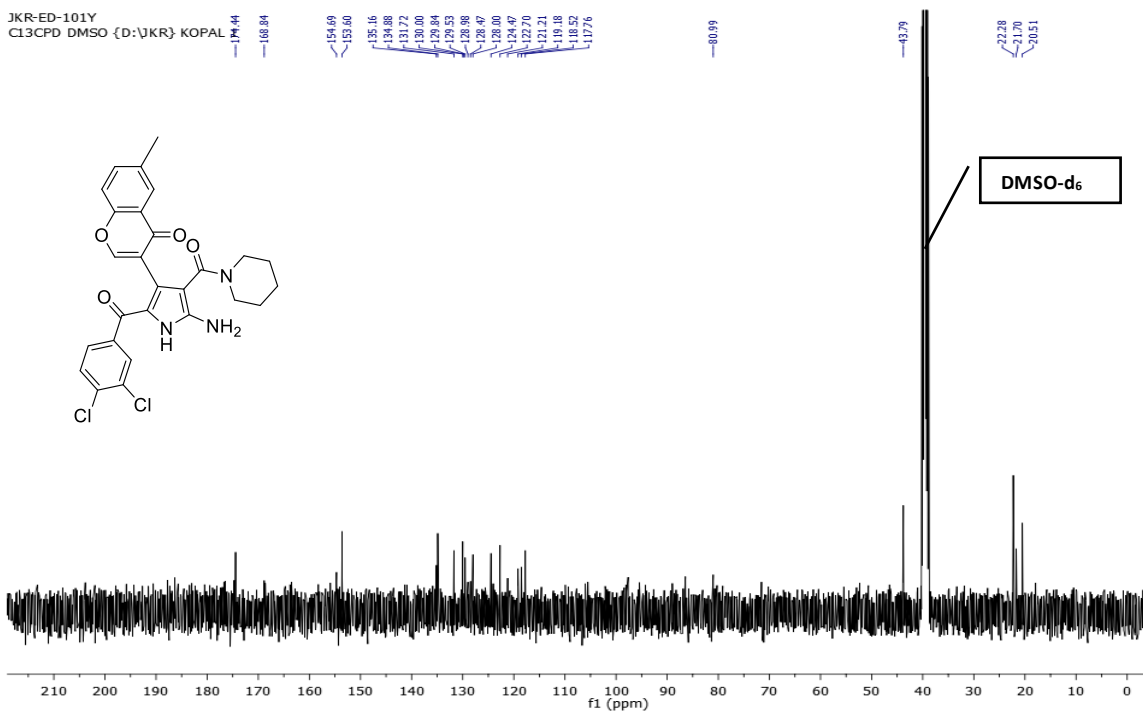
DEPT 135 NMR spectrum of **8b** (100 MHz, DMSO-*d*₆)

JKR-ED-101W
PROTON DMSO {D:\JKR} KOPAL 1



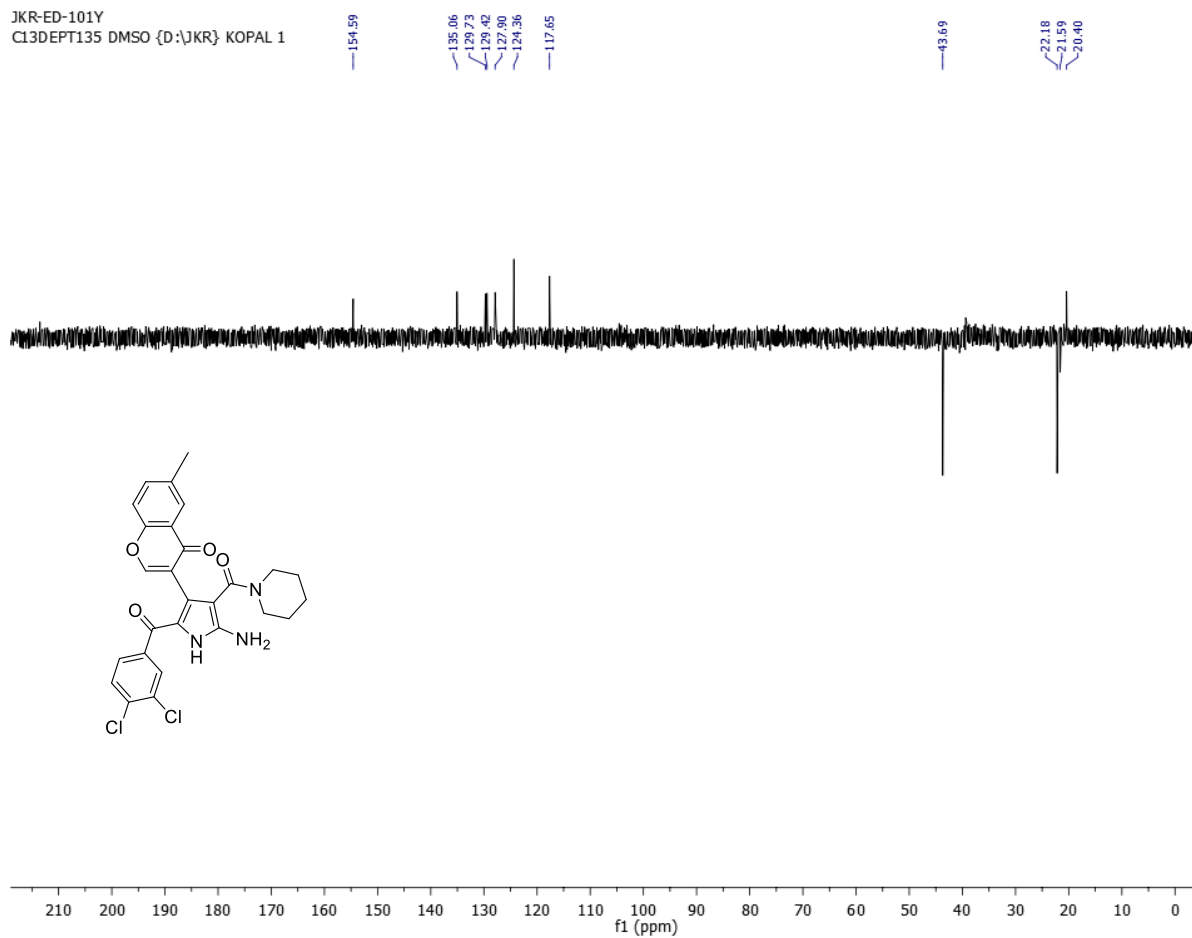
¹H NMR spectrum of **8c** (400 MHz, DMSO-*d*₆)

JKR-ED-101Y
C13CPD DMSO {D:\JKR} KOPAL



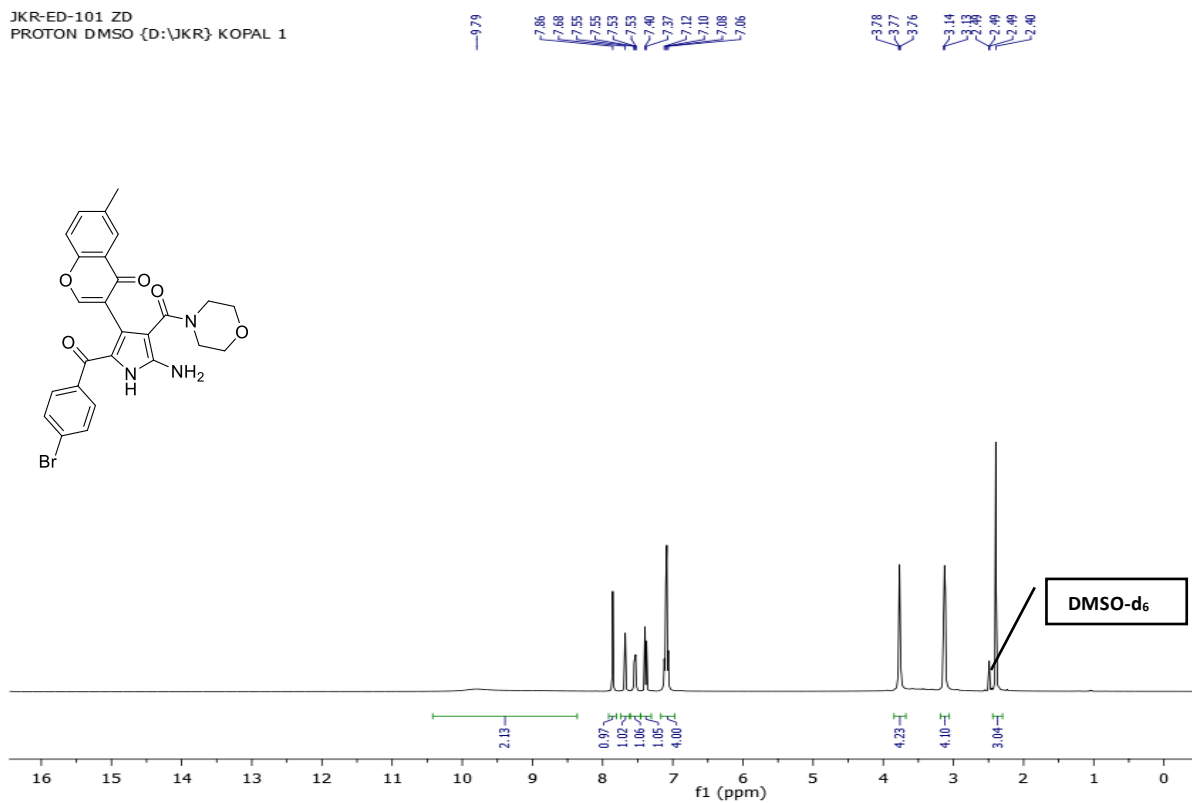
¹³C{¹H} NMR spectrum of **8c** (100 MHz, DMSO-*d*₆)

JKR-ED-101Y
C13DEPT135 DMSO {D:\JKR} KOPAL 1

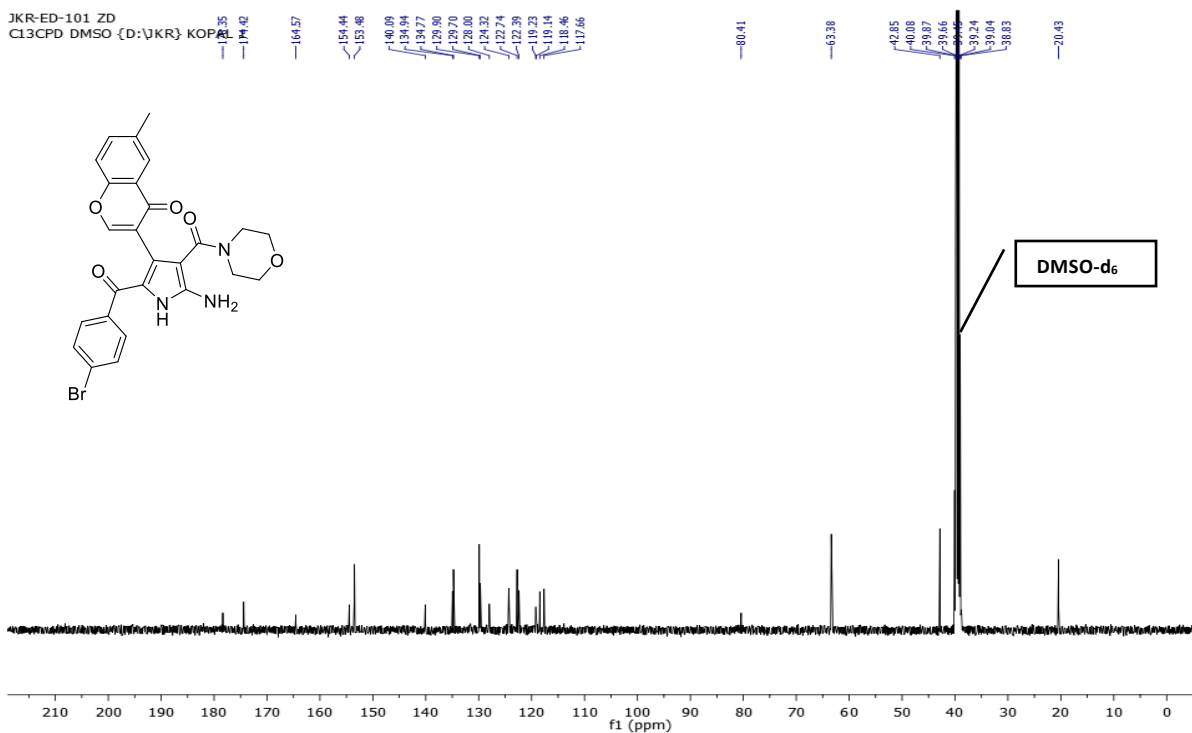


DEPT 135 NMR spectrum of **8c** (100 MHz, DMSO-*d*₆)

JKR-ED-101 ZD
PROTON DMSO {D:\JKR} KOPAL 1

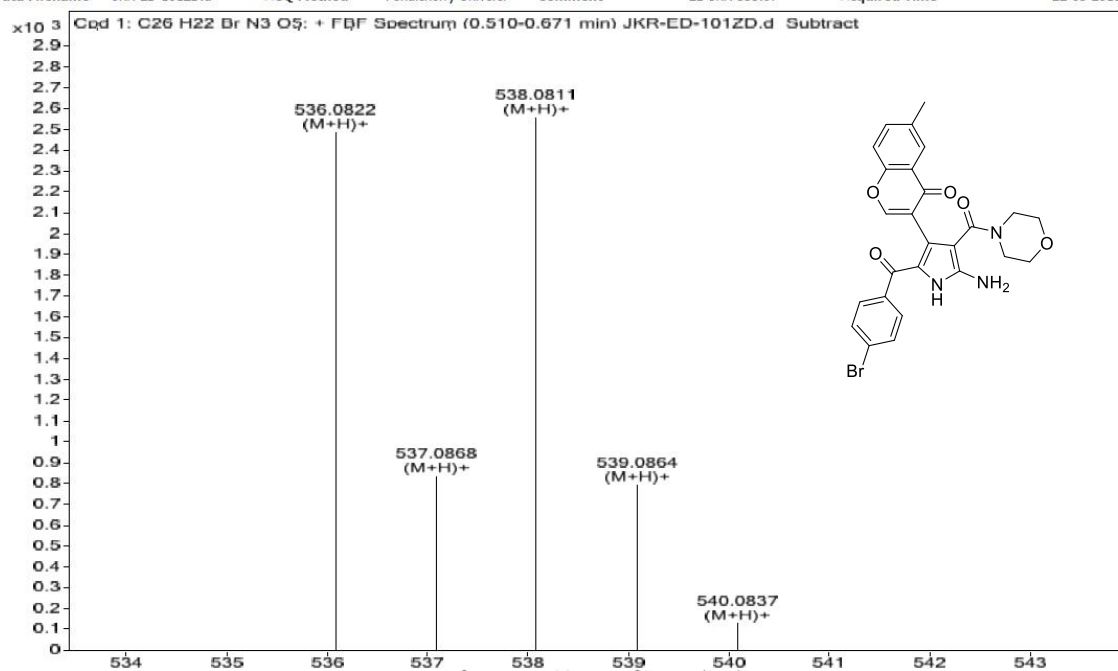


¹H NMR spectrum of **8d** (400 MHz, DMSO-*d*₆)



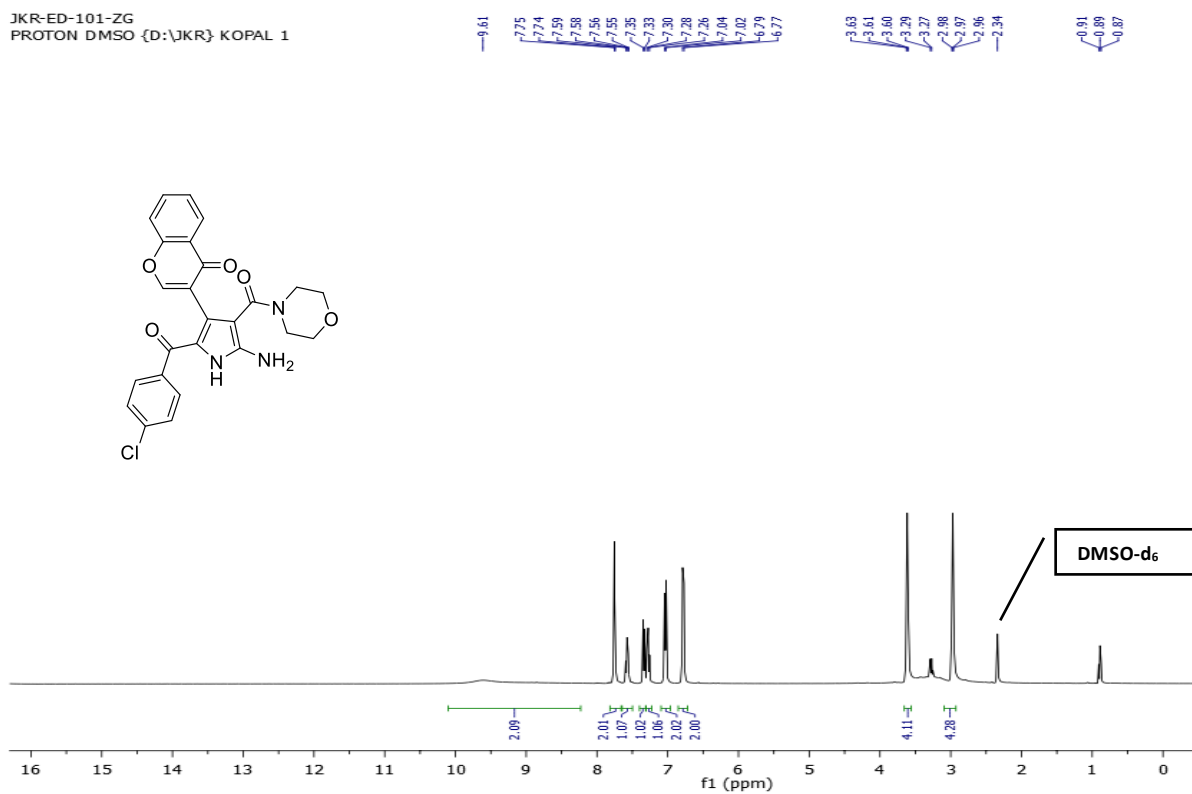
¹³C{¹H} NMR spectrum of **8d** (100 MHz, DMSO-*d*₆)

Sample Name	JKR-ED-101ZD	Position		Instrument Name	Q-TOF	User Name	QTOF-PU\admin
Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	JKR-ED-101ZD.d	ACQ Method	Pondicherry Universi	Comment	ED-JKR-535.07	Acquired Time	22-05-2018 14:14:52

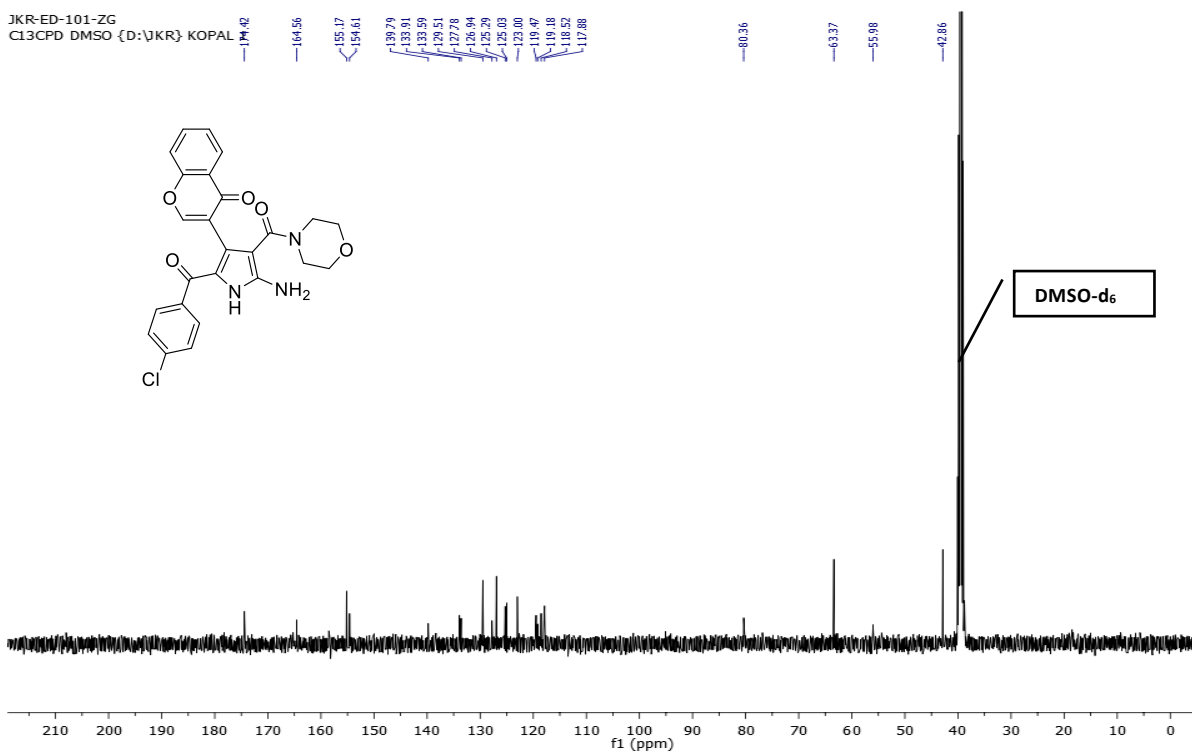


HRMS (ESI) spectrum of **8d**

JKR-ED-101-ZG
PROTON DMSO {D:\JKR} KOPAL 1

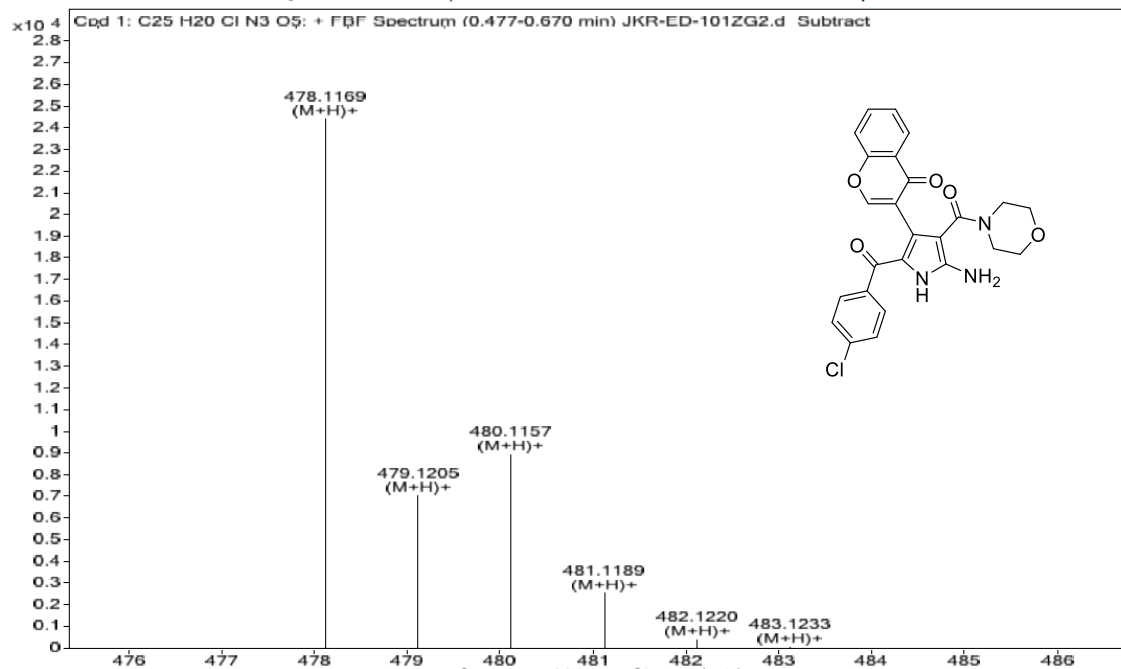


¹H NMR spectrum of **8e** (400 MHz, DMSO-*d*₆)



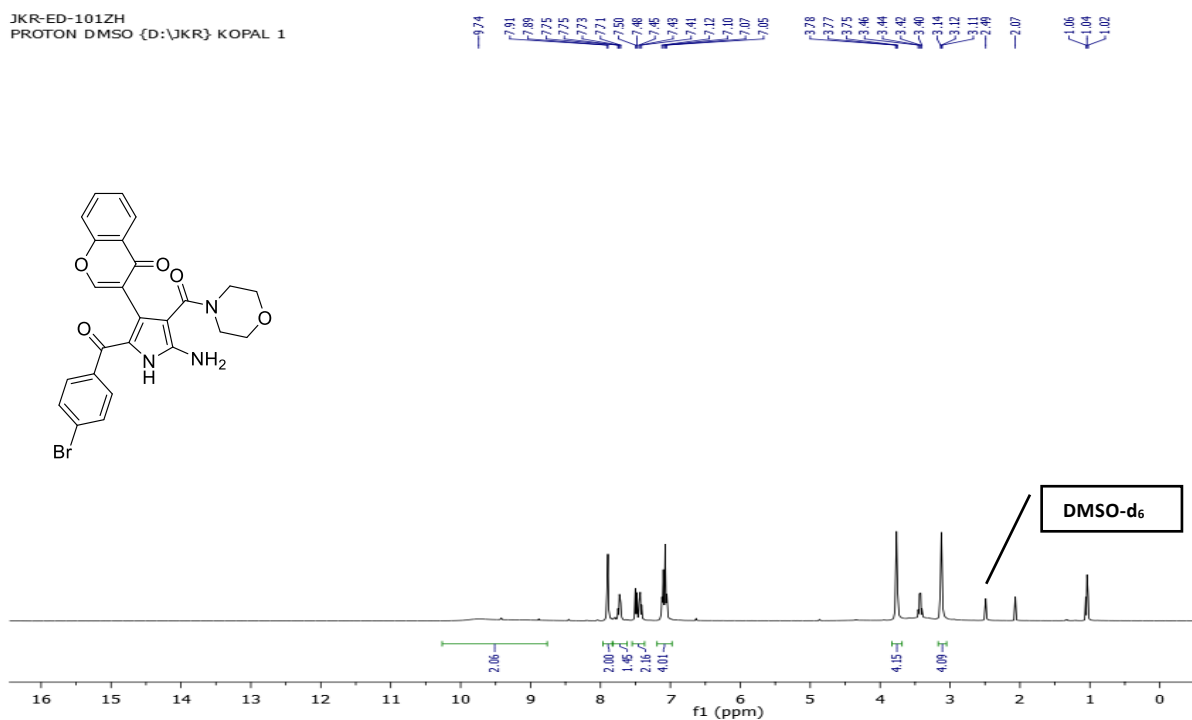
¹³C{¹H} NMR spectrum of **8e** (100 MHz, DMSO-*d*₆)

Sample Name	JKR-ED-101ZG	Position		Instrument Name	Q-TOF	User Name	QTOF-PU\admin
Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	JKR-ED-101ZG2.d	ACQ Method	Pondicherry Universi	Comment	ED-JKR-477.1091	Acquired Time	23-05-2018 12:29:19

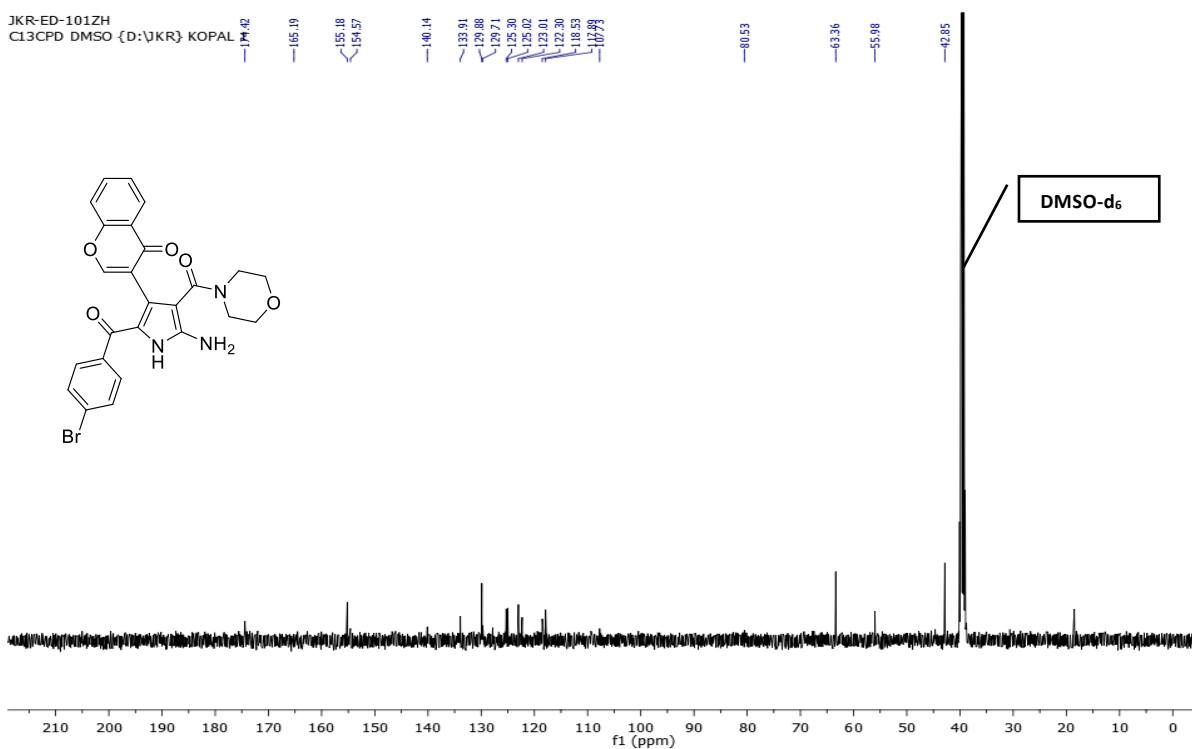


HRMS (ESI) spectrum of **8e**

JKR-ED-101ZH
PROTON DMSO {D:\JKR} KOPAL 1

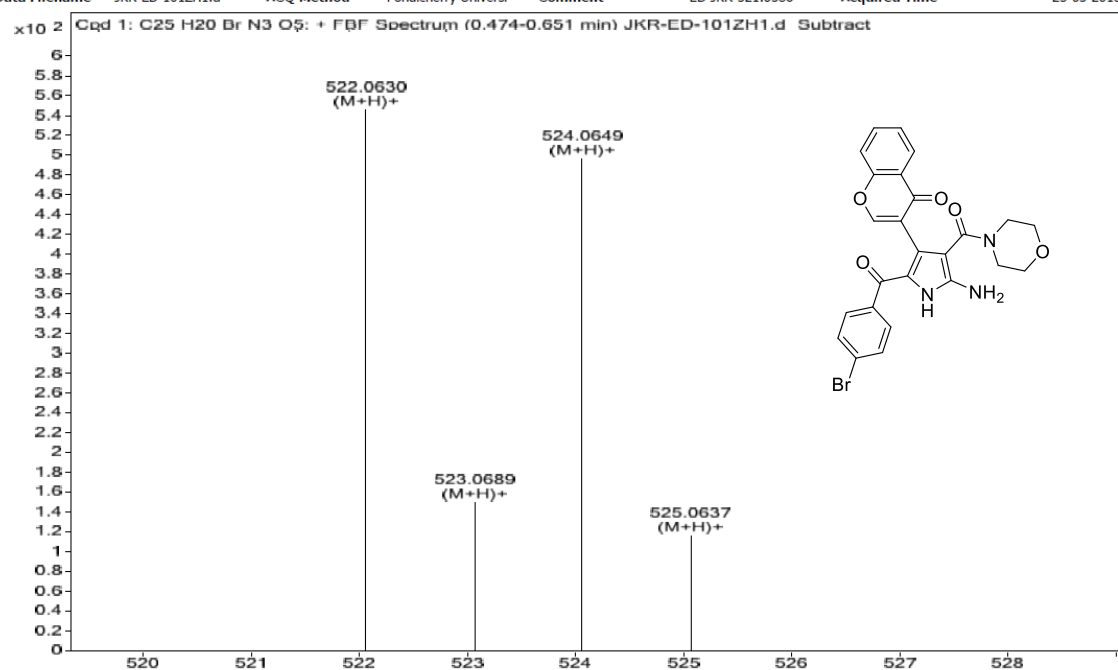


¹H NMR spectrum of **8f** (400 MHz, DMSO-*d*₆)

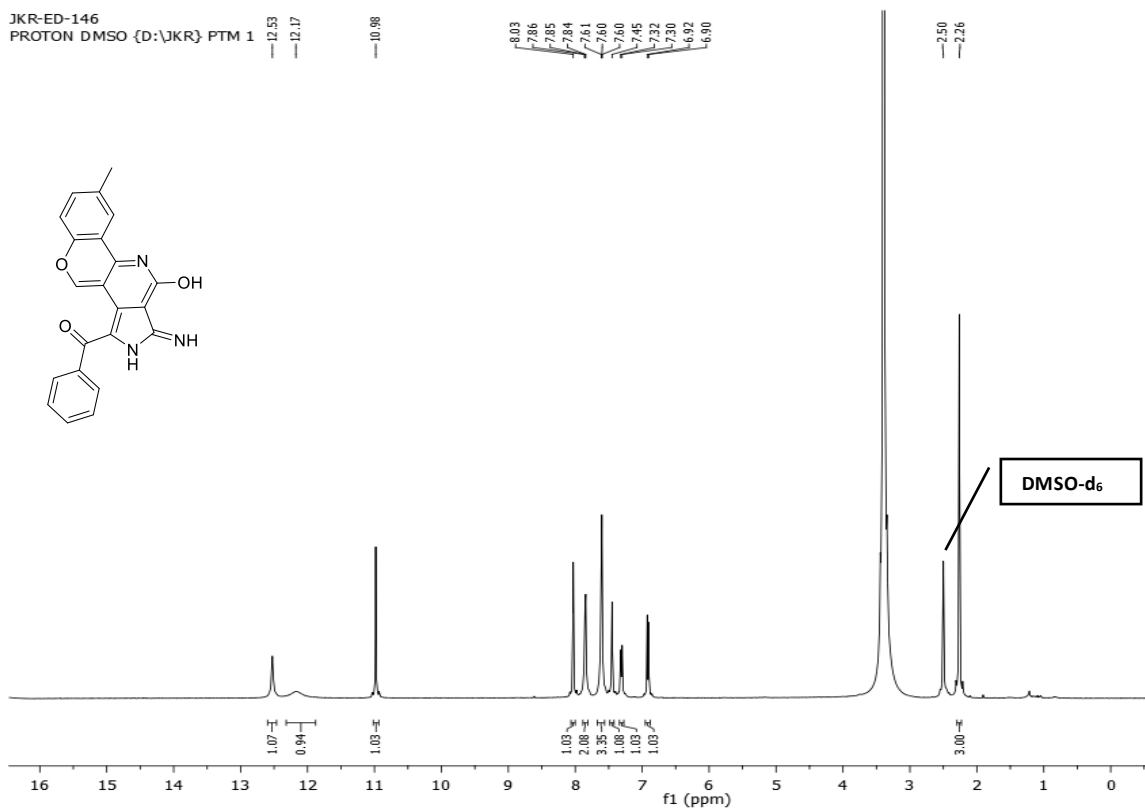


¹³C{¹H} NMR spectrum of **8f** (100 MHz, DMSO-*d*₆)

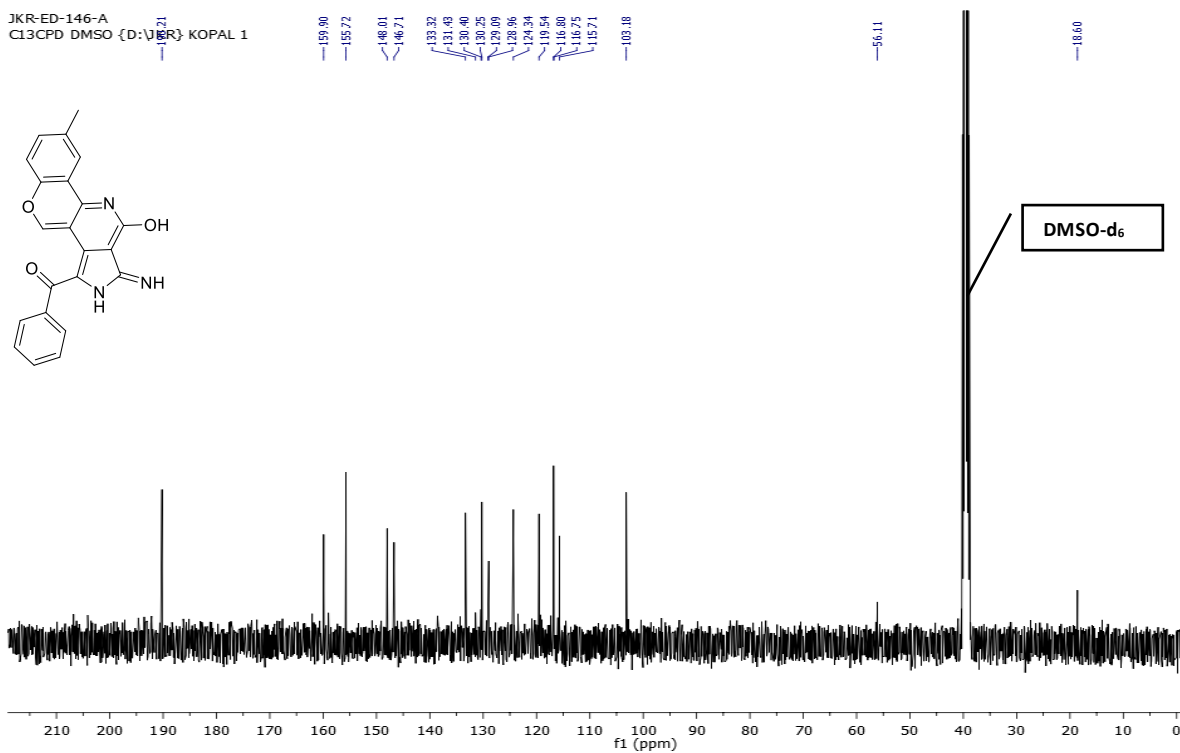
Sample Name	JKR-ED-101ZH	Position		Instrument Name	Q-TOF	User Name	QTOF-PU\admin
Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	JKR-ED-101ZH1.d	ACQ Method	Pondicherry Universi	Comment	ED-JKR-521.0586	Acquired Time	23-05-2018 12:35:41



HRMS (ESI) spectrum of **8f**

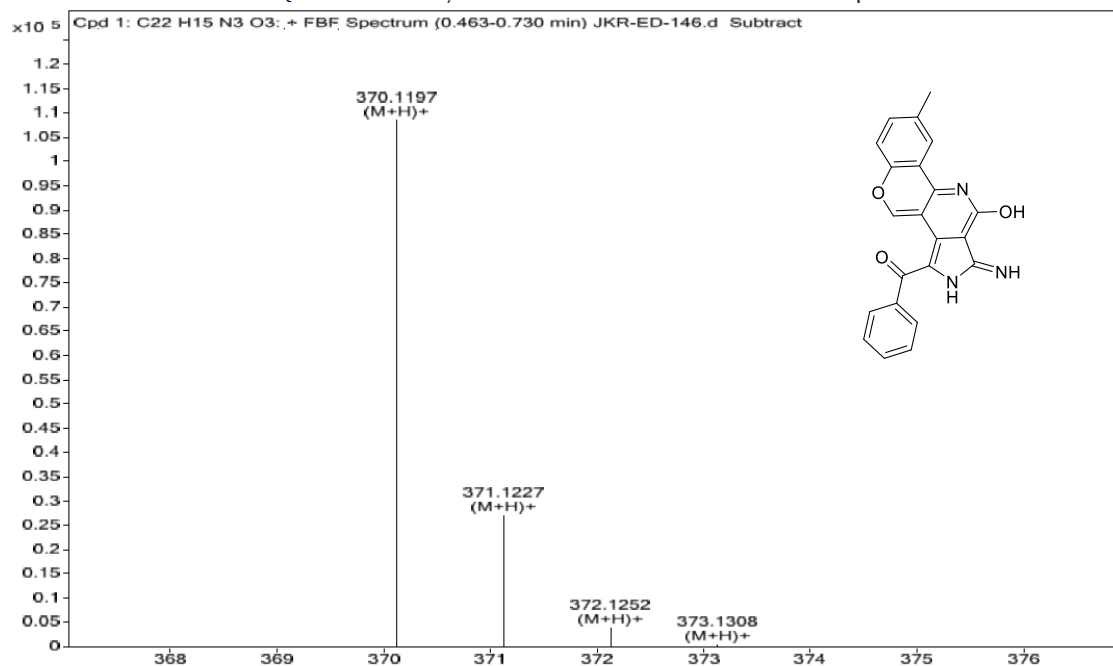


^1H NMR spectrum of **10a** (400 MHz, DMSO- d_6)

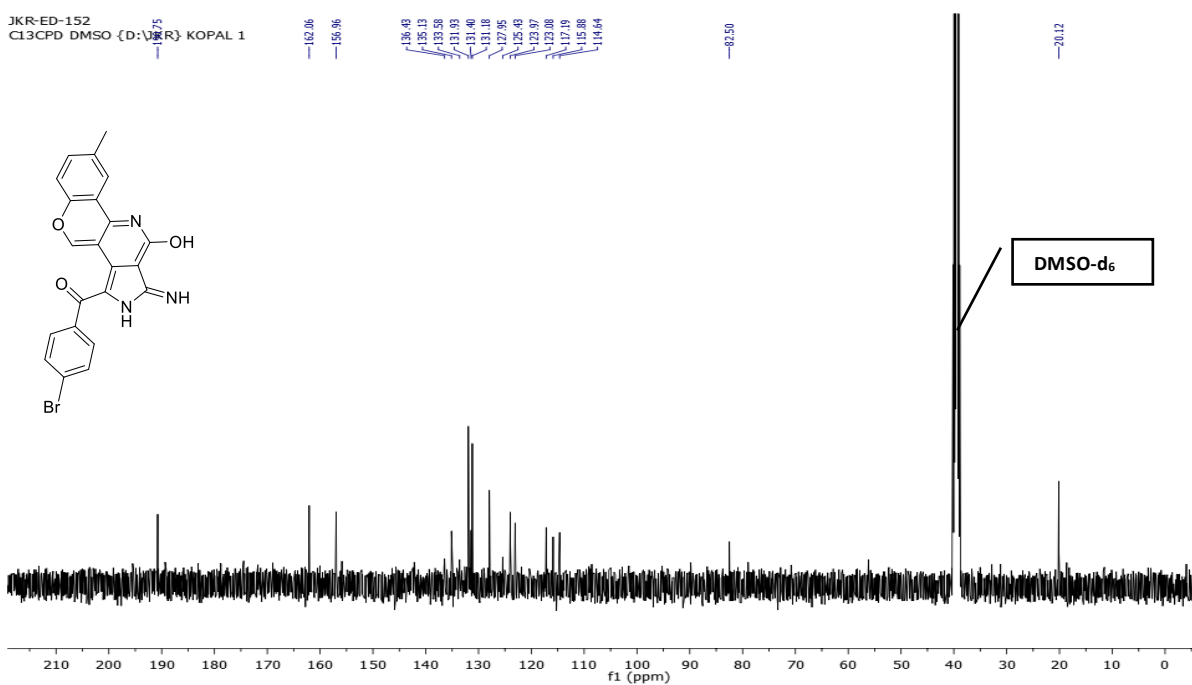
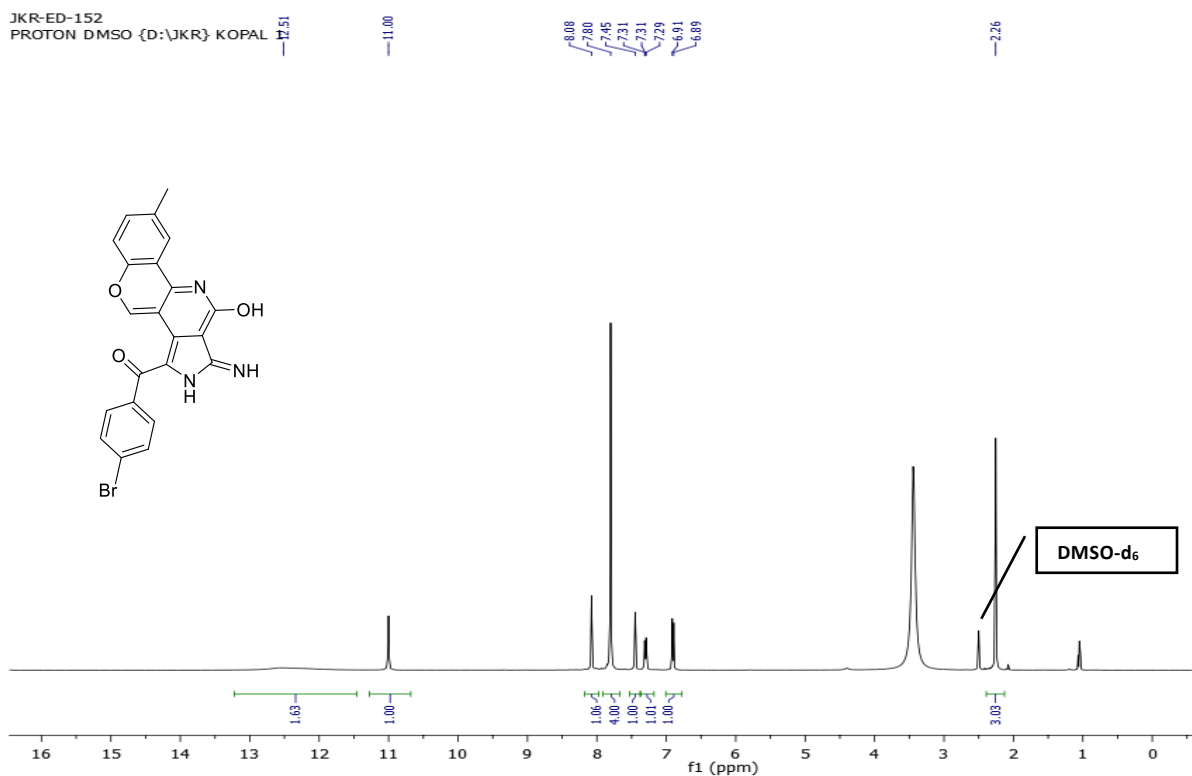


$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **10a** (100 MHz, DMSO- d_6)

Sample Name	JKR-ED-146	Position	Instrument Name	Q-TOF	User Name	QTOF-PU\admin	
Inj Vol	-1	InjPosition	SampleType	Sample	IRM Calibration Status	Success	
Data Filename	JKR-ED-146.d	ACQ Method	Pondicherry Universi	Comment	ED-JKR-387.1219	Acquired Time	20-08-2018 11:53:39



HRMS (ESI) spectrum of **10a**

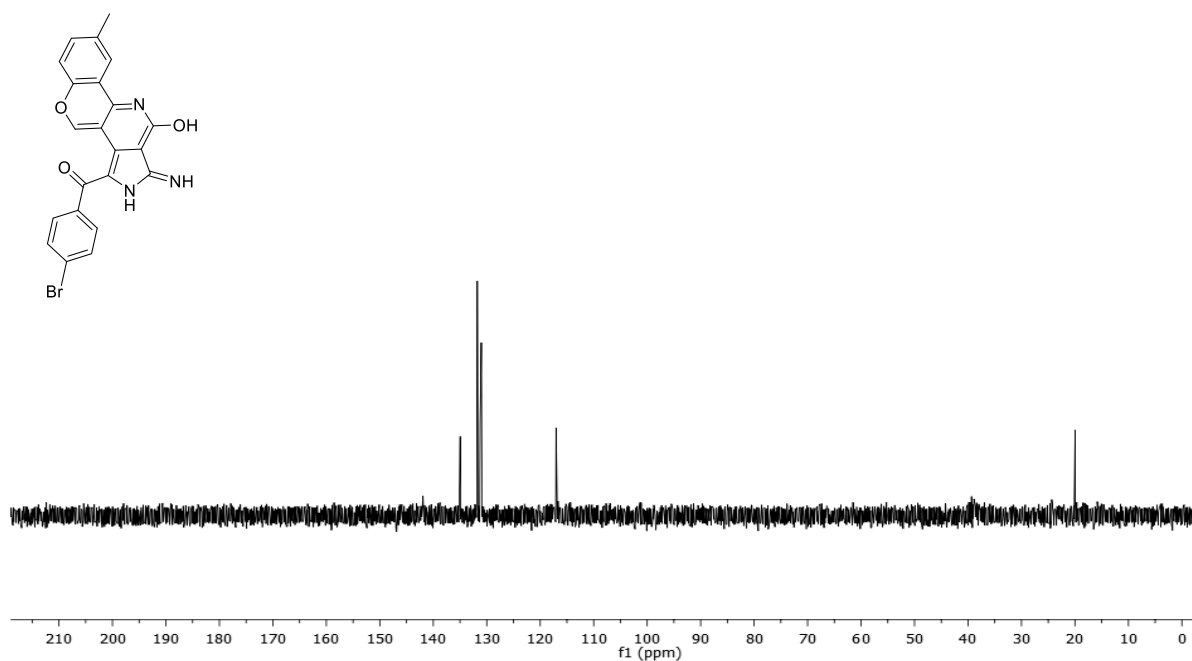


JKR-ED-152
C13DEPT135 DMSO {D-;JKR} KOPAL 1

134.96
131.77
131.24
131.02

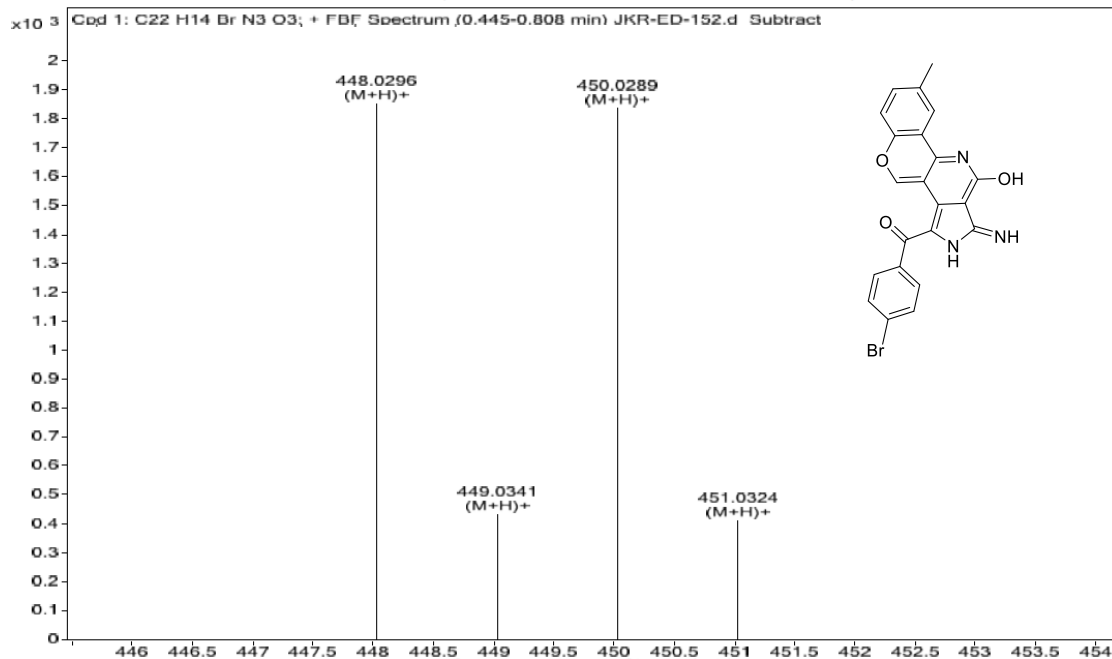
117.03

19.96



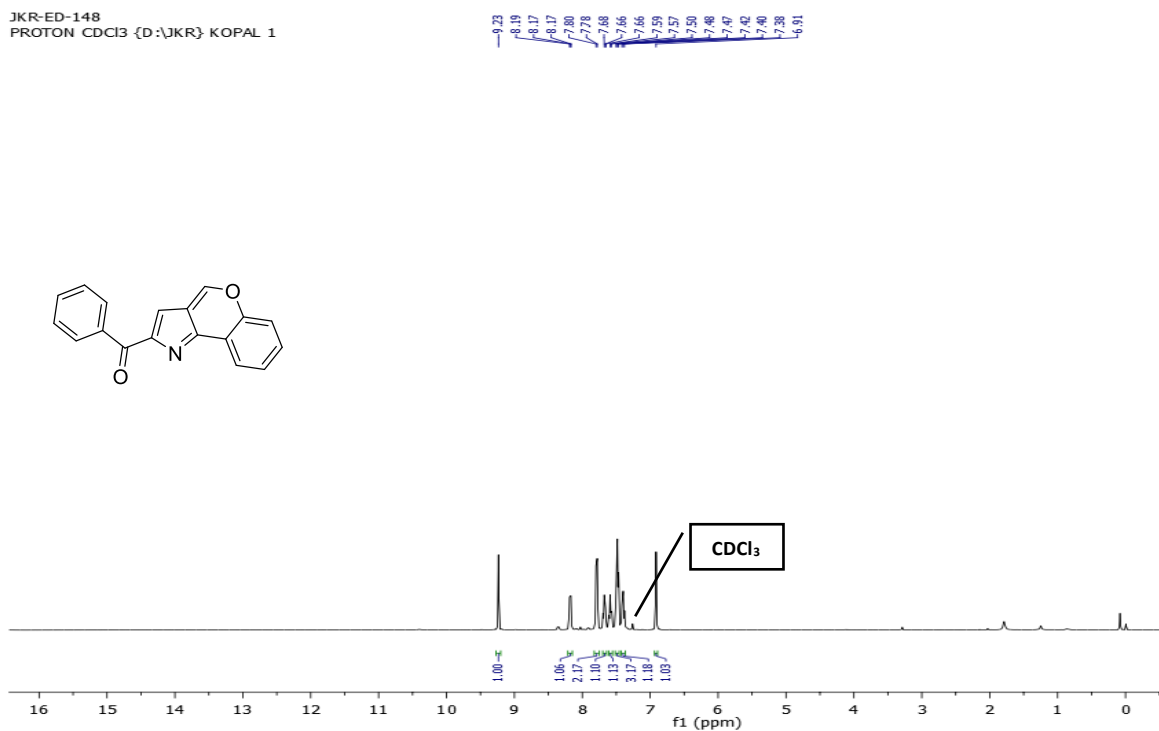
DEPT 135 NMR spectrum of **10b** (100 MHz, DMSO- d_6)

Sample Name	Position	Instrument Name	Q-TOF	User Name	QTOF-PU\admin
JKR-ED-152	-1	Sample	Sample	IRM Calibration Status	Success
Data Filename	ACQ Method	SampleType	Comment	Acquired Time	24-09-2018 12:22:03



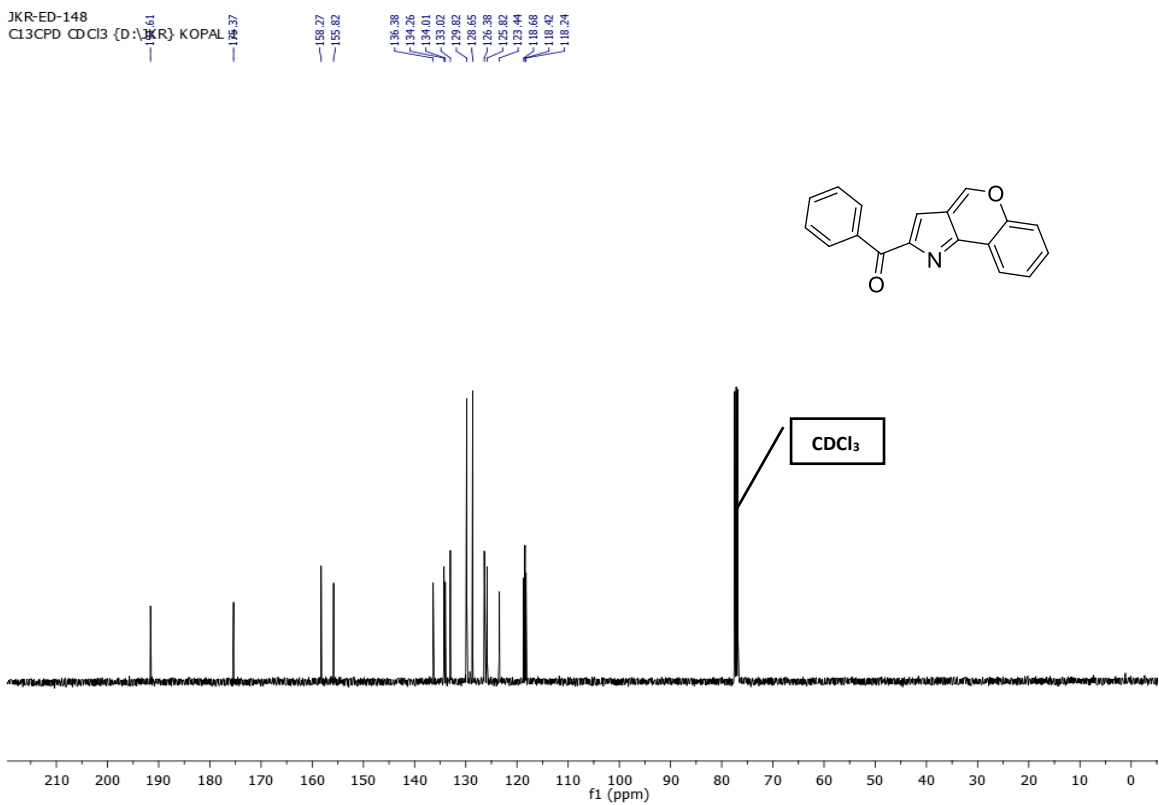
HRMS (ESI) spectrum of **10b**

JKR-ED-148
PROTON CDCl₃ {D:\JKR} KOPAL 1



¹H NMR spectrum of **12a** (400 MHz, CDCl₃)

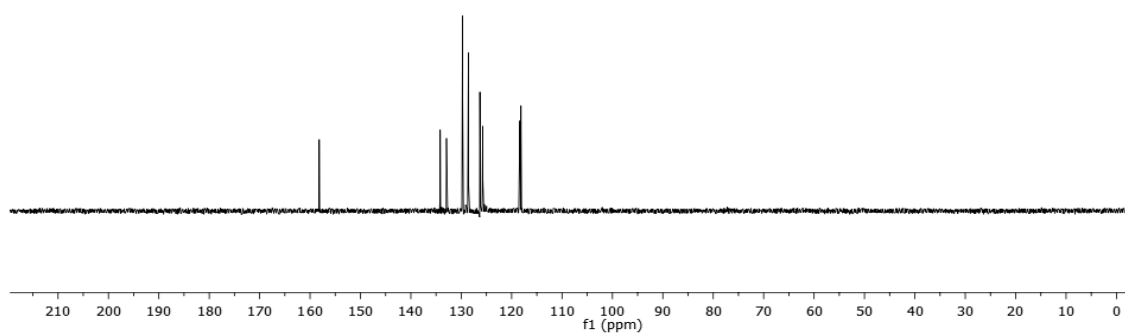
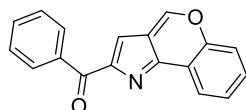
JKR-ED-148
C13CPD CDCl₃ {D:\JKR} KOPAL 1



¹³C{¹H} NMR spectrum of **12a** (100 MHz, CDCl₃)

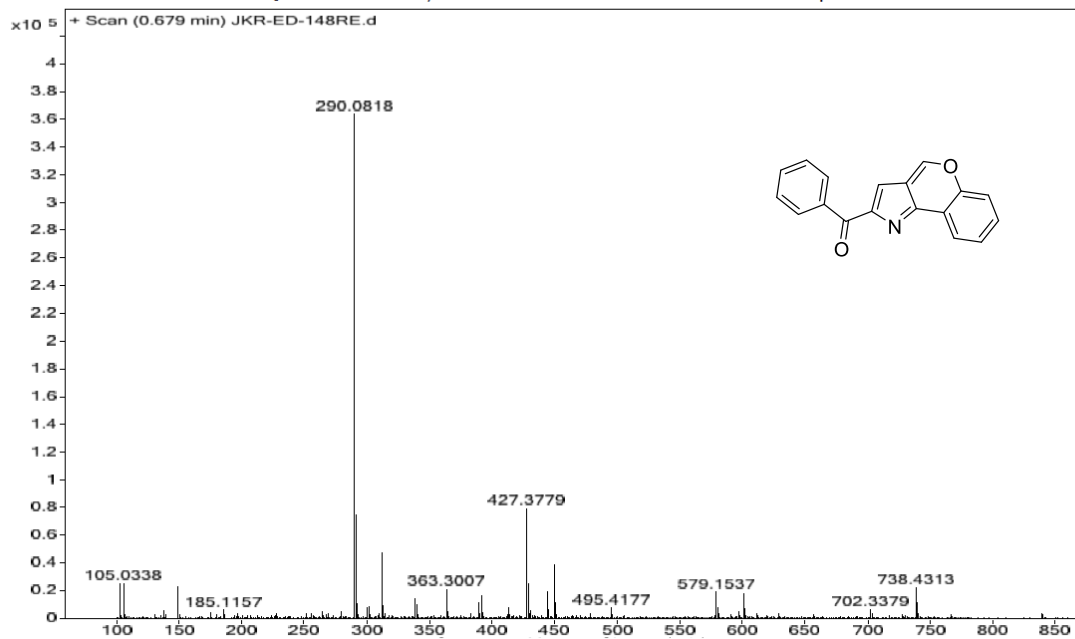
JKR-ED-148
 Cl3DEPT135 CDCl3 {D:\JKR} KOPAL 1

158.18
 134.17
 132.93
 129.73
 128.57
 126.30
 125.73
 118.34
 118.16



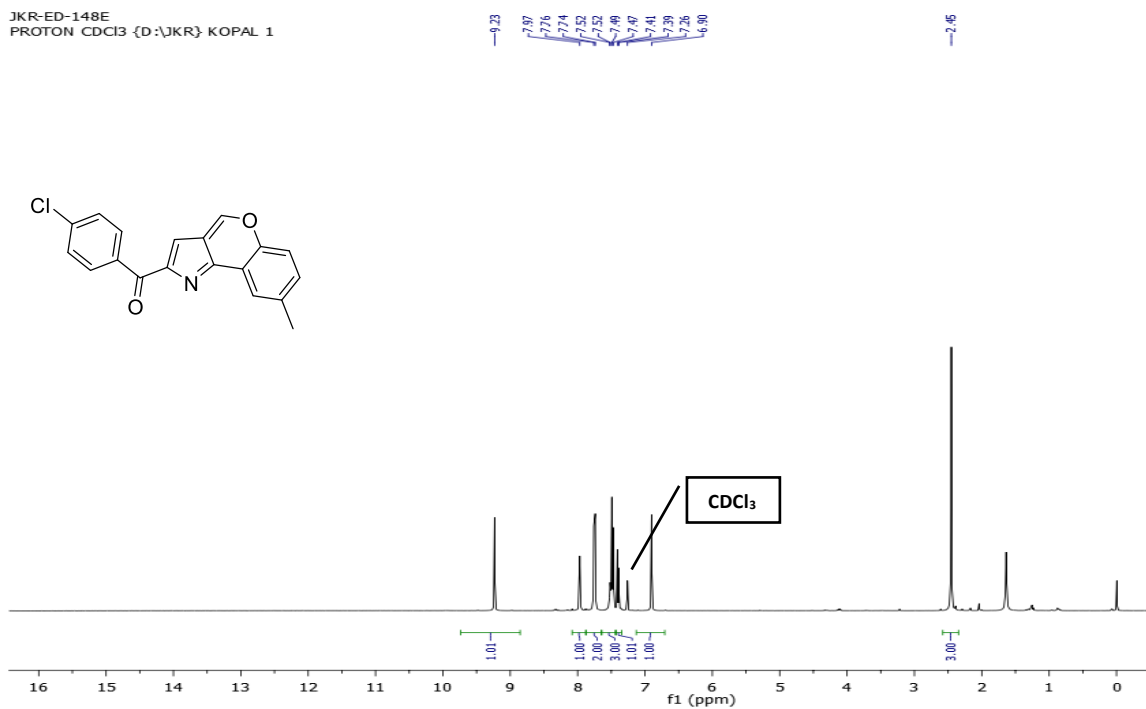
DEPT 135 NMR spectrum of **12a** (100 MHz, CDCl₃)

Sample Name	Position	Instrument Name	User Name
JKR-ED-148RE	JKR-ED-148RE	Q-TOF	QTOF-PU\admin
Inj Vol	-1	Sample	IRM Calibration Status
Data Filename	JKR-ED-148RE.d	Comment	Acquired Time
	Pondicherry Universi	ED-JKR-273.0790	Success
			26-09-2018 12:07:17

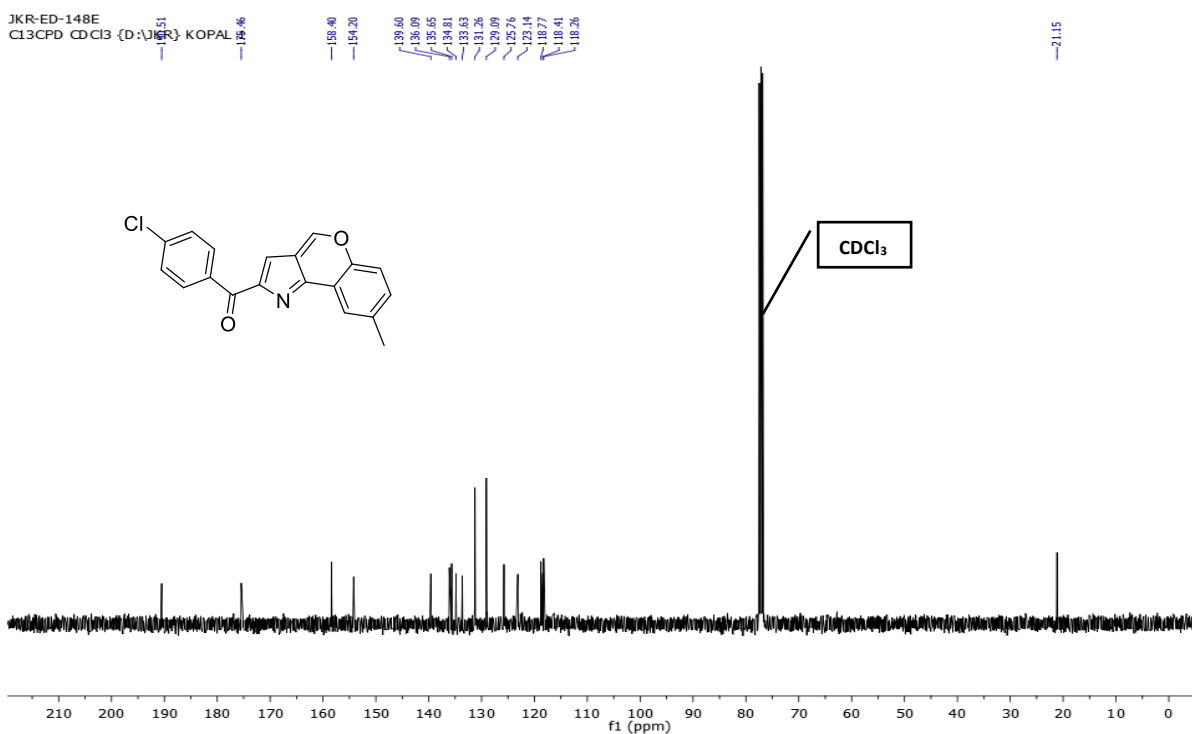


HRMS (ESI) spectrum of **12a**

JKR-ED-148E
PROTON CDCl₃ {D:\JKR} KOPAL 1



¹H NMR spectrum of **12b** (400 MHz, CDCl₃)



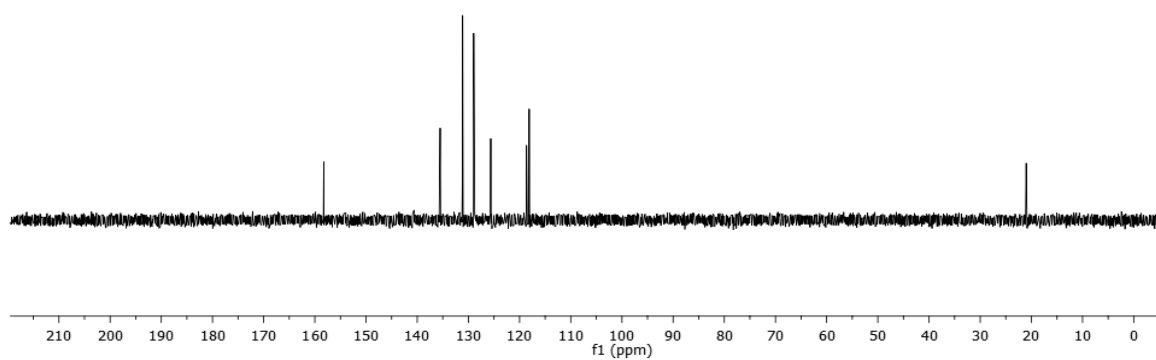
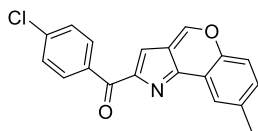
¹³C{¹H} NMR spectrum of **12b** (100 MHz, CDCl₃)

JKR-ED-148E
Cl3DEPT135 CDCl3 {D:\JKR} KOPAL 1

158.26

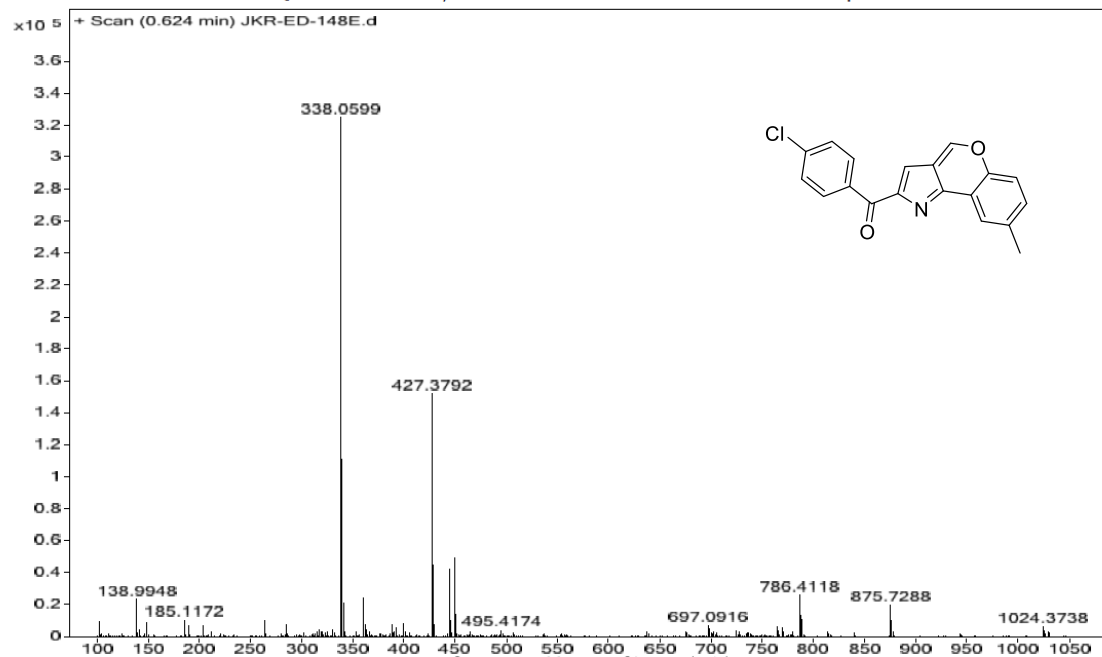
135.51
131.12
128.86
125.63
118.63
118.12

21.01



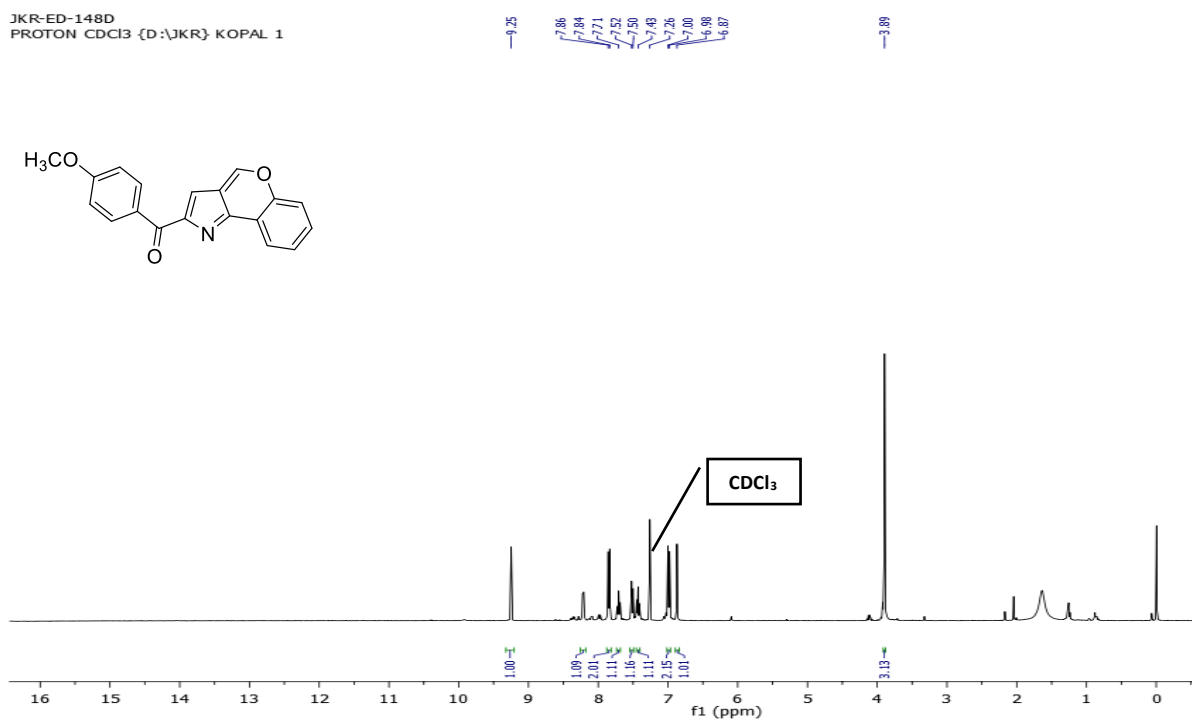
DEPT 135 NMR spectrum of **12b** (100 MHz, CDCl₃)

Sample Name	JKR-ED-148E	Position	Instrument Name	Q-TOF	User Name	QTOF-PU\admin
Inj Vol	-1	InjPosition	SampleType	Sample	IRM Calibration Status	Success
Data Filename	JKR-ED-148E.d	ACQ Method	Comment	ED-JKR-307.0400	Acquired Time	03-10-2018 14:58:17



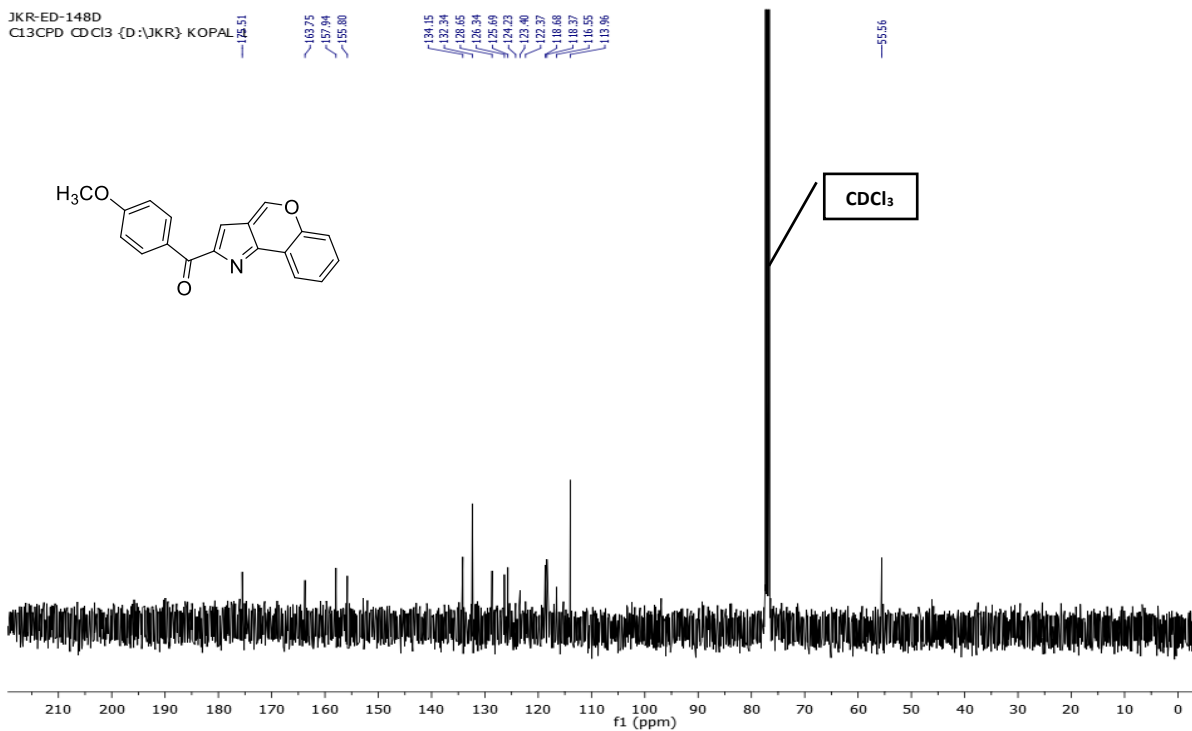
HRMS (ESI) spectrum of **12b**

JKR-ED-148D
PROTON CDCl3 {D:\JKR} KOPAL 1



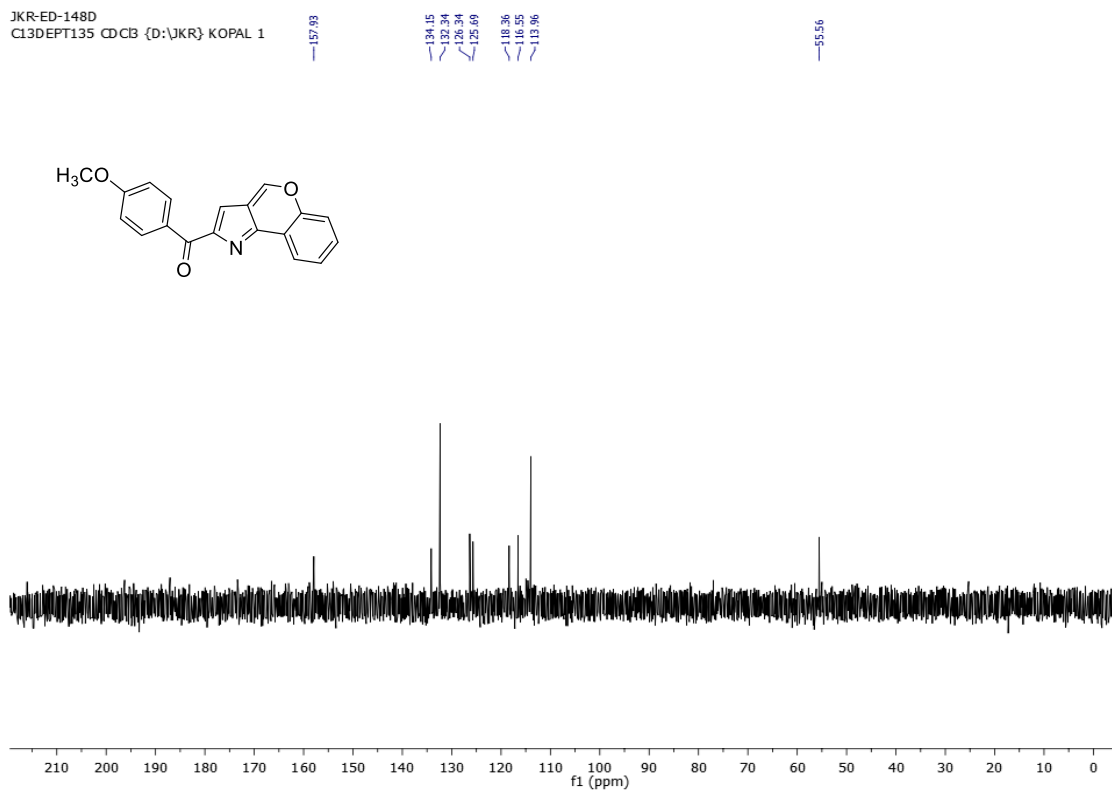
¹H NMR spectrum of **12c** (400 MHz, CDCl₃)

JKR-ED-148D
C13CPD CDCl3 {D:\JKR} KOPAL



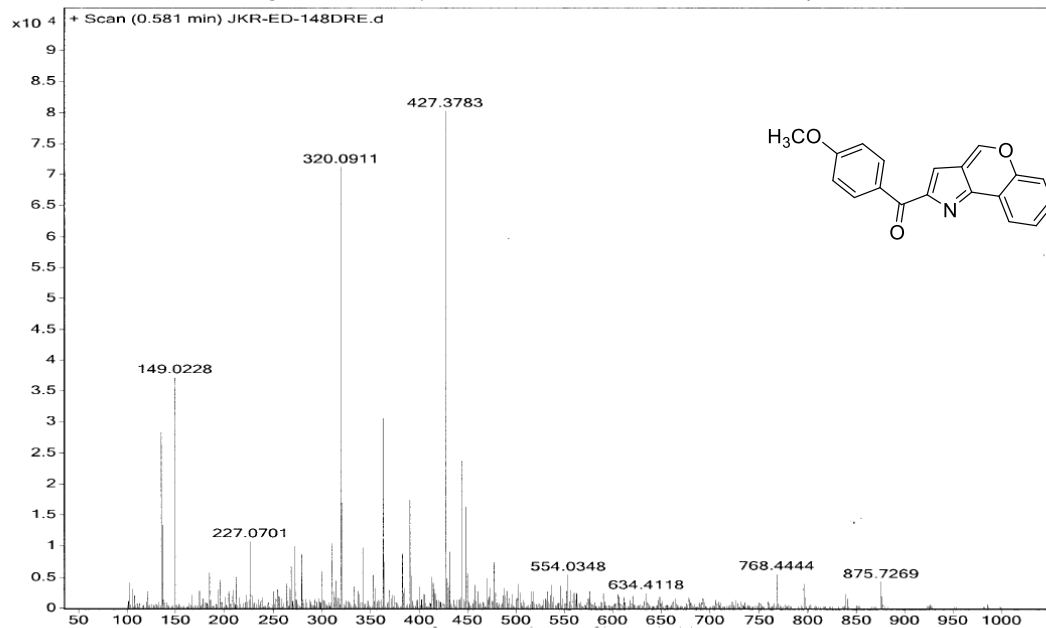
¹³C{¹H} NMR spectrum of **12c** (100 MHz, CDCl₃)

JKR-ED-148D
Cl3DEPT135 CDCl3 {D:\JKR} KOPAL 1



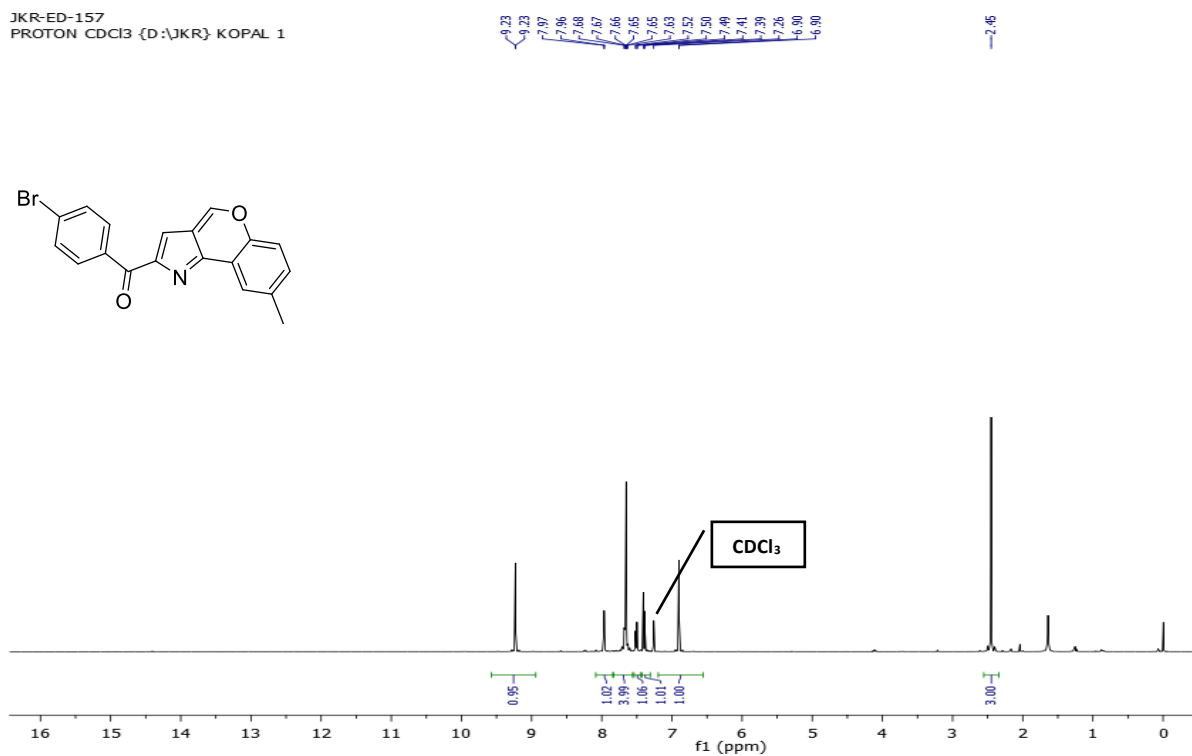
DEPT 135 NMR spectrum of **12c** (100 MHz, CDCl₃)

Sample Name	JKR-ED-148DRE	Position	Instrument Name	Q-TOF	User Name	QTOF-PU\admin
Inj Vol	-1	InjPosition	SampleType	Sample	IRM Calibration Status	Success
Data Filename	JKR-ED-148DRE.d	ACQ Method	Comment	ED-JKR-303.0895	Acquired Time	26-09-2018 12:03:40

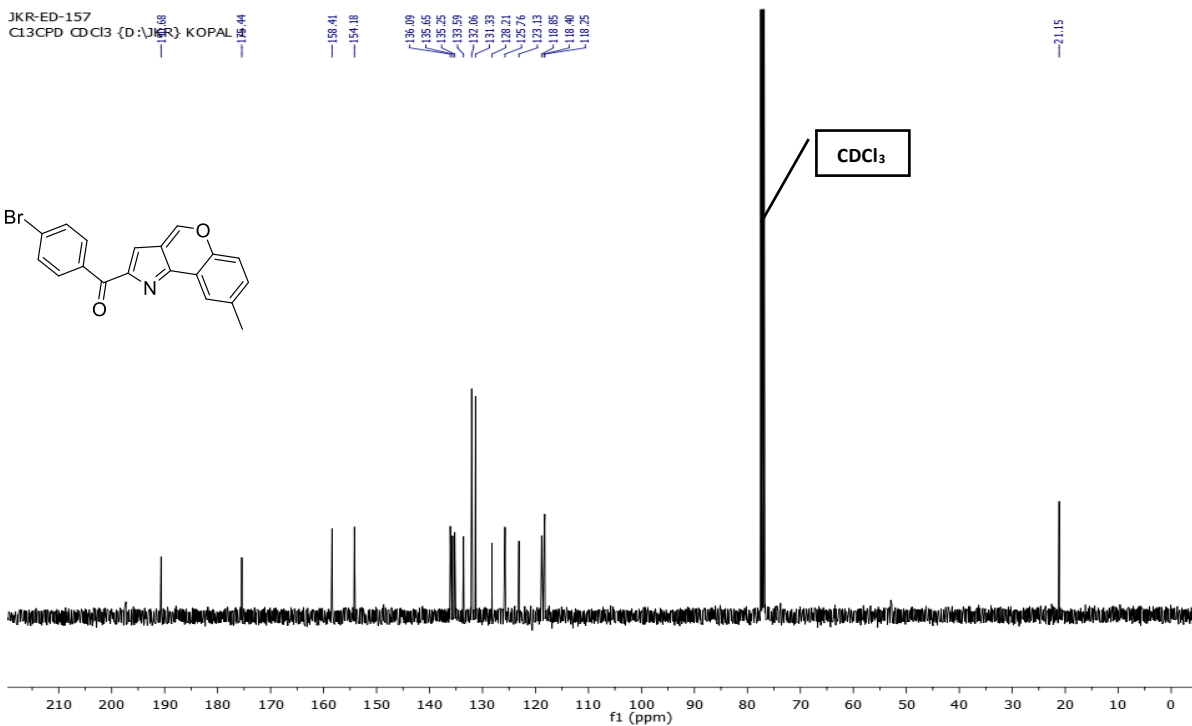


HRMS (ESI) spectrum of **12c**

JKR-ED-157
PROTON CDCl₃ {D:\JKR} KOPAL 1

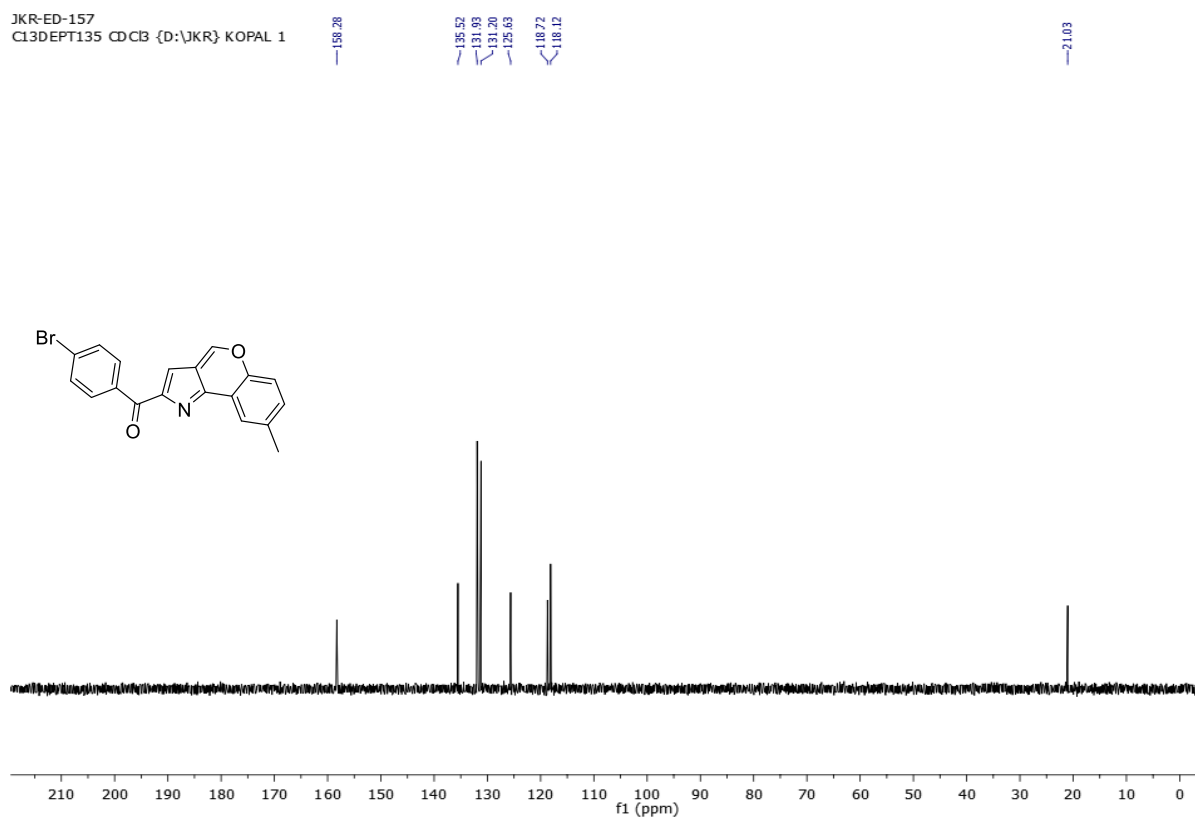


¹H NMR spectrum of **12d** (400 MHz, CDCl₃)



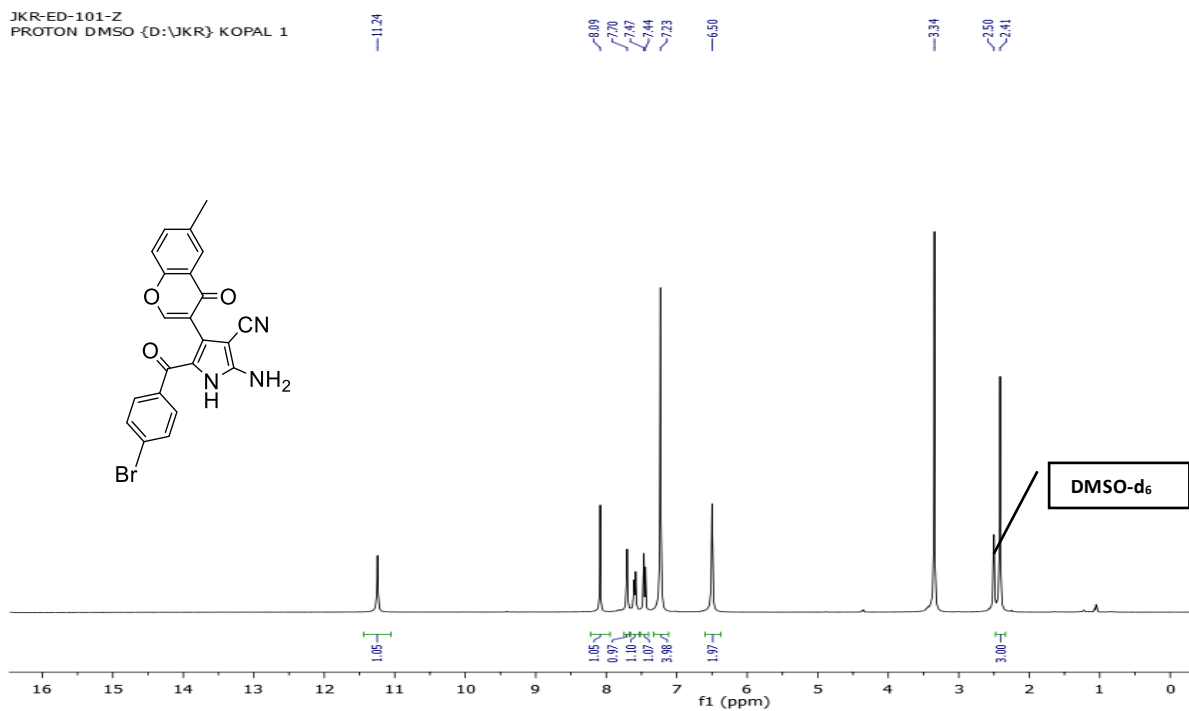
¹³C{¹H} NMR spectrum of **12d** (100 MHz, CDCl₃)

JKR-ED-157
Cl3DEPT135 CDCl3 {D:\JKR\ KOPAL 1



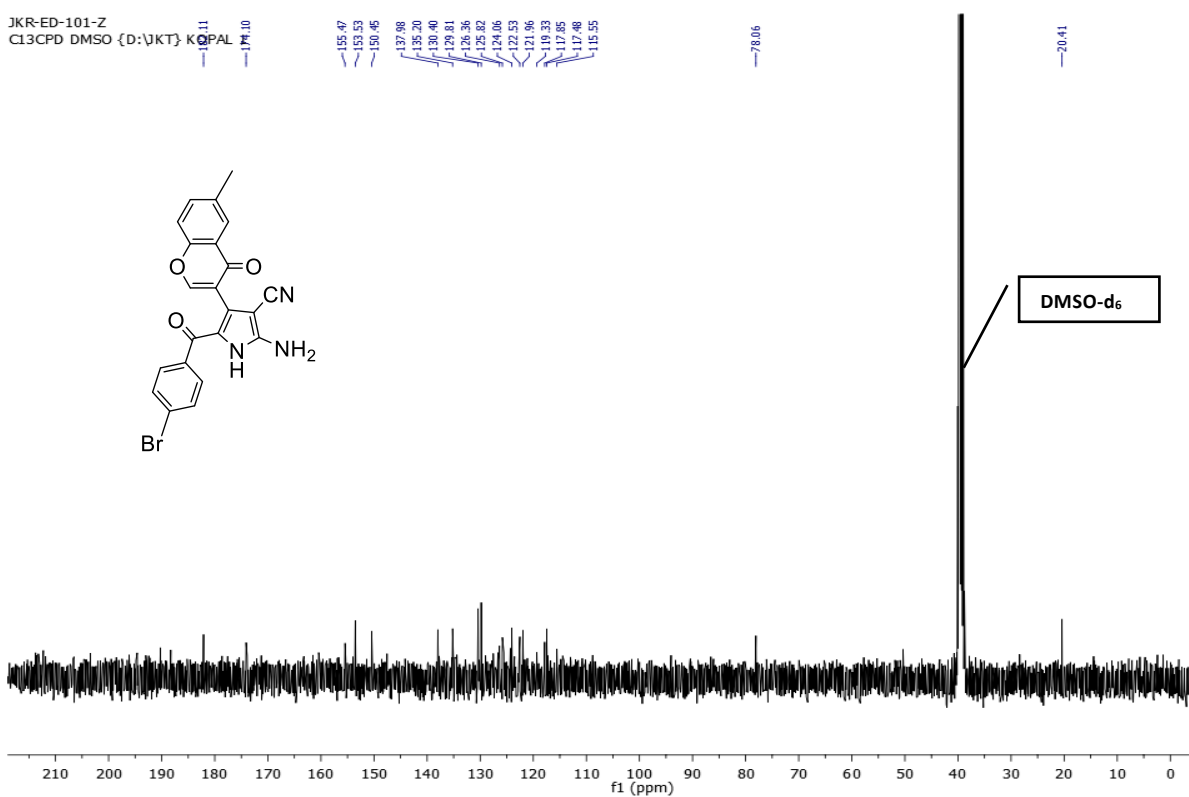
DEPT 135 NMR spectrum of **12d** (100 MHz, CDCl₃)

JKR-ED-101-Z
PROTON DMSO {D:\JKR} KOPAL 1



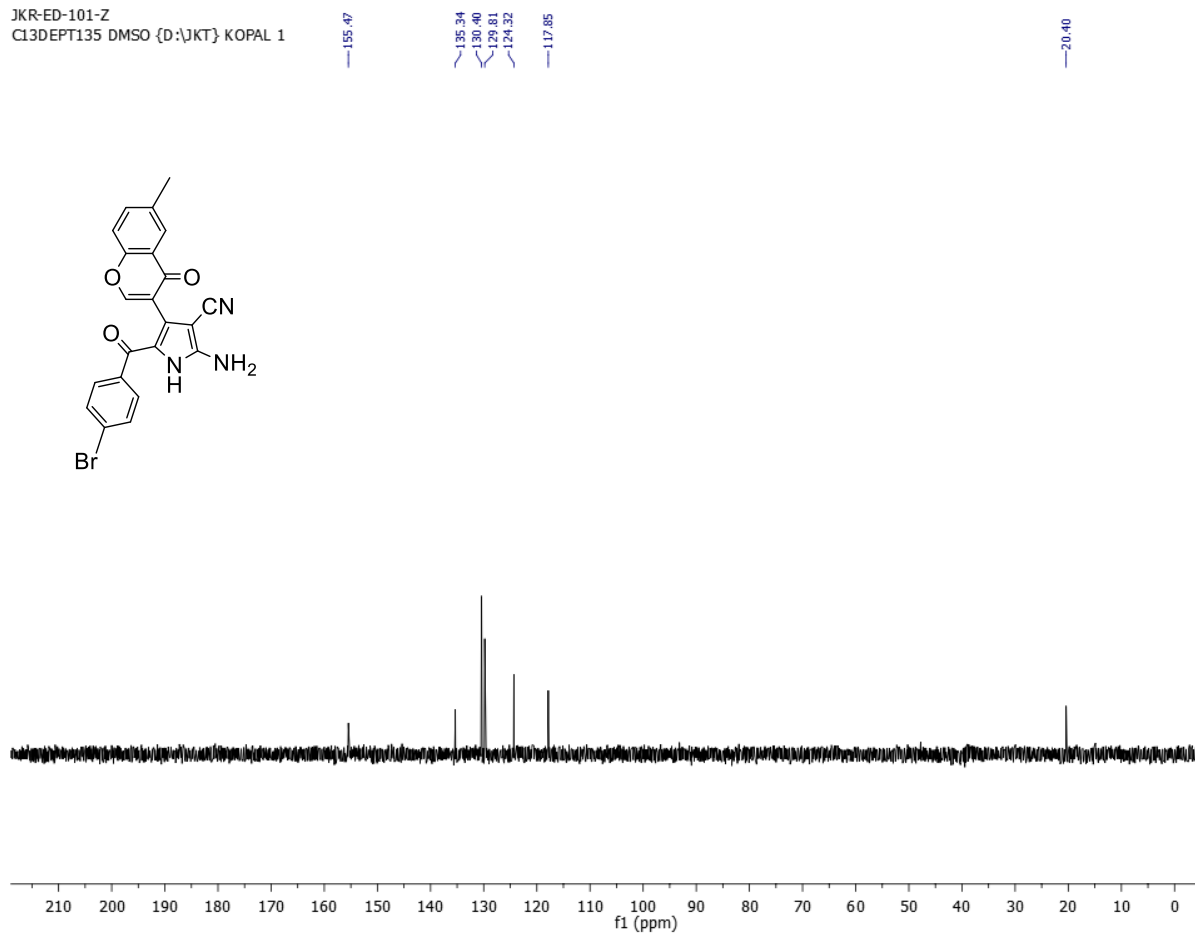
^1H NMR spectrum of **15a** (400 MHz, $\text{DMSO-}d_6$)

JKR-ED-101-Z
C13CPD DMSO {D:\JKT} KOPAL



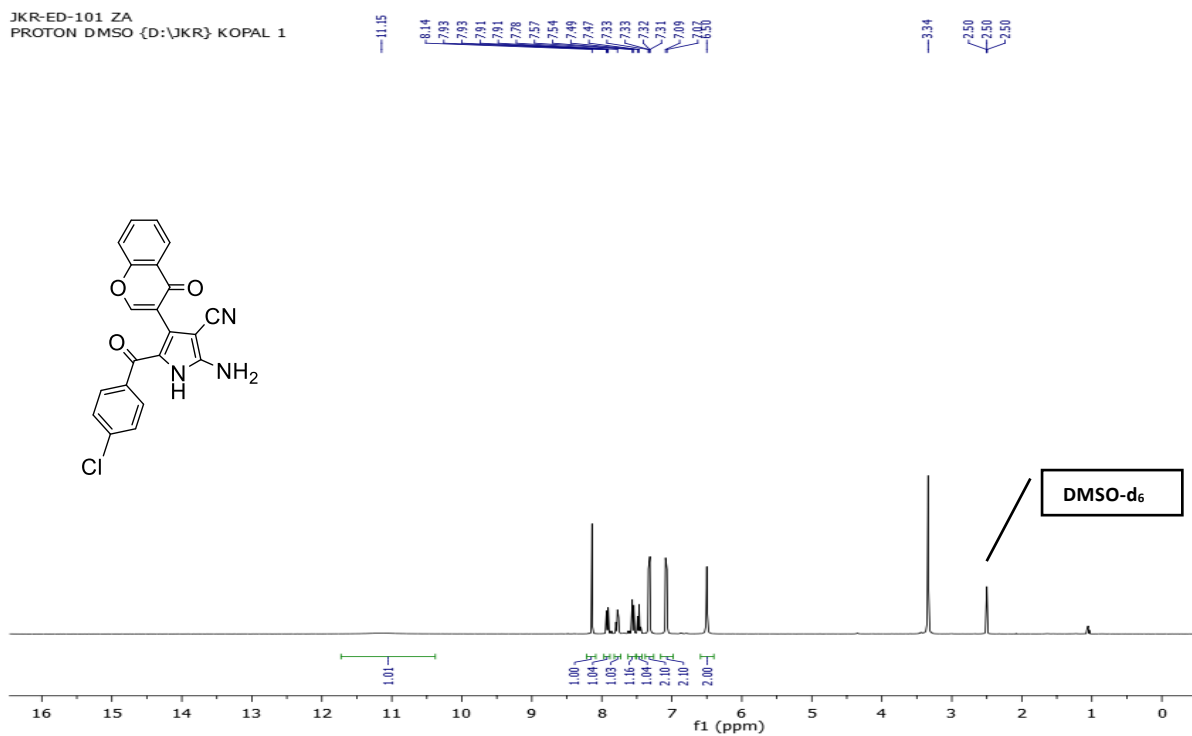
$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **15a** (100 MHz, $\text{DMSO-}d_6$)

JKR-ED-101-Z
C13DEPT135 DMSO {D:\JKT} KOPAL 1

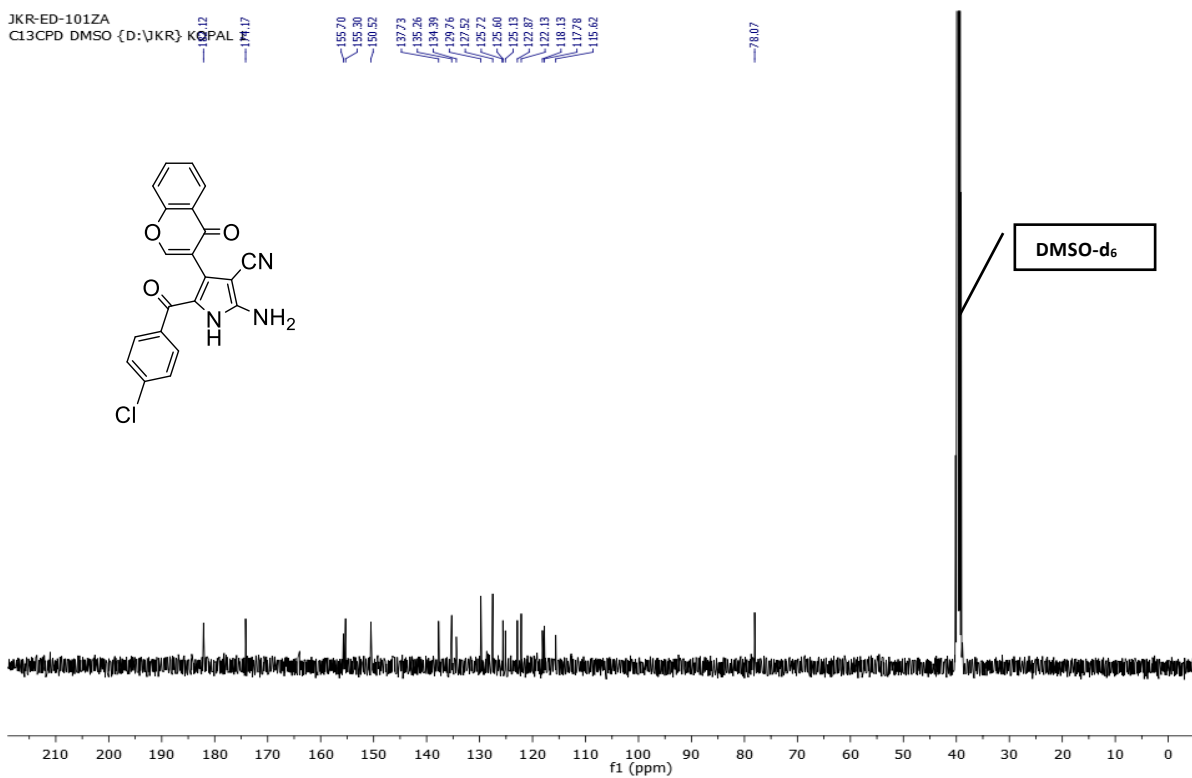


DEPT 135 NMR spectrum of **15a** (100 MHz, DMSO-*d*₆)

JKR-ED-101 ZA
PROTON DMSO {D:\JKR} KOPAL 1



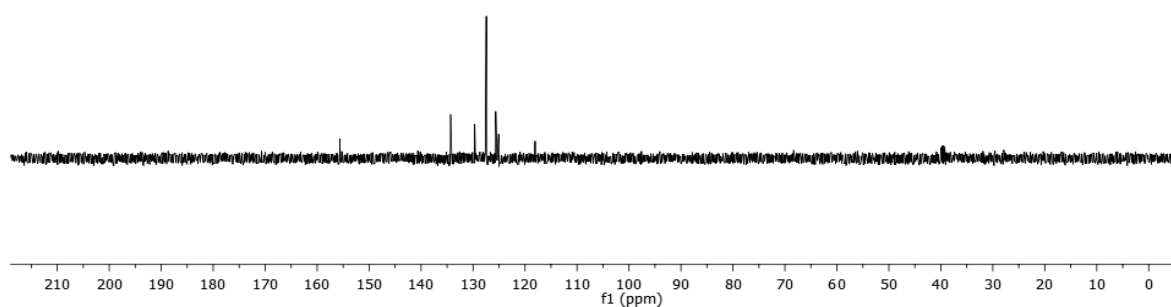
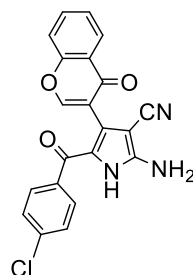
¹H NMR spectrum of **15b** (400 MHz, DMSO-*d*₆)



¹³C{¹H} NMR spectrum of **15b** (100 MHz, DMSO-*d*₆)

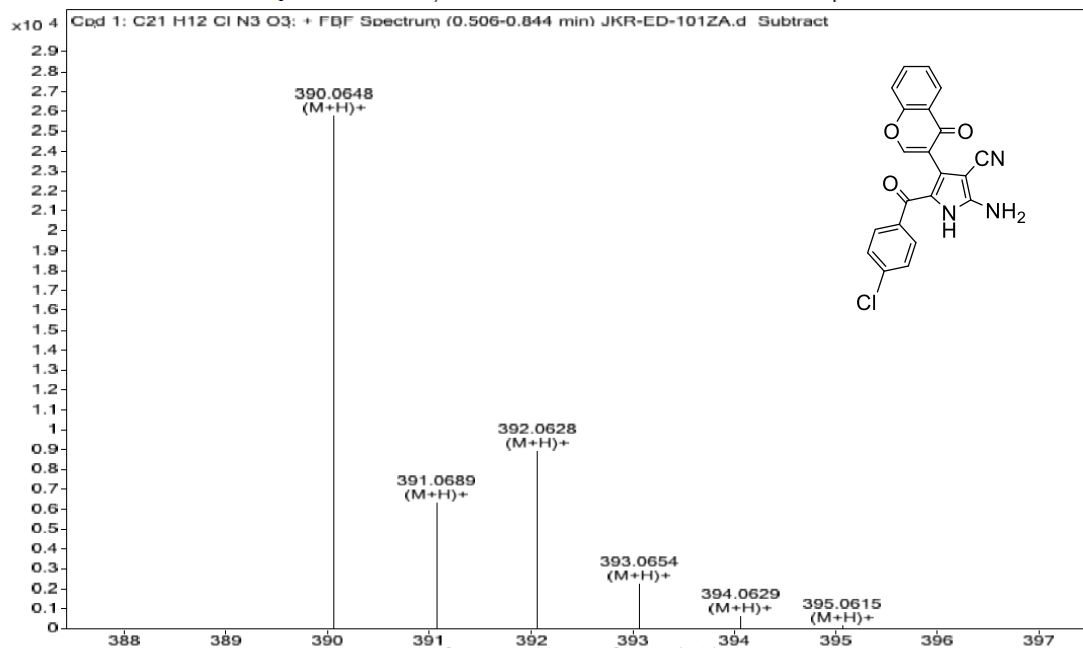
JKR-ED-101 ZA
CL3DEPT135 DMSO {D:\JKR} KOPAL 1

155.61
134.31
129.86
127.45
125.86
118.06

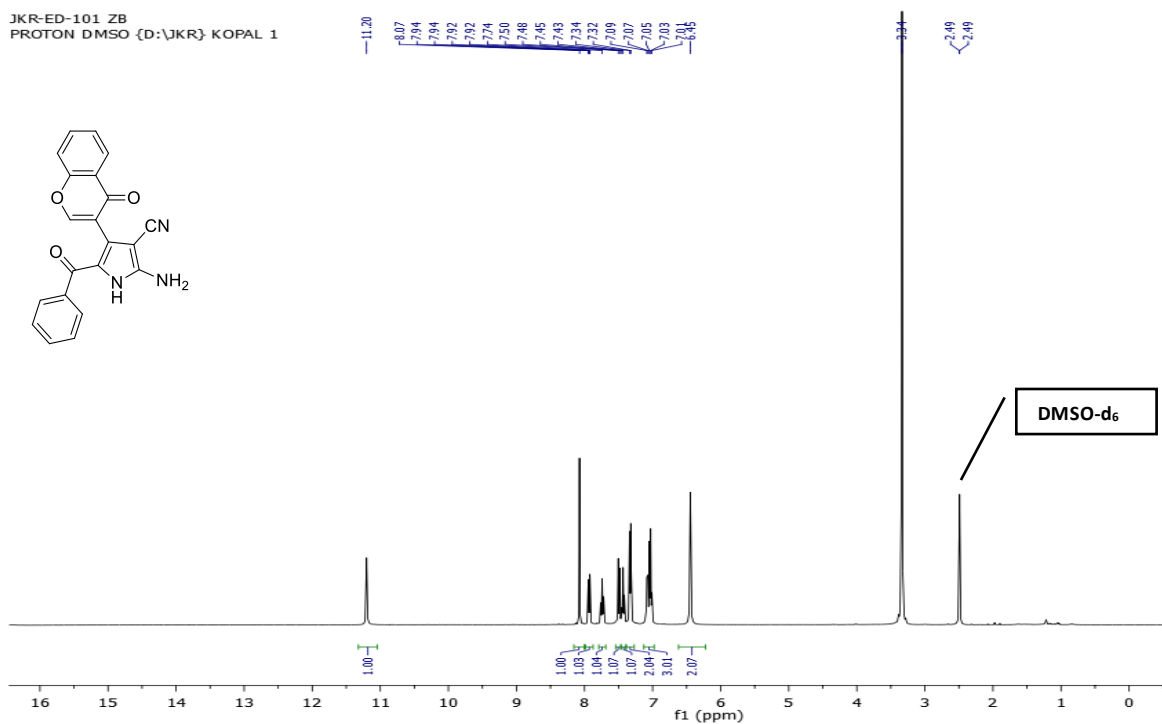


DEPT 135 NMR spectrum of **15b** (100 MHz, DMSO- d_6)

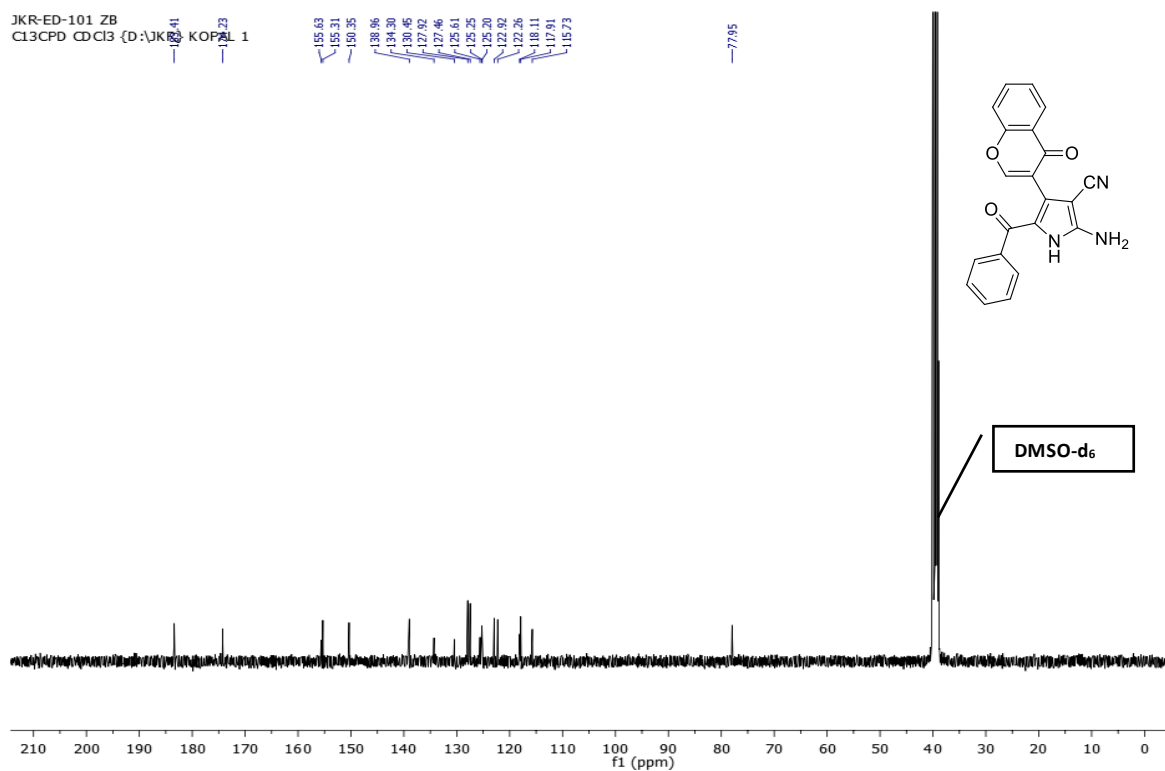
Sample Name	JKR-ED-101ZA	Position		Instrument Name	Q-TOF	User Name	QTOF-PU\admin
Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	JKR-ED-101ZA.d	ACQ Method	Pondicherry Universi	Comment	ED-JKR-389.06	Acquired Time	16-05-2018 13:21:45



HRMS (ESI) spectrum of **15b**



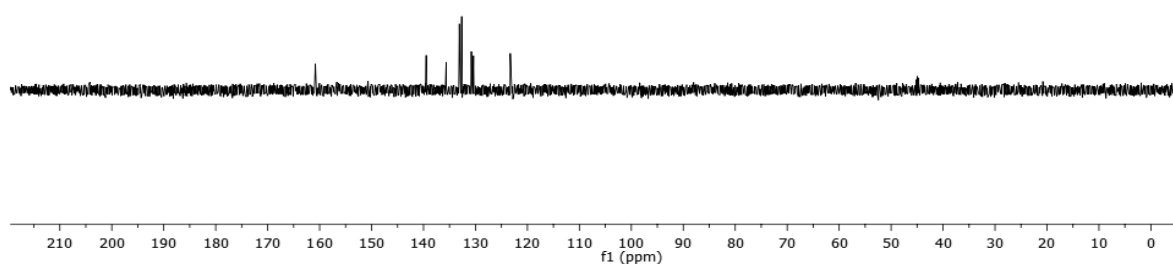
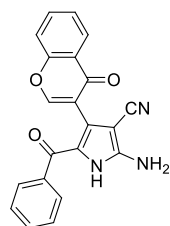
^1H NMR spectrum of **15c** (400 MHz, DMSO- d_6)



$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **15c** (100 MHz, DMSO- d_6)

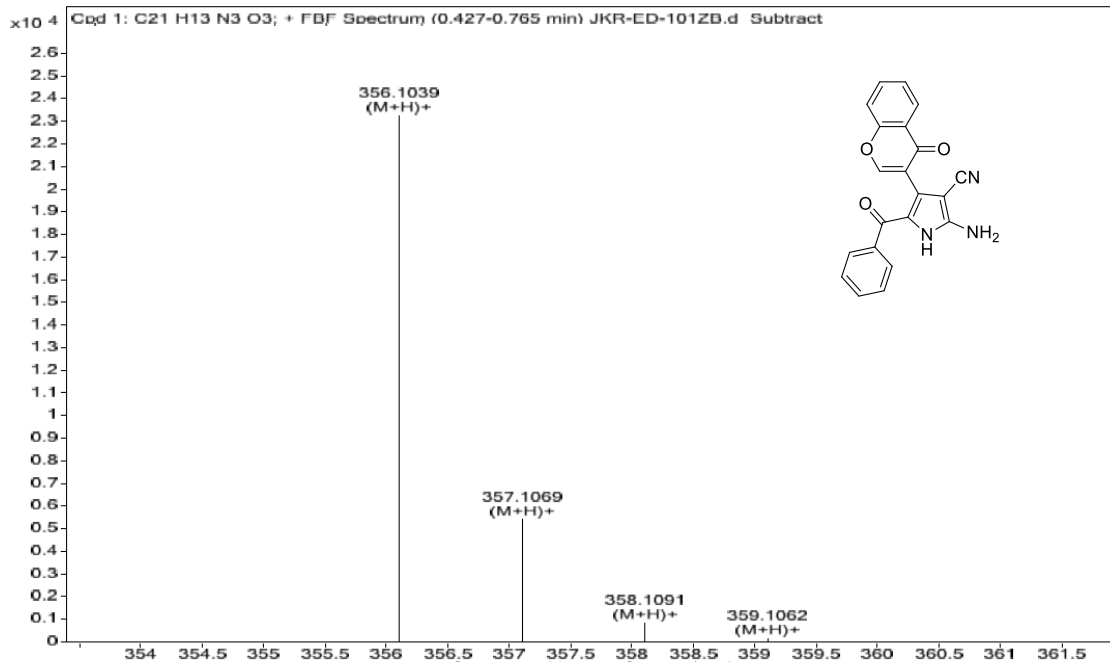
JKR-ED-101 ZB
CL3DEPT135 CD CB {D:\JKR} KOPAL 1

160.81
136.46
135.64
133.10
132.65
130.79
130.30
123.30



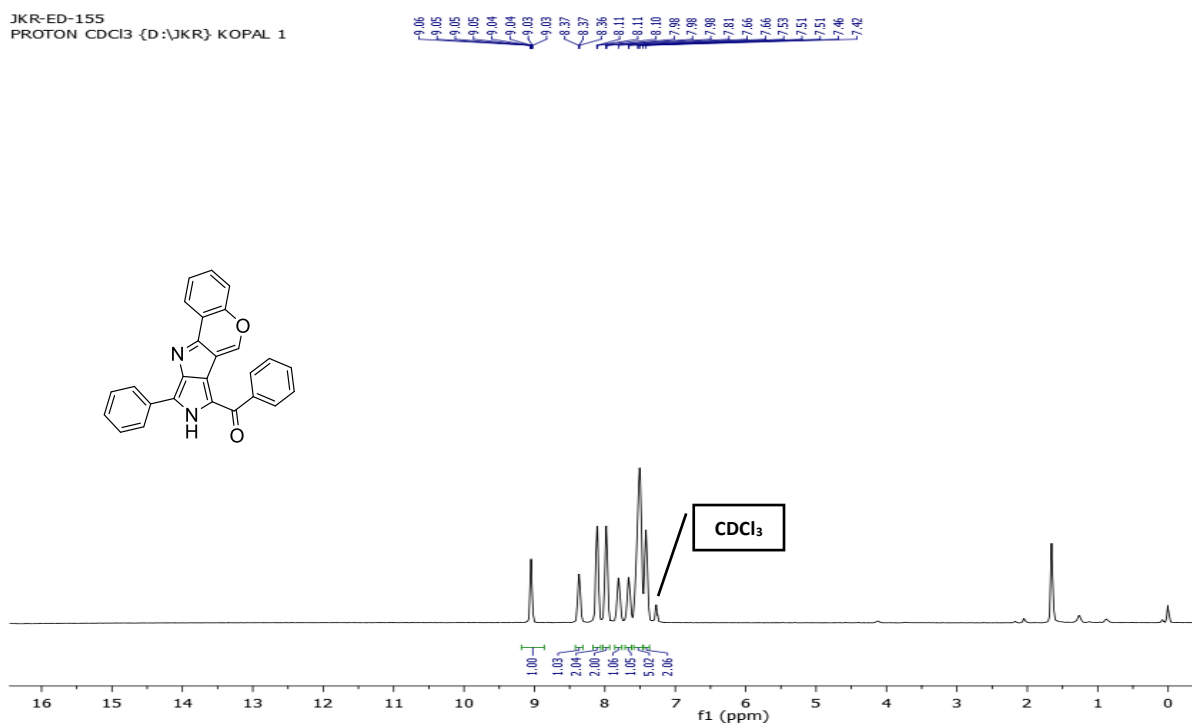
DEPT 135 NMR spectrum of **15c** (100 MHz, DMSO- d_6)

Sample Name	JKR-ED-101ZB	Position		Instrument Name	Q-TOF	User Name	QTOF-PU\admin
Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	JKR-ED-101ZB.d	ACQ Method	Pondicherry Universi	Comment	ED-JKR-355.10	Acquired Time	16-05-2018 13:18:10



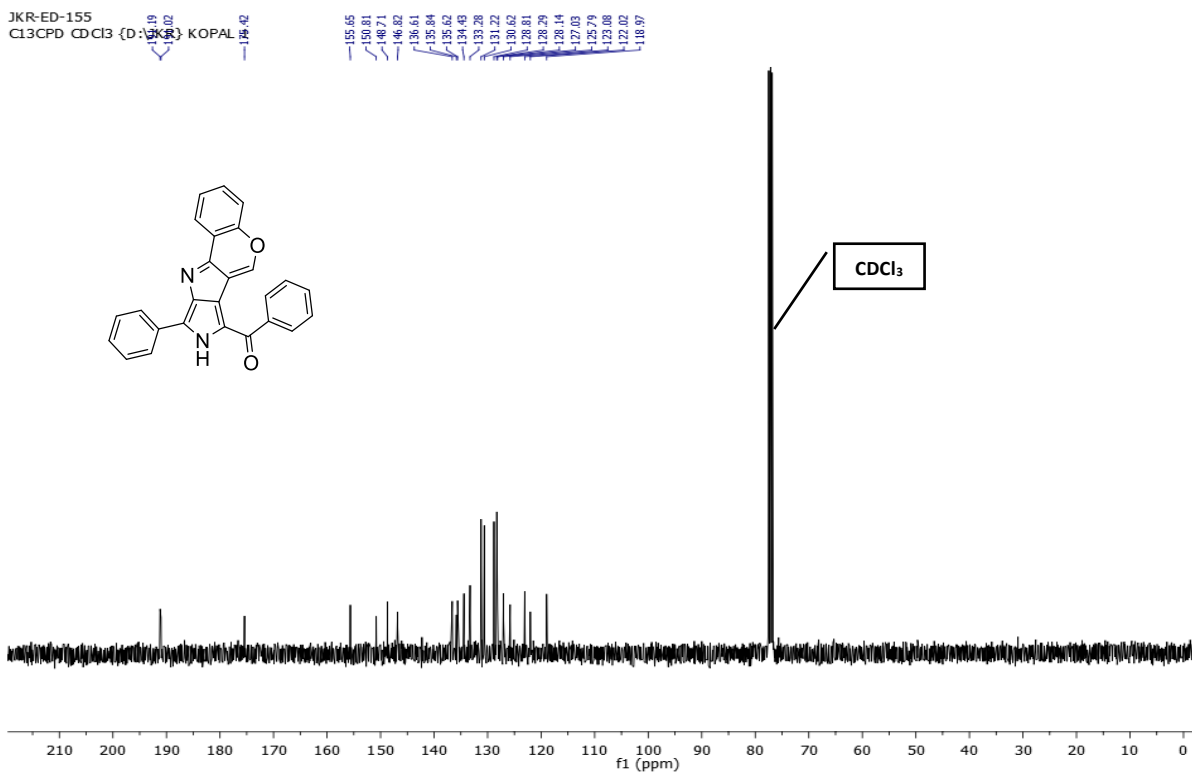
HRMS (ESI) spectrum of **15c**

JKR-ED-155
PROTON CDCl₃ {D:\JKR} KOPAL 1



¹H NMR spectrum of **17a** (400 MHz, CDCl₃)

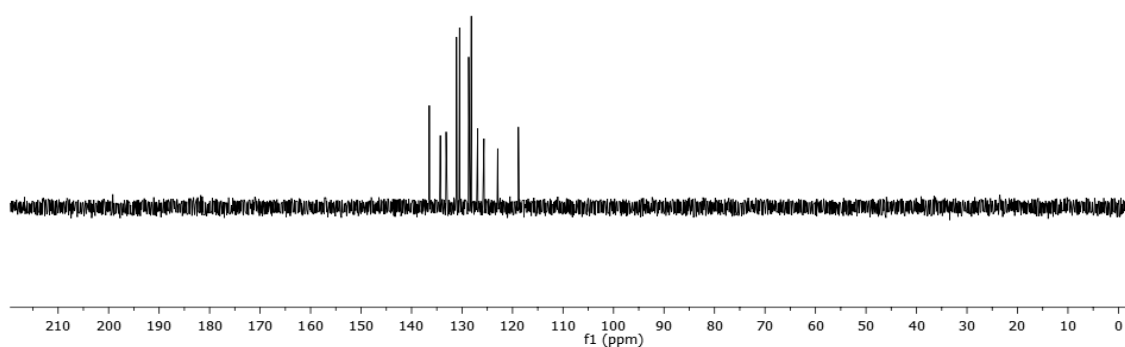
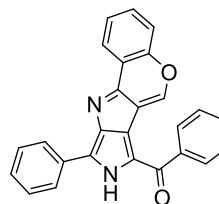
JKR-ED-155
C13CPD CDCl₃ {D:\JKR} KOPAL 1



¹³C{¹H} NMR spectrum of **17a** (100 MHz, CDCl₃)

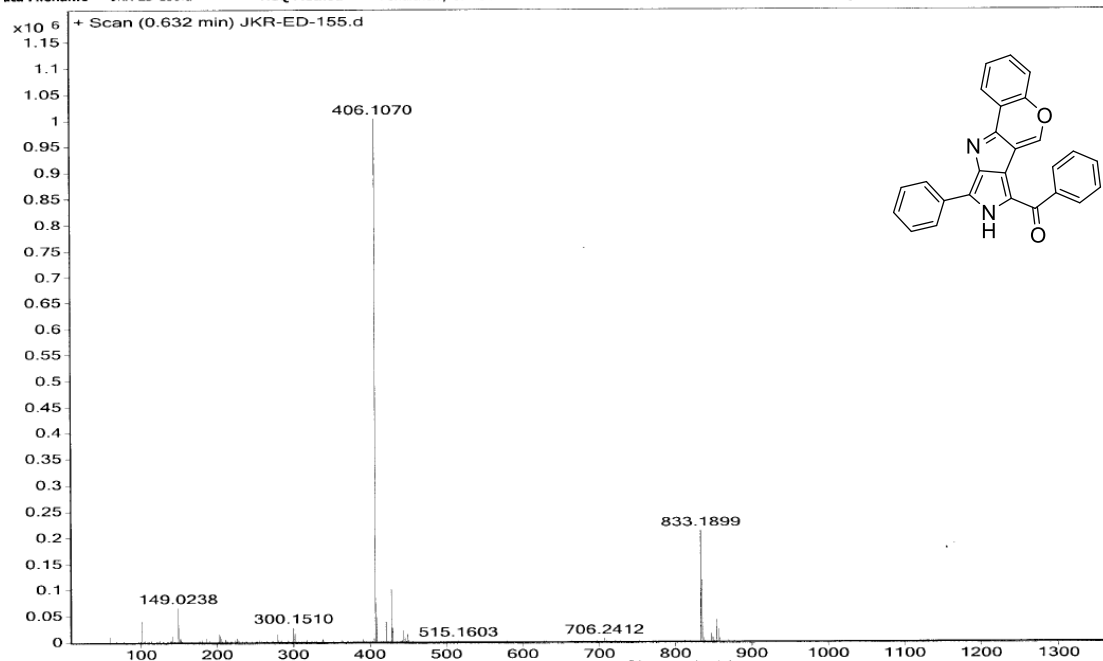
JKR-ED-155
 Cl3DEPT135 CDCl3 {D:\JKR} KOPAL 1

136.48
 134.30
 133.15
 131.10
 129.09
 128.69
 128.16
 128.91
 125.66
 122.94
 118.84

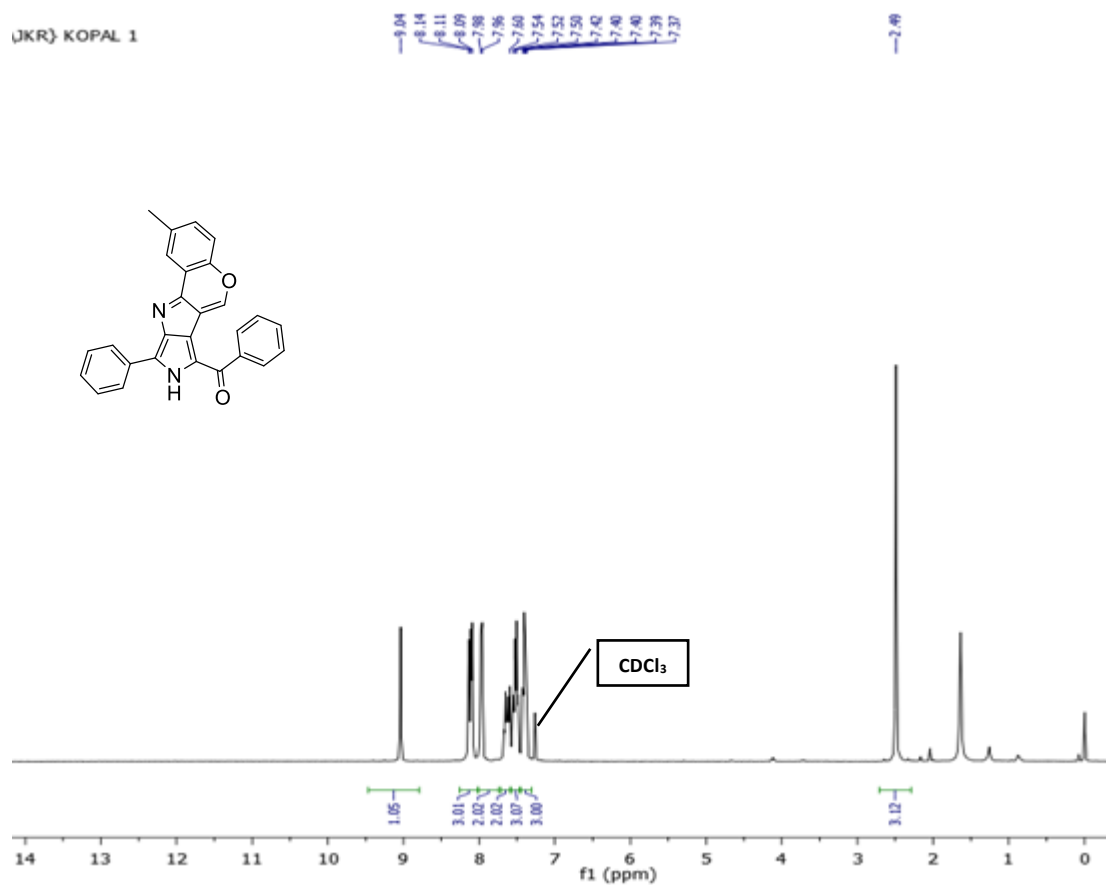


DEPT 135 NMR spectrum of **17a** (100 MHz, CDCl₃)

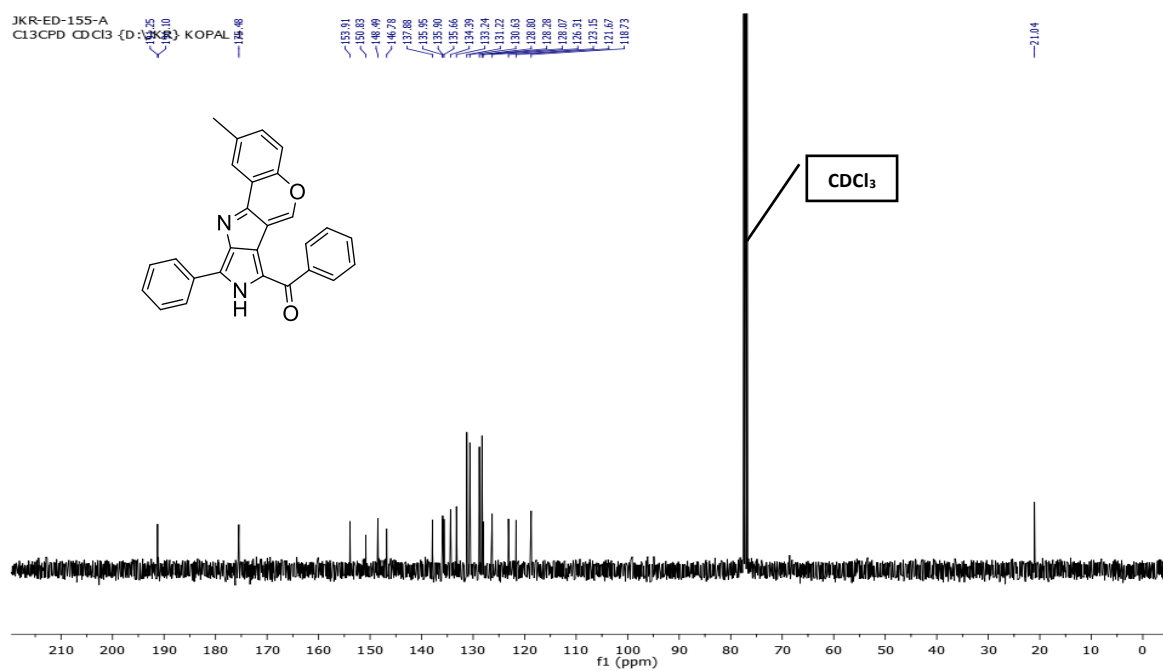
Sample Name	Position	Instrument Name	Q-TOF	User Name	QTOF-PU/admin
JKR-ED-155	-1	Sample	Sample	IRM Calibration Status	Success
ata Filename	JKR-ED-155.d	ACQ Method	Pondicherry Universi	Comment	ED-JKR-373.0950
				Acquired Time	12-10-2018 14:03:22



HRMS (ESI) spectrum of **17a**



¹H NMR spectrum of **17b** (400 MHz, CDCl₃)

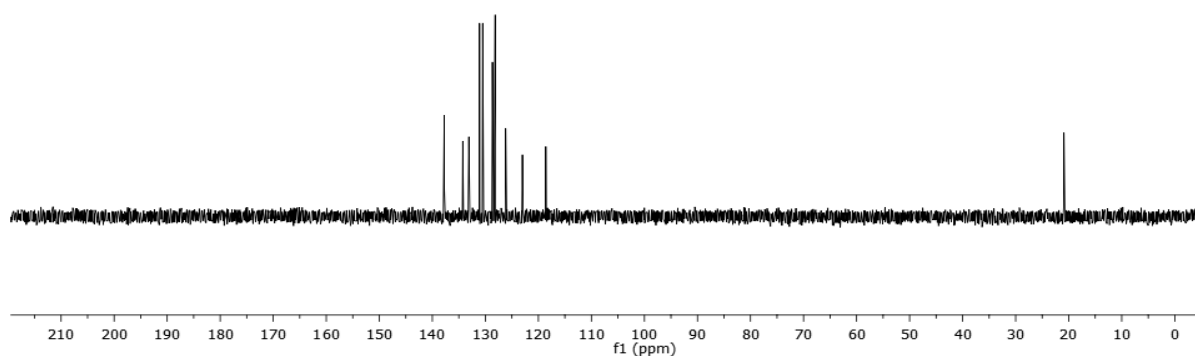
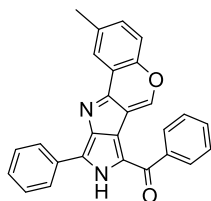


¹³C{¹H} NMR spectrum of **17b** (100 MHz, CDCl₃)

JKR-ED-155-A
 CL3DEPT135 CDCl₃ {D:\JKR} KOPAL 1

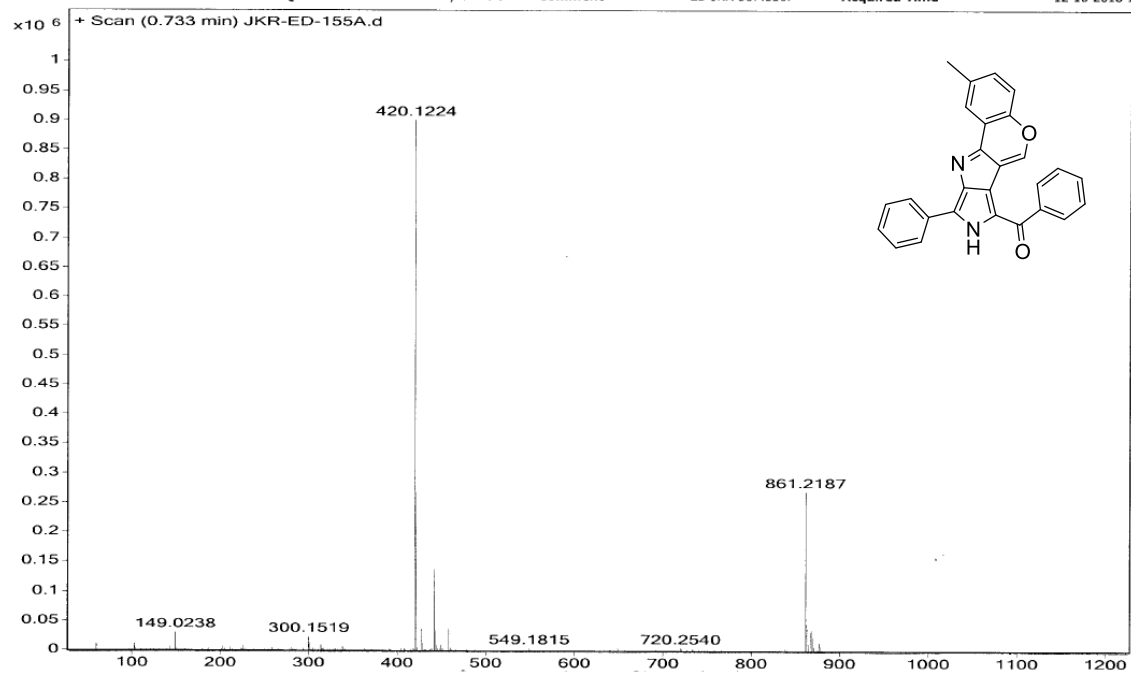
137.4
 134.26
 133.11
 131.09
 130.50
 128.66
 128.15
 126.17
 123.01
 118.60

20.90

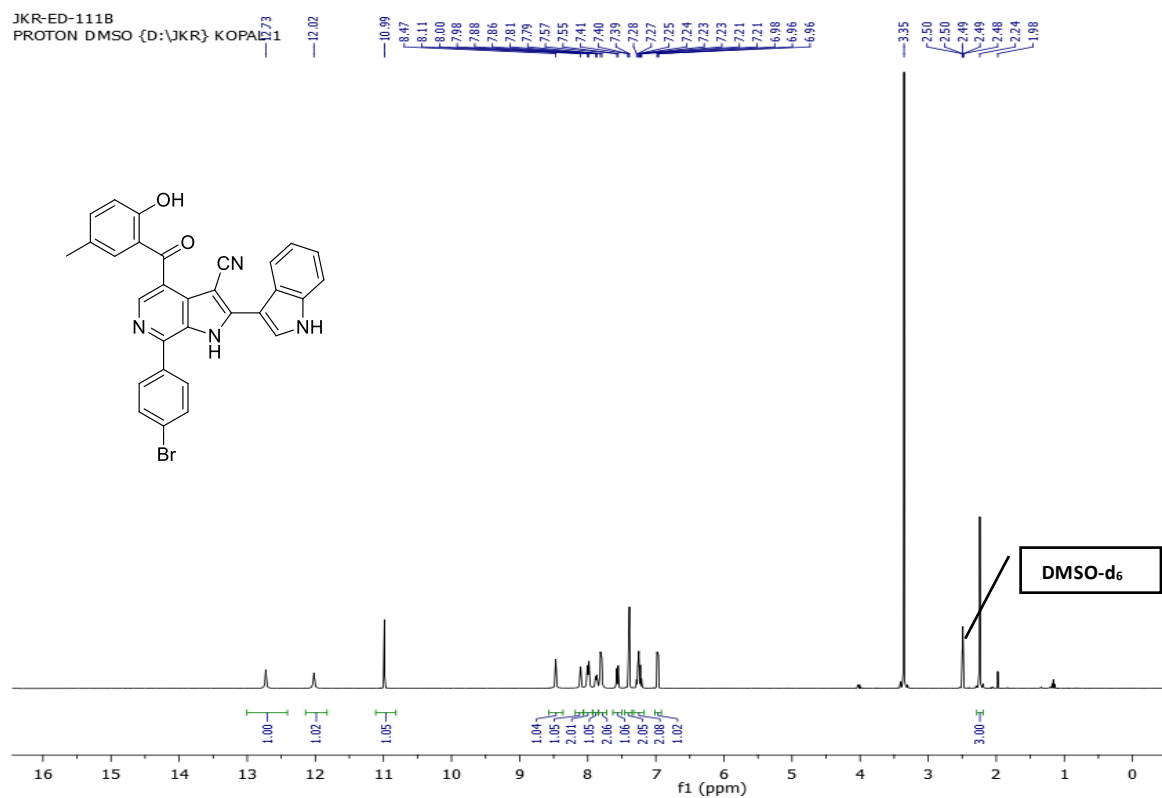


DEPT 135 NMR spectrum of **17b** (100 MHz, CDCl₃)

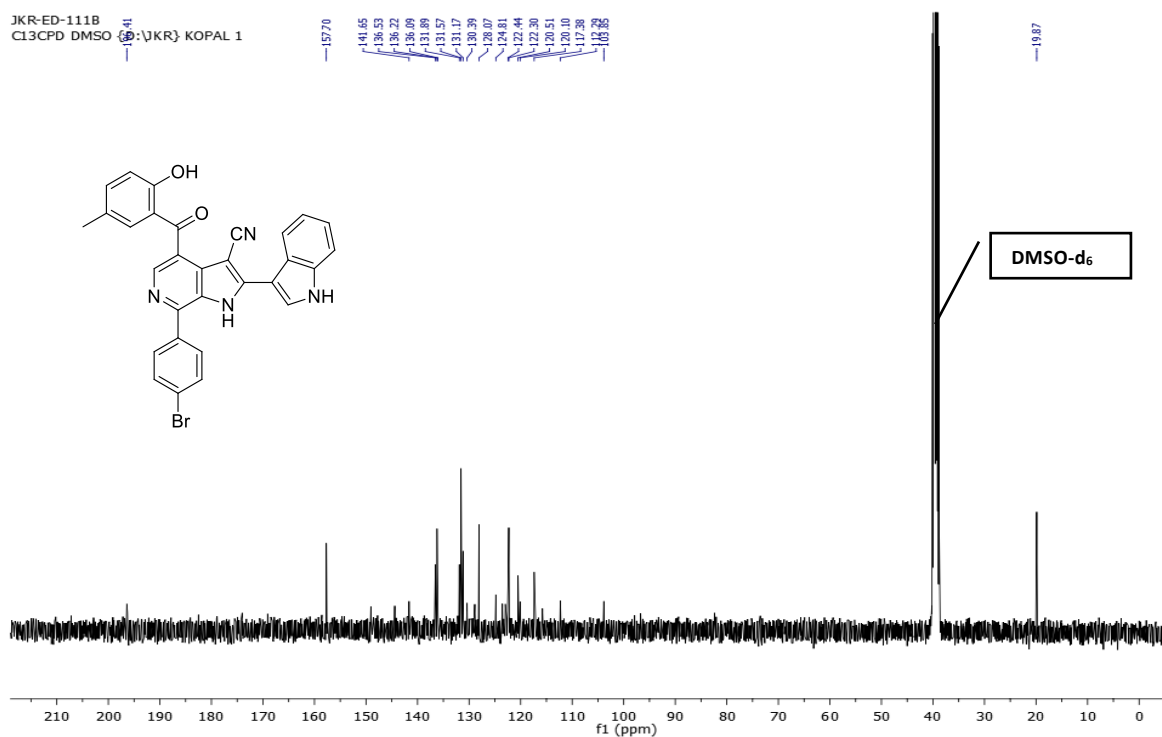
Sample Name	JKR-ED-155A	Position		Instrument Name	Q-TOF	User Name	QTOF-PU\admin
Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	JKR-ED-155A.d	ACQ Method	Pondicherry Universi	Comment	ED-JKR-387.1107	Acquired Time	12-10-2018 13:59:46



HRMS (ESI) spectrum of **17b**

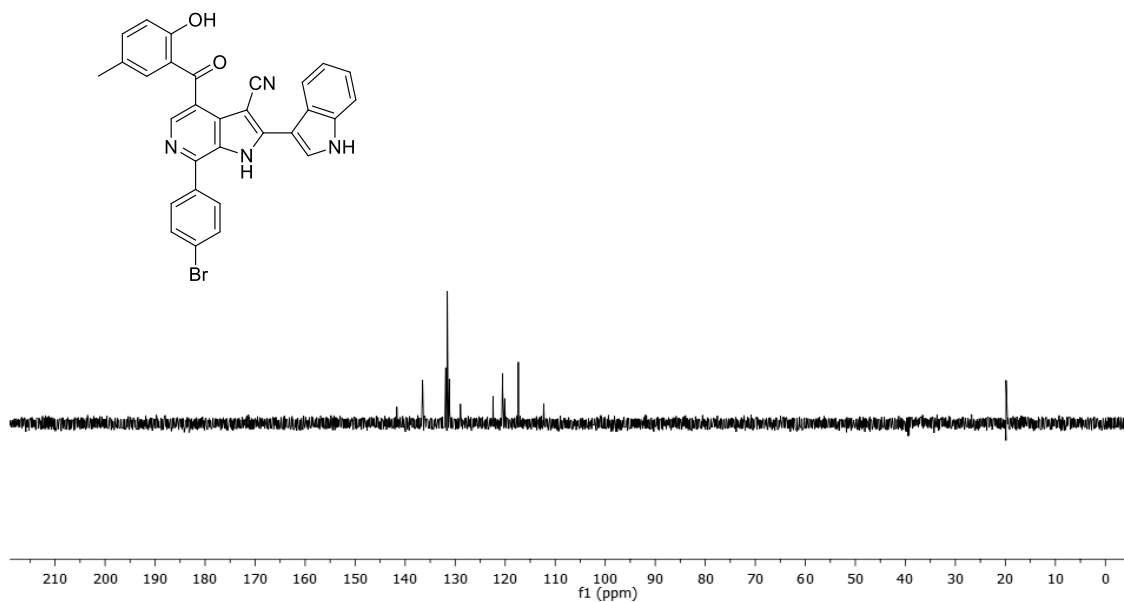
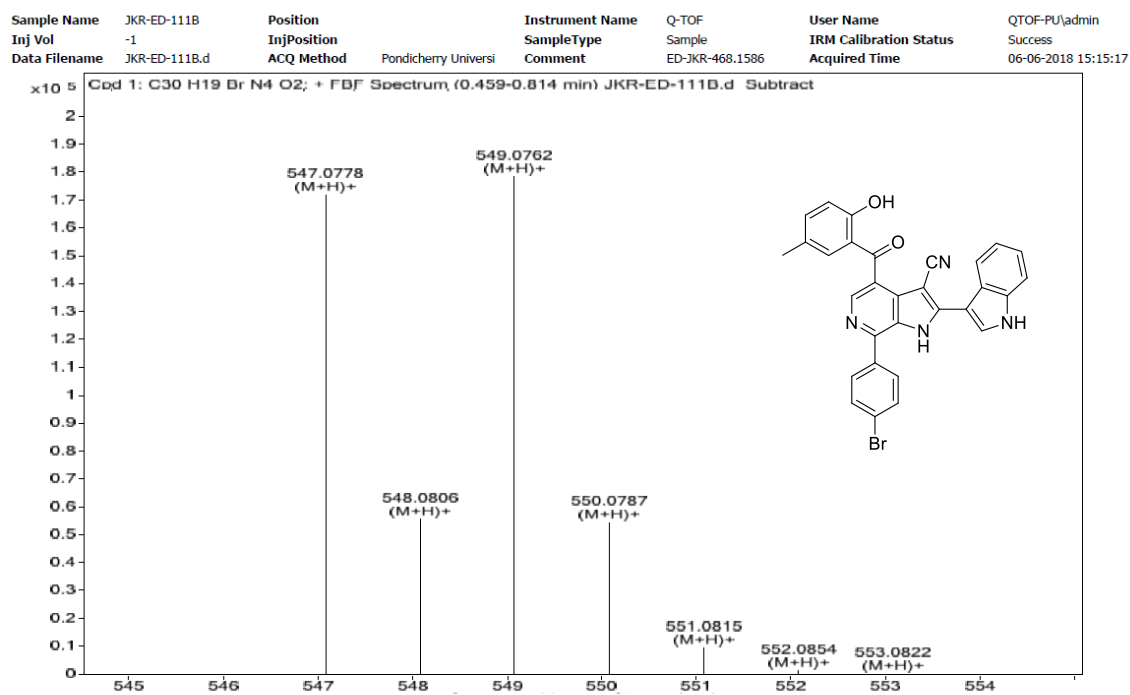


^1H NMR spectrum of **18a** (400 MHz, $\text{DMSO}-d_6$)

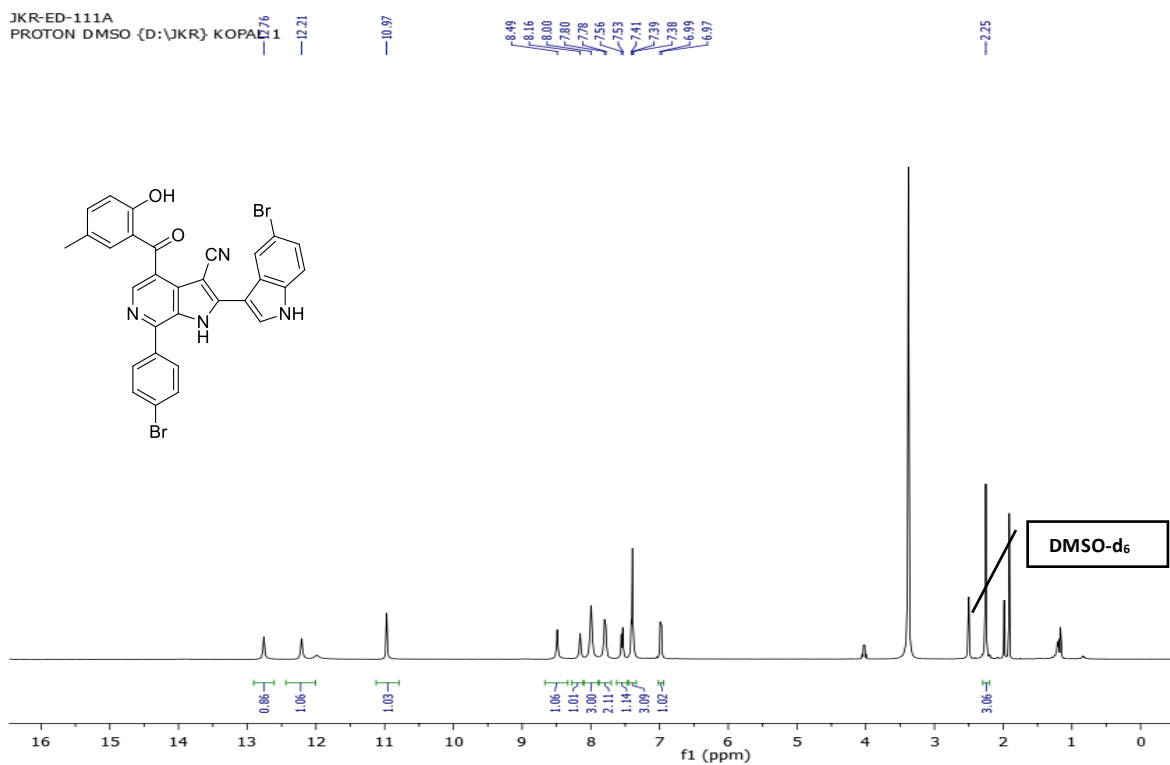


$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **18a** (100 MHz, $\text{DMSO}-d_6$)

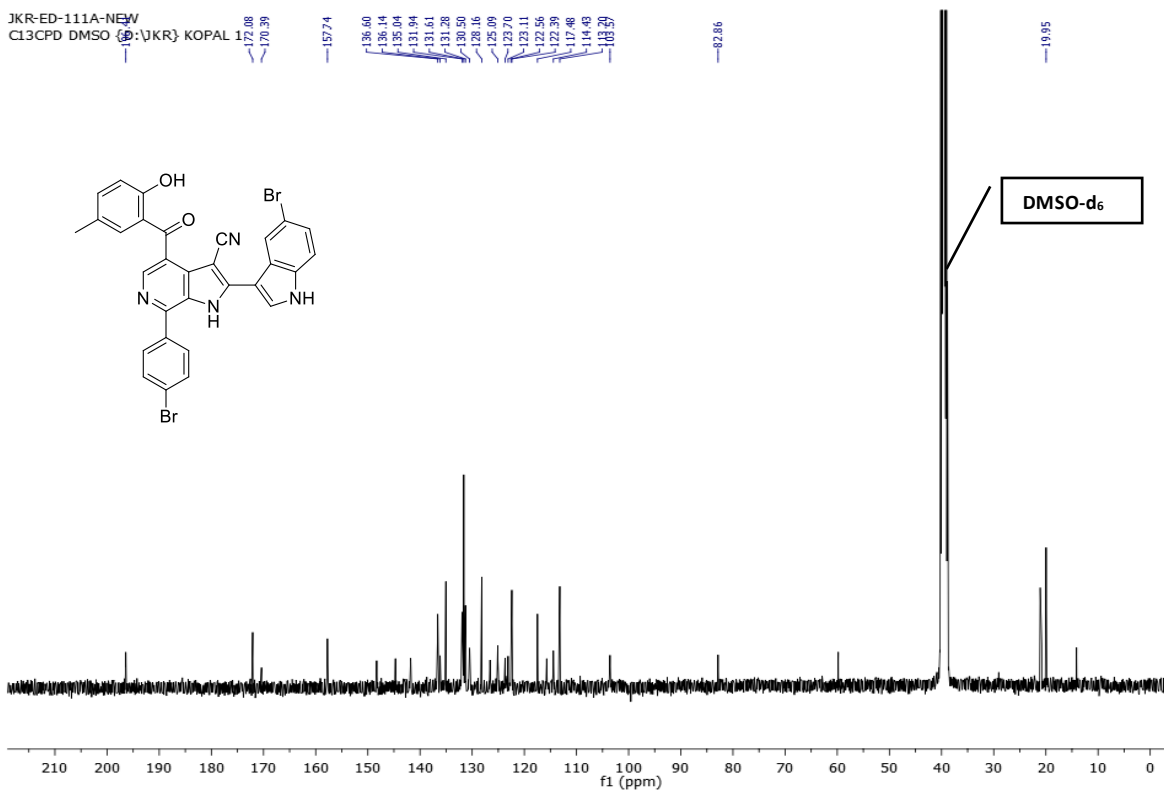
—19.86

DEPT 135 NMR spectrum of **18a** (100 MHz, DMSO-*d*₆)

HRMS (ESI) spectrum of **18a**



^1H NMR spectrum of **18b** (400 MHz, DMSO- d_6)

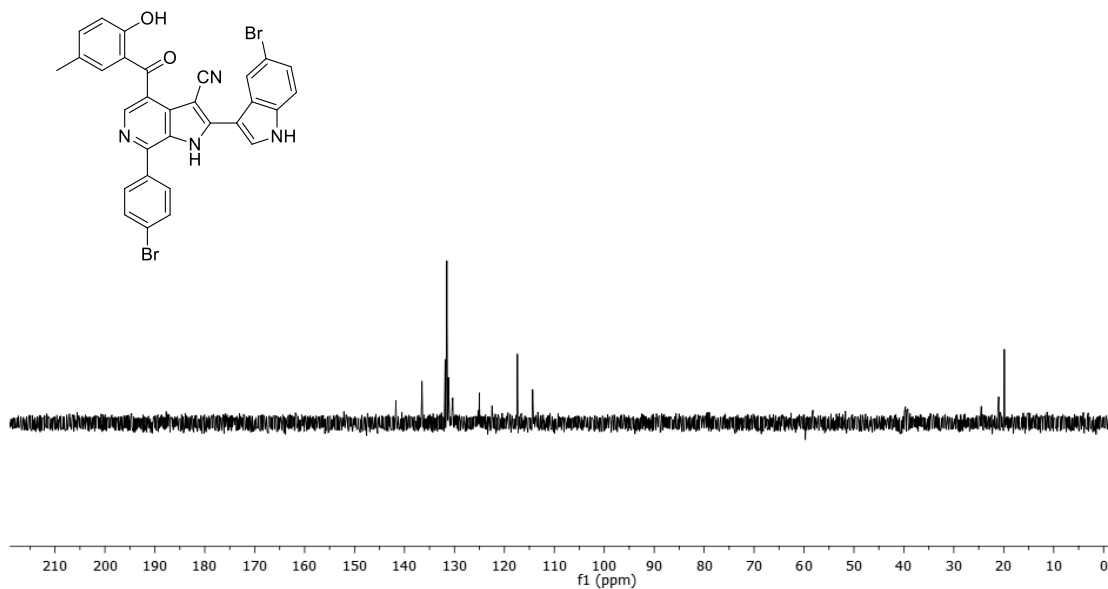


$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **18b** (100 MHz, DMSO- d_6)

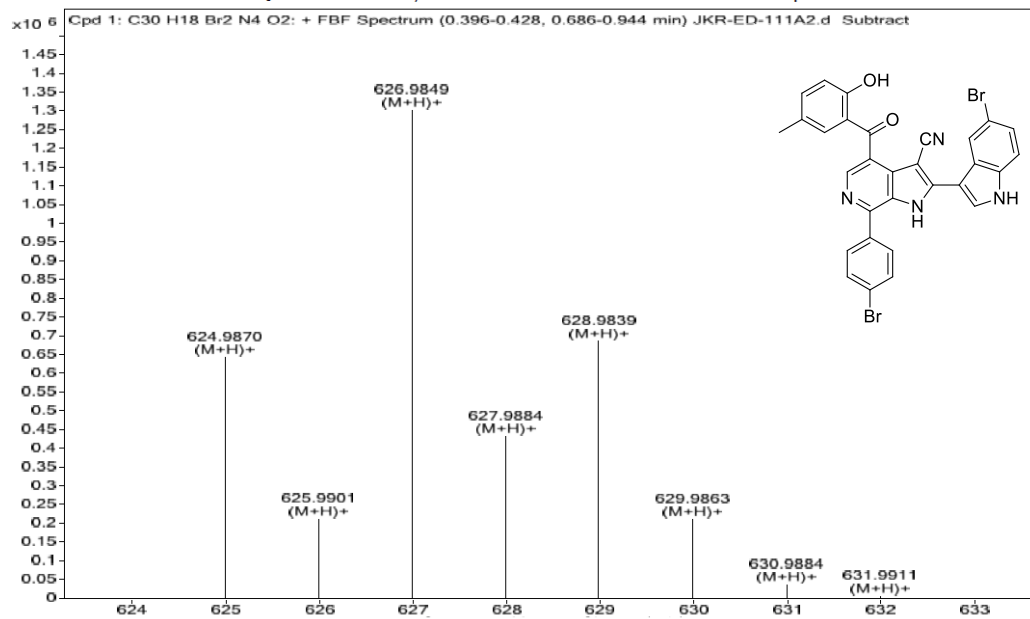
JKR-ED-111A
C13DEPT135 DMSO {D:\JKR} KOPAL 1

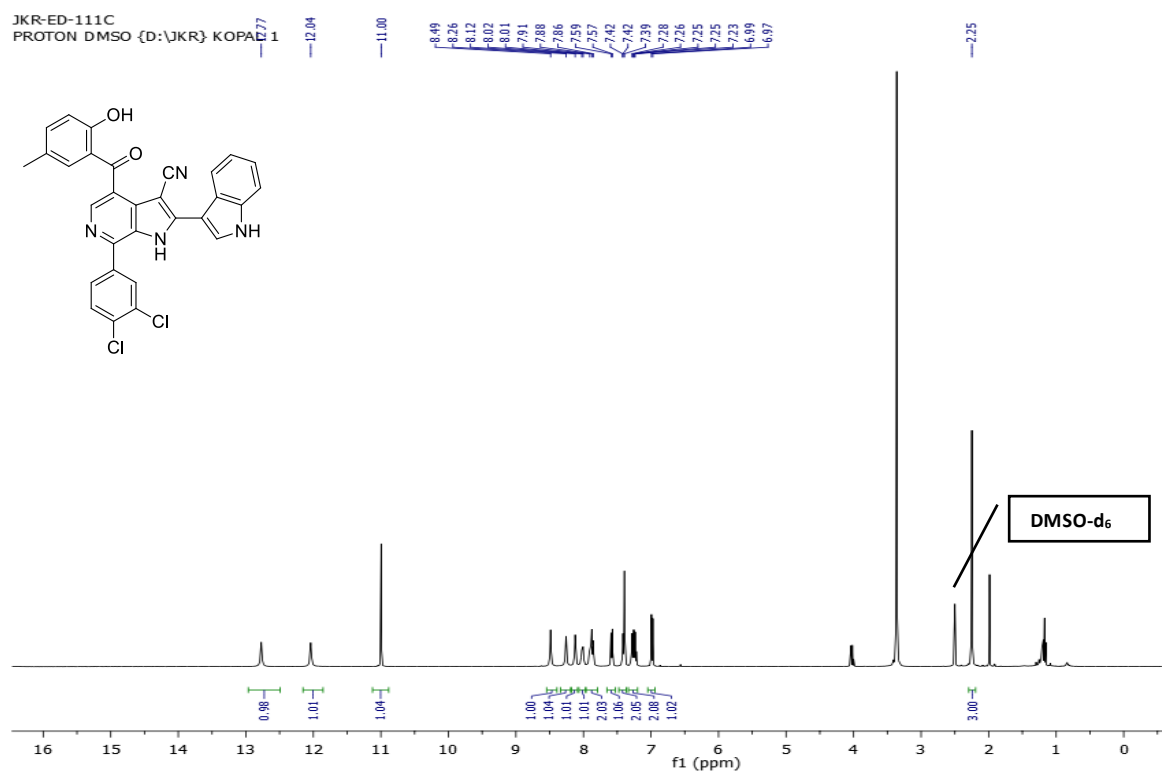
141.23
136.51
135.85
131.62
131.20
130.34
125.01
122.49
117.39
114.34

19.87

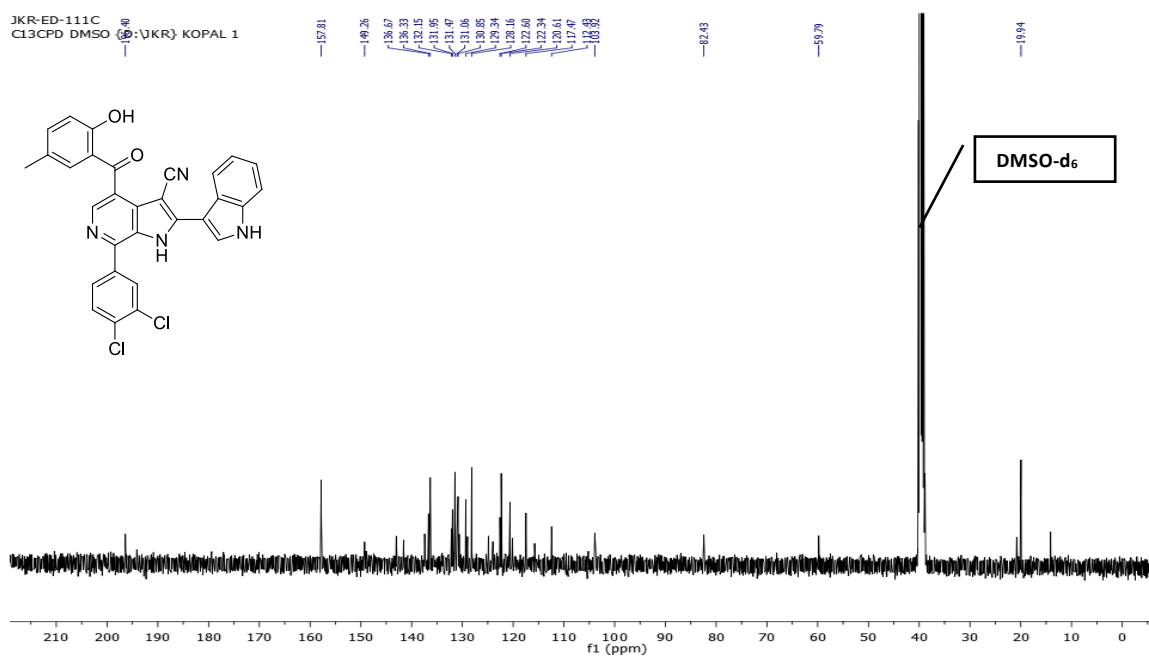


Sample Name	JKR-ED-111A	Position	Instrument Name	Q-TOF	User Name	QTOF-PU\admin
Inj Vol	-1	InjPosition	SampleType	Sample	IRM Calibration Status	Success
Data Filename	JKR-ED-111A2.d	ACQ Method	Comment	ED-JKR-454.1430	Acquired Time	24-05-2018 12:18:43





^1H NMR spectrum of **18c** (400 MHz, DMSO- d_6)

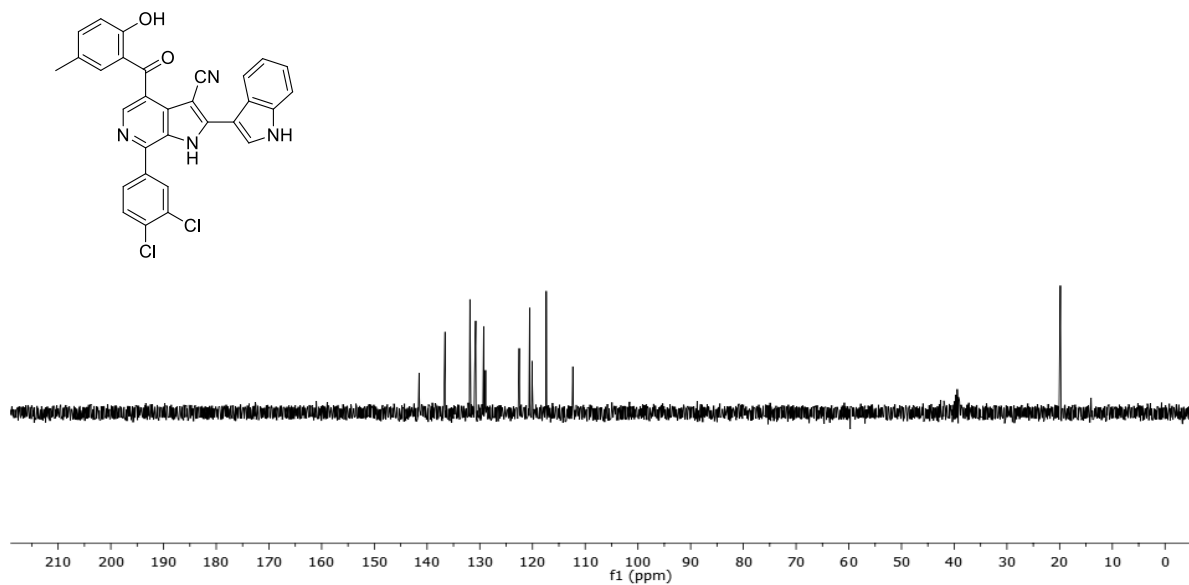


$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **18c** (100 MHz, DMSO- d_6)

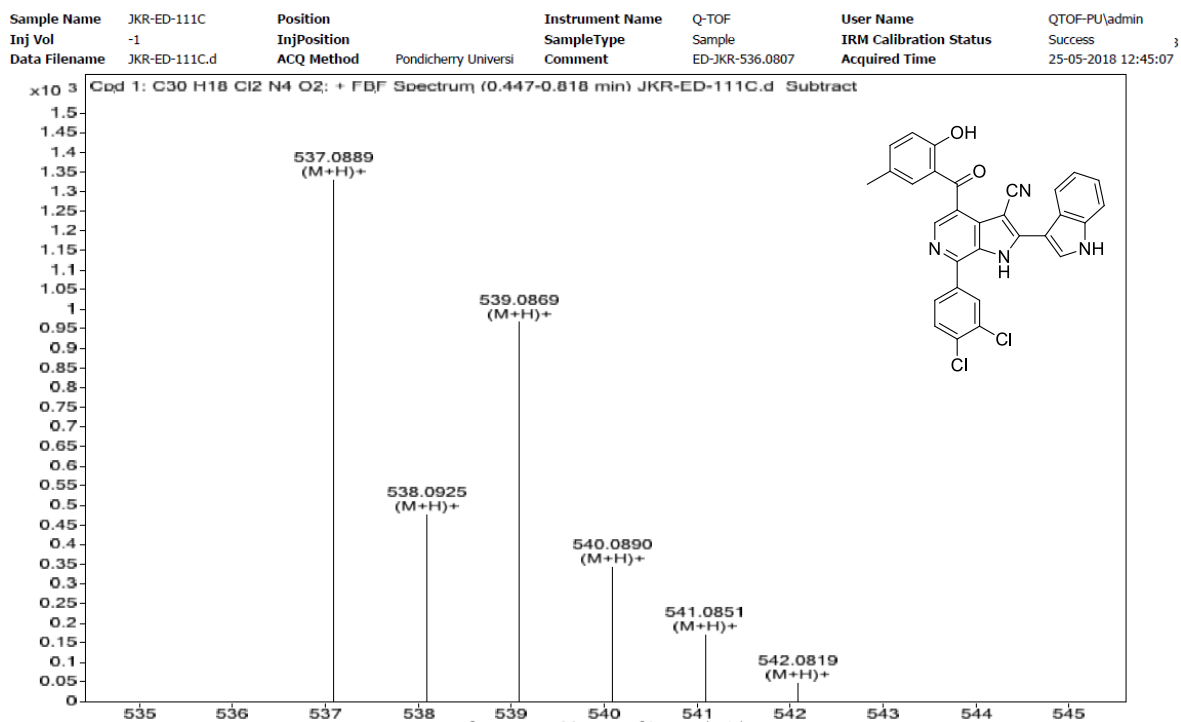
JKR-ED-111C
CL3DEPT135 DMSO {D:\JKR} KOPAL 1

141.51
136.59
131.87
130.97
130.78
129.26
128.91
122.52
120.54
120.06
117.39
112.35

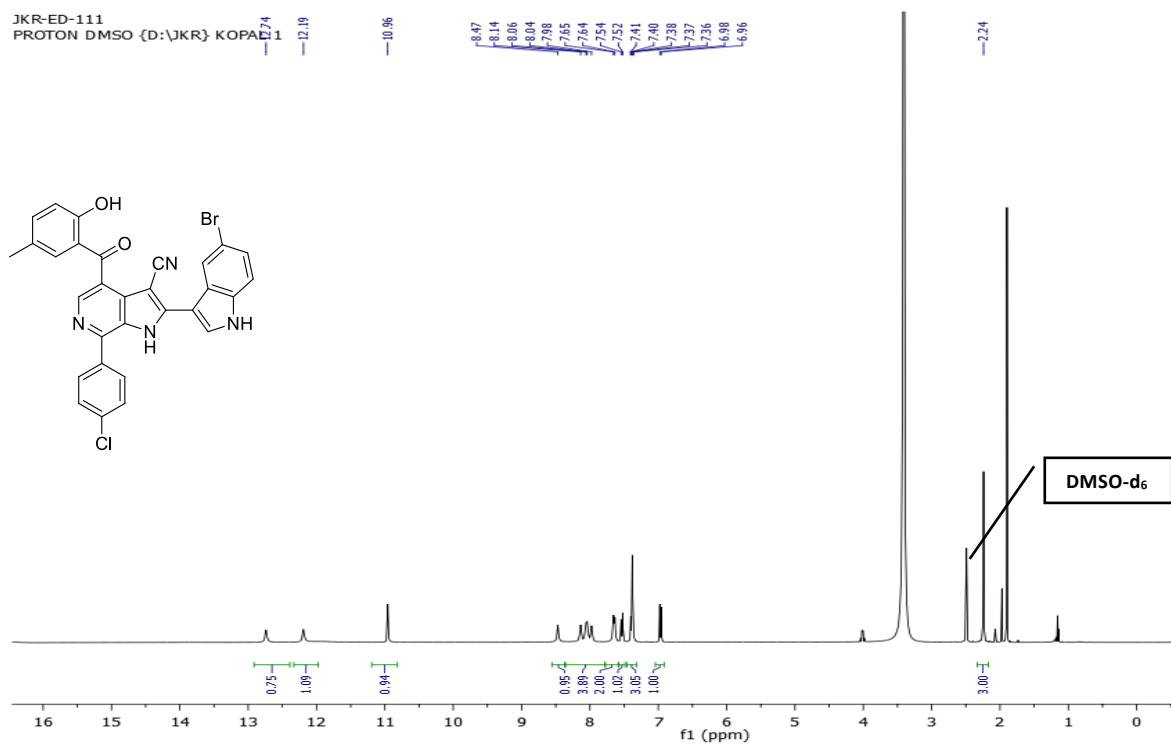
19.86



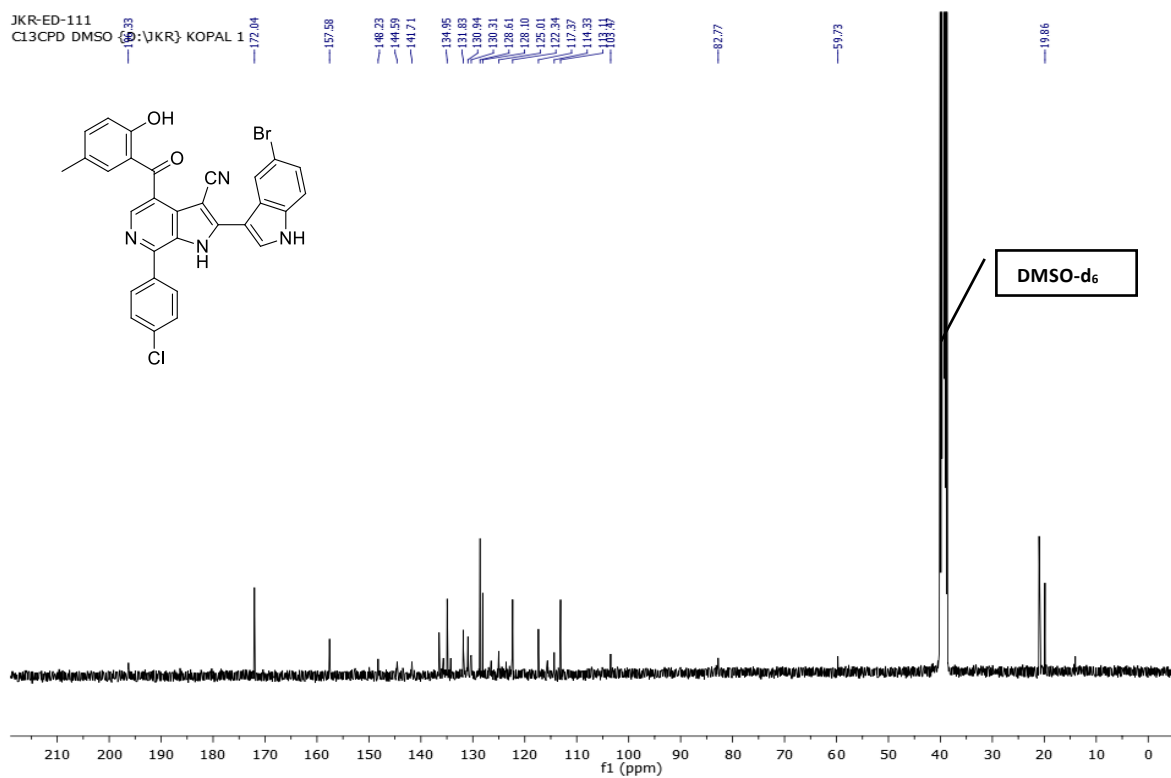
DEPT 135 NMR spectrum of **18c** (100 MHz, DMSO- d_6)



HRMS (ESI) spectrum of **18c**



^1H NMR spectrum of **18d** (400 MHz, DMSO- d_6)

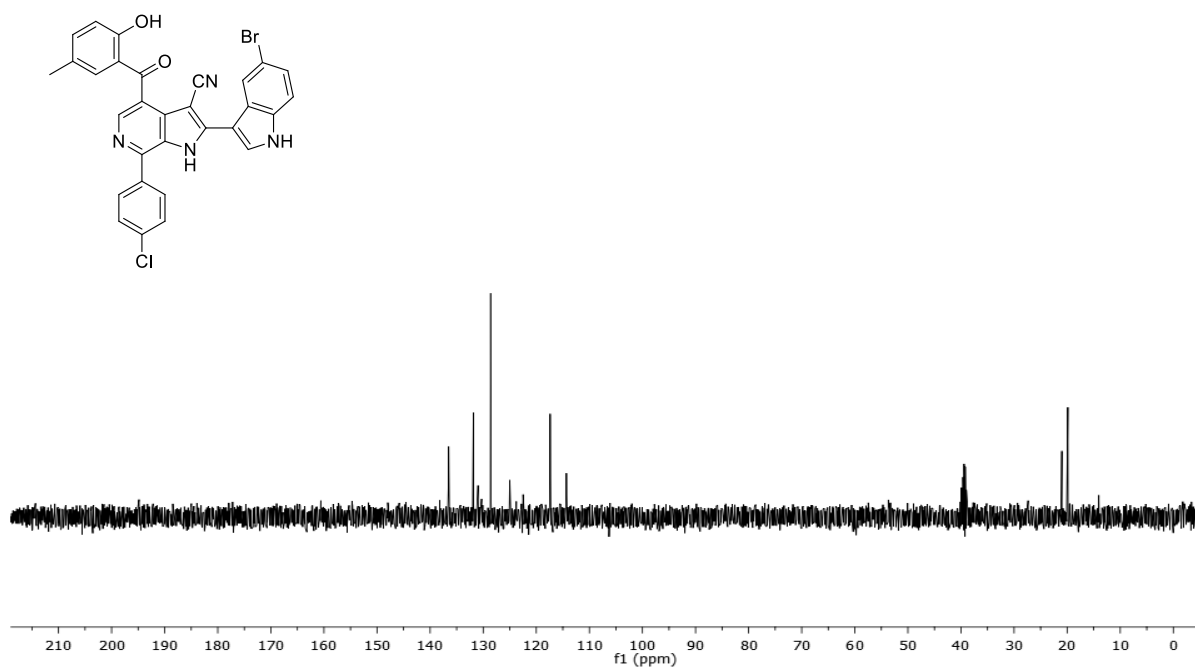


$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **18d** (100 MHz, DMSO- d_6)

JKR-ED-111E
C13DEPT135 DMSO {D:\JKR} KOPAL 1

36.51
31.85
30.97
30.30
28.60
25.00
23.76
22.49
17.39
14.32

198.7



DEPT 135 NMR spectrum of **18d** (100 MHz, DMSO-*d*₆)

III. Experimental Details of X-ray analysis of Compound 4i

Single crystal of compound **4i** was prepared using DMSO solvent by a slow evaporation method. X-ray diffraction data were collected using Bruker AXS Kappa ApexII CCD diffractometer equipped with graphite monochromated MoK α ($\lambda=0.71073\text{\AA}$) radiation. The single crystal of size ca. 0.25 x 0.22 x 0.18 mm was used for data collection. Data collection, data reduction and absorption correction were performed by APEX2, SAINT-plus and SADABS [v2014/5] programs¹. The structure was solved by direct methods procedure using SHELXS-97 (Sheldrick, 2008) and refined by full-matrix least-squares procedure on F² using SHELXL-2014(Sheldrick, 2015) program². All the non-hydrogen atoms were subjected to anisotropic refinement whereas the hydrogen atoms were refined isotropically. The H-atoms bound to the C-atoms were treated as riding atoms with Uiso(H) set to 1.5Ueq \odot and C–H distance of 0.96 \AA for CH₃ groups and Uiso(H) set to 1.2Ueq \odot and C–H distance of 0.93 \AA for aromatic CH. The H atoms bounded to amine nitrogen were refined to constrained distances with Uiso(H) = 1.2 Ueq(N), N—H distances of 0.90(1) \AA . The final refinement converged to the R-value of 0.0531 for 3824 observed reflections. Crystallographic data **4i** have been deposited with the Cambridge Crystallographic Data Center, (39) CCDC 1881467. Copies of this information may be obtained free of charge from the Director, CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (Fax: +44 1223 336033; e-mail: deposit@ccdc.cam.ac.uk or www.ccdc.cam.ac.uk). Crystal structure determination was performed in the Department of Chemistry, Indian Institute of Technology Madras, Chennai – 600036, INDIA.

1. Bruker, **2014**, SADABS v2014/5, Bruker AXS Inc., Madison, Wisconsin, USA.
2. Sheldrick, G. M. **2015**, *Acta Cryst.* C71, 3–8.

IV. ORTEP diagram of compound 4i

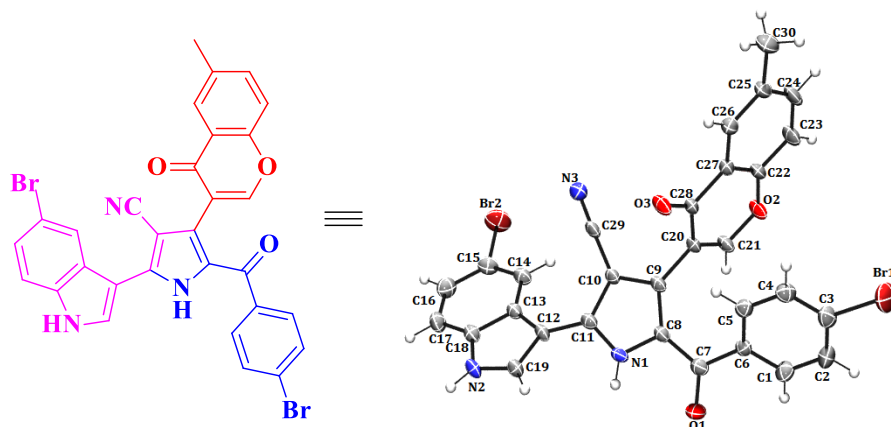


Figure S1. Molecular configuration and the atom numbering structure of **4i** crystal. Displacement ellipsoids are drawn at 30% probability level.

V. Table S1. Crystal data and structure refinement for 4i

Bond precision:	C-C = 0.0066 Å		Wavelength = 0.71073
Cell:	a = 11.6878(4)	b = 12.5438(4)	c = 13.3312(4)
	alpha = 70.9079(14)	beta = 72.8568(15)	gamma = 81.4490(16)
Temperature:	296 K		
	Calculated		Reported
Volume	1761.95(10)		1761.95(10)
Space group	P -1		P -1
Hall group	-P 1		-P 1
Moiety formula	C30 H17 Br2 N3 O3, 2(C2 H6 O S)		C34 H29 Br2 N3 O5 S2
Sum formula	C34 H29 Br2 N3 O5 S2		C34 H29 Br2 N3 O5 S2
Mr	783.52		783.52
Dx,g cm-3	1.477		1.477
Z	2		2
Mu (mm-1)	2.463		2.463
F000	792.0		792.0
F000'	791.65		
h,k,lmax	13,14,15		13,14,15
Nref	6187		6171
Tmin,Tmax	0.546,0.642		0.578,0.666
Tmin'	0.535		

Correction method= # Reported T Limits: Tmin= 0.578 Tmax=0.666

AbsCorr = MULTI-SCAN

Data completeness = 0.997

Theta(max) = 25.000

R(reflections) = 0.0531(3824)

wR2(reflections) = 0.1477(6171)

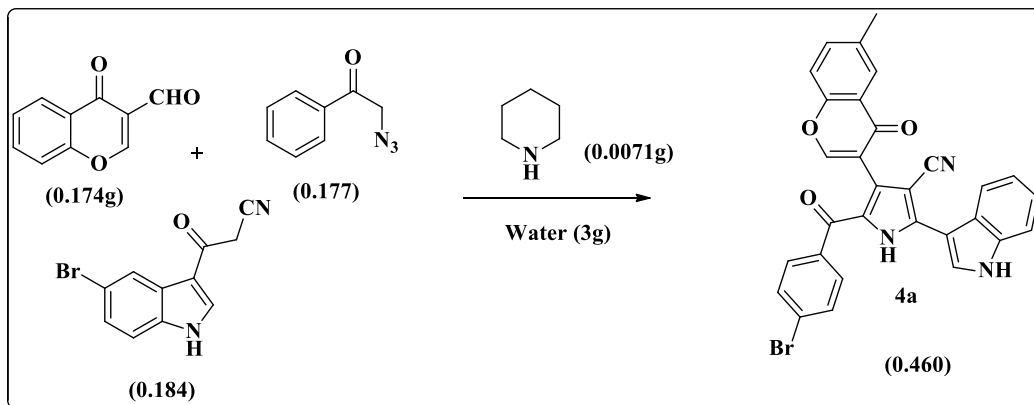
S = 1.034

Npar = 428

VI. Green matrix Factors: Atom Economy and E-Factor Calculations

E-Factor and Atom Economy for each class of compounds

E- Factor for compound 4a



Weight of total starting material – Product weight

$$\text{E-Factor} = \frac{\text{Weight of total starting material} - \text{Product weight}}{\text{Product weight}}$$

$$\text{E-Factor} = \frac{3.5427 - 0.46}{0.46}$$

$$\text{E-Factor} = 6.69$$

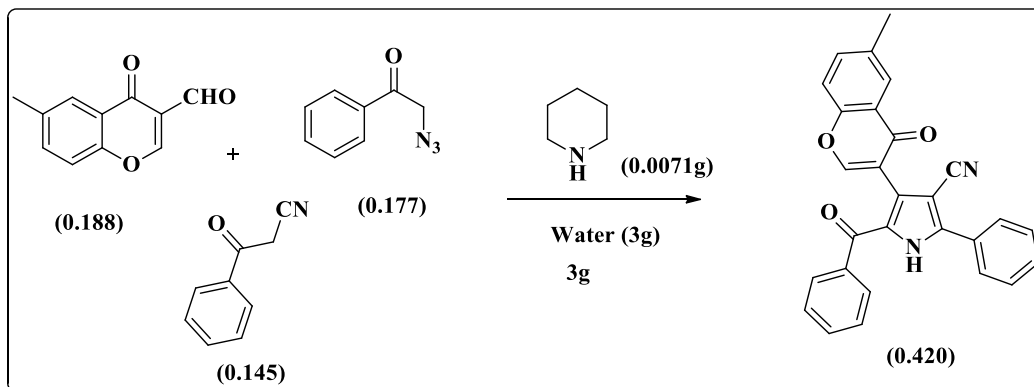
Atom economy for compound 4a

$$\text{Atom Economy} = \frac{\text{Mass of atoms in the desired product}}{\text{Mass of atoms in the reactant}}$$

$$\text{Atom Economy} = \frac{455 \times 100}{650}$$

$$\text{Atom Economy} = 70.03$$

E- Factor for compound **4q**



$$\text{E-Factor} = \frac{\text{Weight of total starting material} - \text{Product weight}}{\text{Product weight}}$$

$$\text{E-Factor} = \frac{3.5171 - 0.425}{0.425}$$

$$\text{E-Factor} = 7.27$$

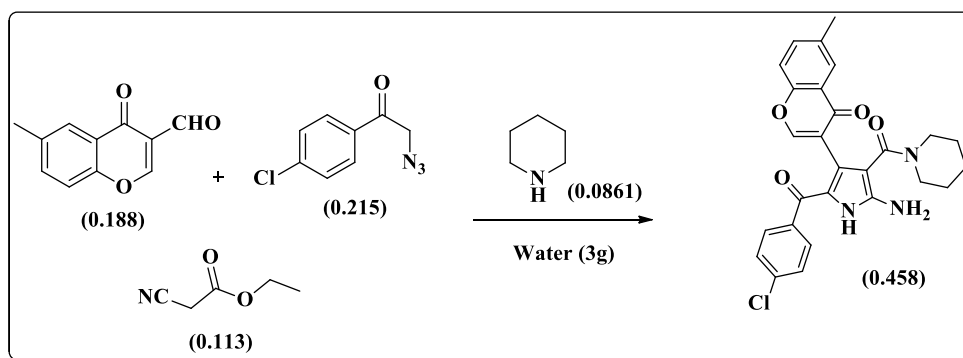
Atom economy for compound **4q**

$$\text{Atom Economy} = \frac{\text{Mass of atoms in the desired product}}{\text{Mass of atoms in the reactant}}$$

$$\text{Atom Economy} = \frac{430 \times 100}{494}$$

$$\text{Atom Economy} = 87.04$$

E- Factor for compound 8a



Weight of total starting material – Product weight

$$\text{E-Factor} = \frac{\text{Weight of total starting material} - \text{Product weight}}{\text{Product weight}}$$

$$\text{E-Factor} = \frac{3.602 - 0.458}{0.458}$$

$$\text{E-Factor} = 6.86$$

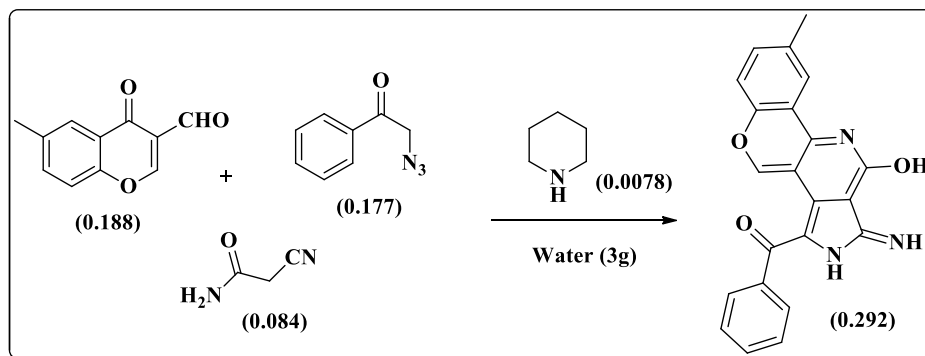
Atom economy for compound 8a

$$\text{Atom Economy} = \frac{\text{Mass of atoms in the desired product}}{\text{Mass of atoms in the reactant}}$$

$$\text{Atom Economy} = \frac{489}{627} \times 100$$

$$\text{Atom Economy} = 78.13$$

E- Factor for compound **10a**



Weight of total starting material – Product weight

$$\text{E-Factor} = \frac{\text{Weight of total starting material} - \text{Product weight}}{\text{Product weight}}$$

$$\text{E-Factor} = \frac{3.456 - 0.292}{0.292}$$

$$\text{E-Factor} = 10.83$$

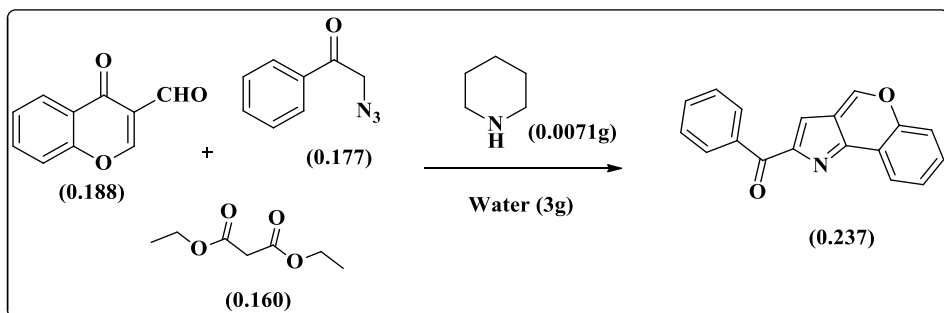
Atom economy for compound **10a**

$$\text{Atom Economy} = \frac{\text{Mass of atoms in the desired product}}{\text{Mass of atoms in the reactant}}$$

$$\text{Atom Economy} = \frac{369}{564} \times 100$$

$$\text{Atom Economy} = 65.49$$

E- Factor for compound **12a**



Weight of total starting material – Product weight

$$\text{E-Factor} = \frac{\text{Weight of total starting material} - \text{Product weight}}{\text{Product weight}}$$

$$\text{E-Factor} = \frac{3.53 - 0.237}{0.237}$$

$$\text{E-Factor} = 13.90$$

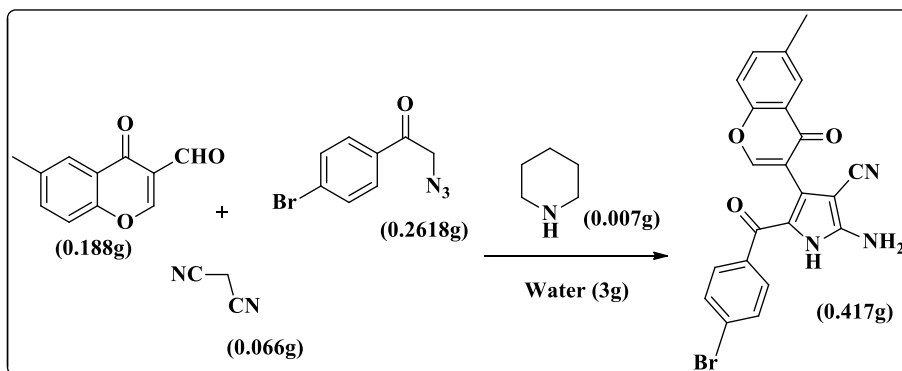
Atom economy for compound **12a**

$$\text{Atom Economy} = \frac{\text{Mass of atoms in the desired product}}{\text{Mass of atoms in the reactant}}$$

$$\text{Atom Economy} = \frac{273 \times 100}{640}$$

$$\text{Atom Economy} = 42.70$$

E- Factor for compound **15a**



Weight of total starting material – Product weight

$$\text{E-Factor} = \frac{\text{Weight of total starting material} - \text{Product weight}}{\text{Product weight}}$$

$$\text{E-Factor} = \frac{3.523 - 0.417}{0.417}$$

$$\text{E-Factor} = 7.43$$

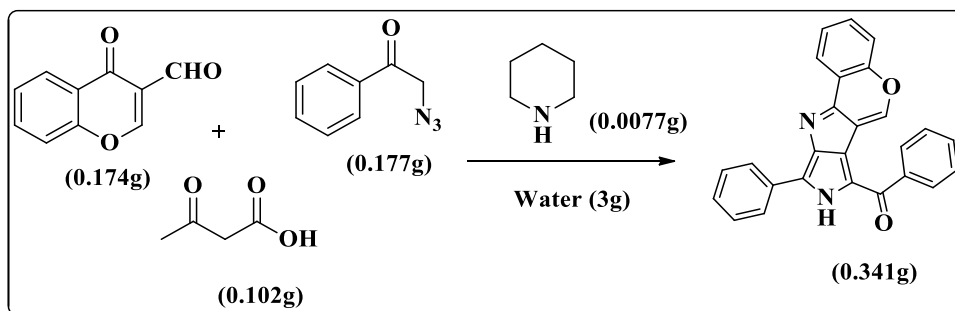
Atom economy for compound **15a**

$$\text{Atom Economy} = \frac{\text{Mass of atoms in the desired product}}{\text{Mass of atoms in the reactant}}$$

$$\text{Atom Economy} = \frac{447}{625} \times 100$$

$$\text{Atom Economy} = 71.52$$

E- Factor for compound **17a**



Weight of total starting material – Product weight

$$\text{E-Factor} = \frac{\text{Weight of total starting material} - \text{Product weight}}{\text{Product weight}}$$

$$\text{E-Factor} = \frac{3.489 - 0.341}{0.341}$$

$$\text{E-Factor} = 9.23$$

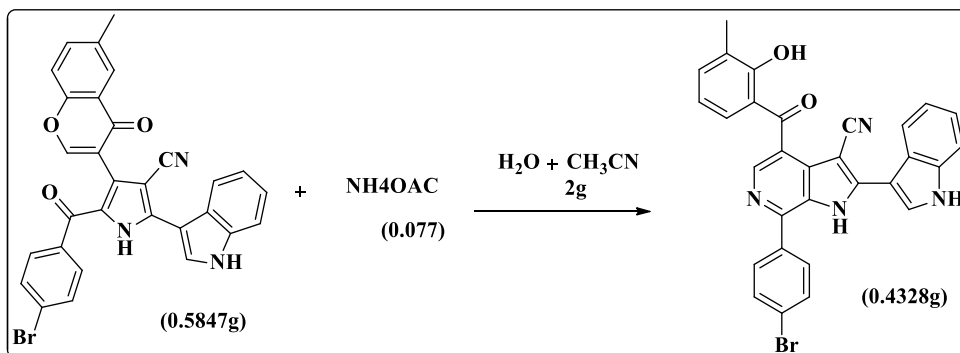
Atom economy for compound **17a**

$$\text{Atom Economy} = \frac{\text{Mass of atoms in the desired product}}{\text{Mass of atoms in the reactant}}$$

$$\text{Atom Economy} = \frac{388}{556} \times 100$$

$$\text{Atom Economy} = 69.80$$

E- Factor for compound **18a**



$$\text{E-Factor} = \frac{\text{Weight of total starting material} - \text{Product weight}}{\text{Product weight}}$$

$$\text{E-Factor} = \frac{2.624 - 0.4328}{0.4328}$$

$$\text{E-Factor} = 5.06$$

Atom economy for compound **18a**

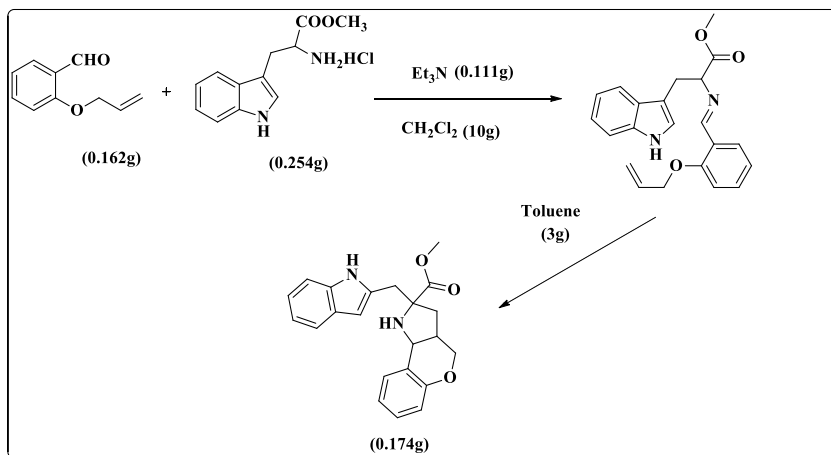
$$\text{Atom Economy} = \frac{\text{Mass of atoms in the desired product}}{\text{Mass of atoms in the reactant}}$$

$$\text{Atom Economy} = \frac{547}{684} \times 100$$

$$\text{Atom Economy} = 80.03$$

Comparison of E- Factor and Atom Economy of our methodology with other similar reports compound

E- Factor for similarly reported compound



Ref: N. Arumugam R. Raghunathan, , A. I. Almansour, U. Karama, *Bioorg. Med. Chem. Lett.* **2012**, 22, 1375–1379.

Weight of total starting material – Product weight

$$\text{E-Factor} = \frac{\text{Weight of total starting material} - \text{Product weight}}{\text{Product weight}}$$

$$\text{E-Factor} = \frac{13.527 - 0.174}{0.174}$$

$$\text{E-Factor} = 76.74$$

Comparison of E- Factor and Atom Economy

	E-Factor	Atom Economy
<p> </p> <p>Our methodology</p>	6.69	70.03
<p> </p> <p>Reported methodology</p>	76.74	50.2

Advantages of our methodology:

- 1) Higher atom economy
- 2) Low E factor
- 3) Remarkably eco-friendly solvent *viz* water used as reaction medium