Supporting Information

Synthesis, SAR and biological studies of sugar amino acid based almiramide analogues: *N*-methylation leads the way

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General Experimental Details:

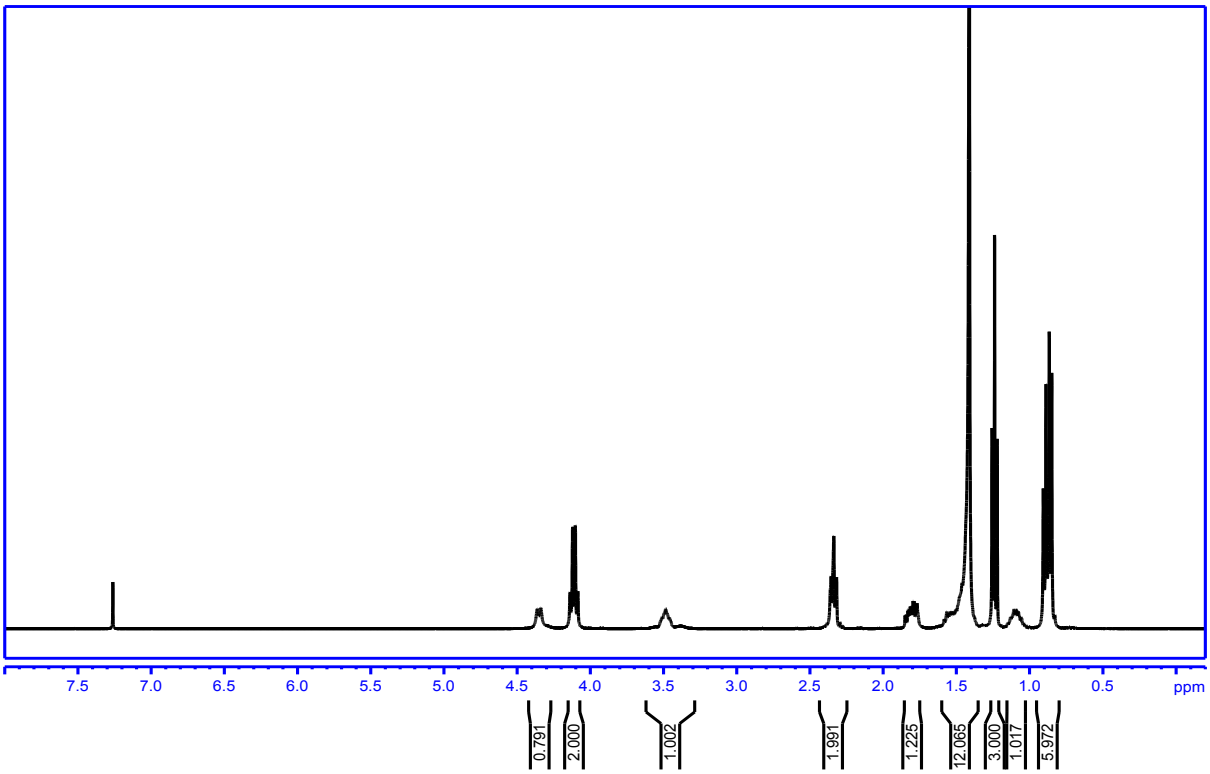
All the reactions were carried out under an inert atmosphere in oven-dried glassware using dry solvents, unless otherwise stated. All chemicals purchased from commercial suppliers were used as received unless otherwise stated. Reactions and chromatography fractions were monitored by Merck silica gel 60 F-254 glass TLC plates and visualized using UV light, 7% ethanolic phosphomolybdic acid-heat, 2.5% ethanolic anisaldehyde (with 1% AcOH and 3.3% conc. H_2SO_4), ninhydrin or chlorine/*o*-tolidine-heat as developing agents. Flash column chromatography was performed with 100-200 mesh silica gel and yields refer to chromatographically and spectroscopically pure compounds.

Instrumentation:

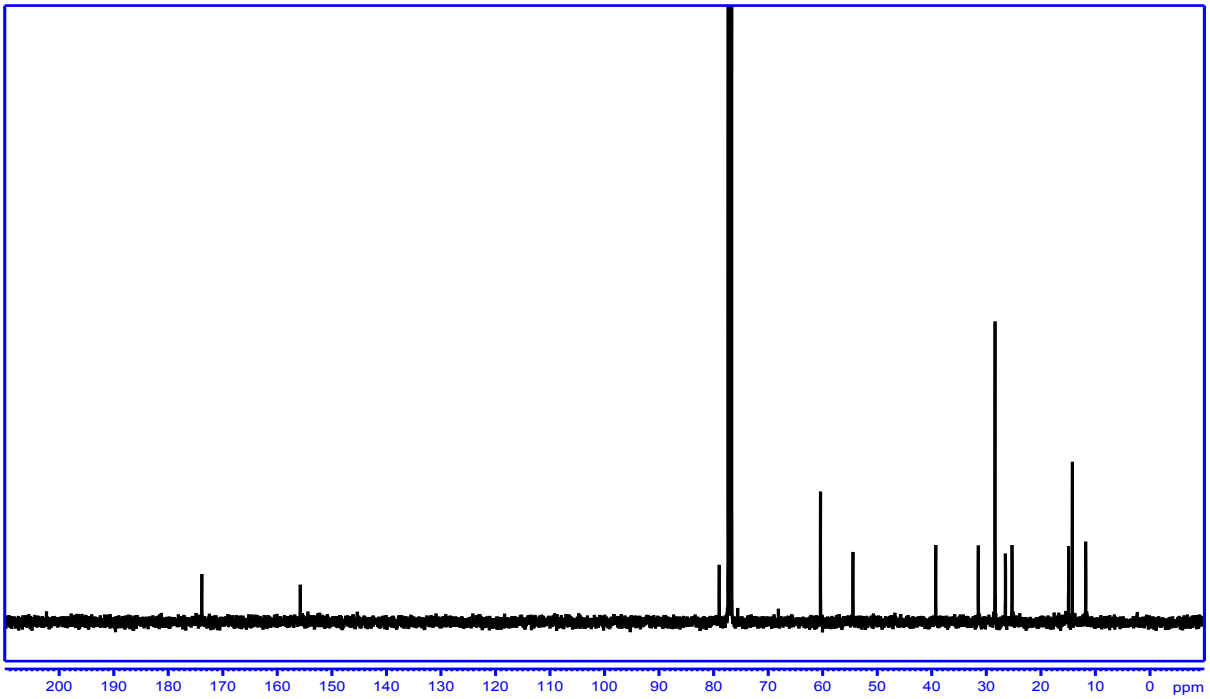
All NMR spectra were recorded in $CDCl_3$ or in DMSO-d_6 on a 300, 400 and 500 MHz instruments at 300 K and are calibrated to residual solvent peaks ($CHCl_3$ 7.26 ppm and 77.0 ppm, DMSO 2.50 ppm and 40 ppm). Multiplicities are abbreviated as: s = singlet; d = doublet; t = triplet; q = quartet; m = multiplate. All IR data were recorded as neat liquid or KBr pellets using a Perkin Elmer's RX I FTIR spectrophotometer. Mass spectra were obtained under electron spray ionisation (ESI) and HRMS spectra were taken with a 3000 mass spectrometer using Waters Agilent 6520-Q-TofMS/MS system and JEOL-AccuTOF JMS-T100 LC. RP-HPLC was performed on a waters HPLC system and Shimadzu's ISO 9001 HPLC system (model no. LC-20AD) equipped with a 5 µ SunFire C18 column (4.6 × 250 mm) and 5 µ Shimadzu's C18 column (4.6 × 250 mm) respectively in combination with eluants A (H_2O) and B (MeCN) with flow rate: 0.8 mL/min and photodiode array detector setting of λ = 210-254 nm.

Spectra (^{1}H and ^{13}C NMR) of Compounds:

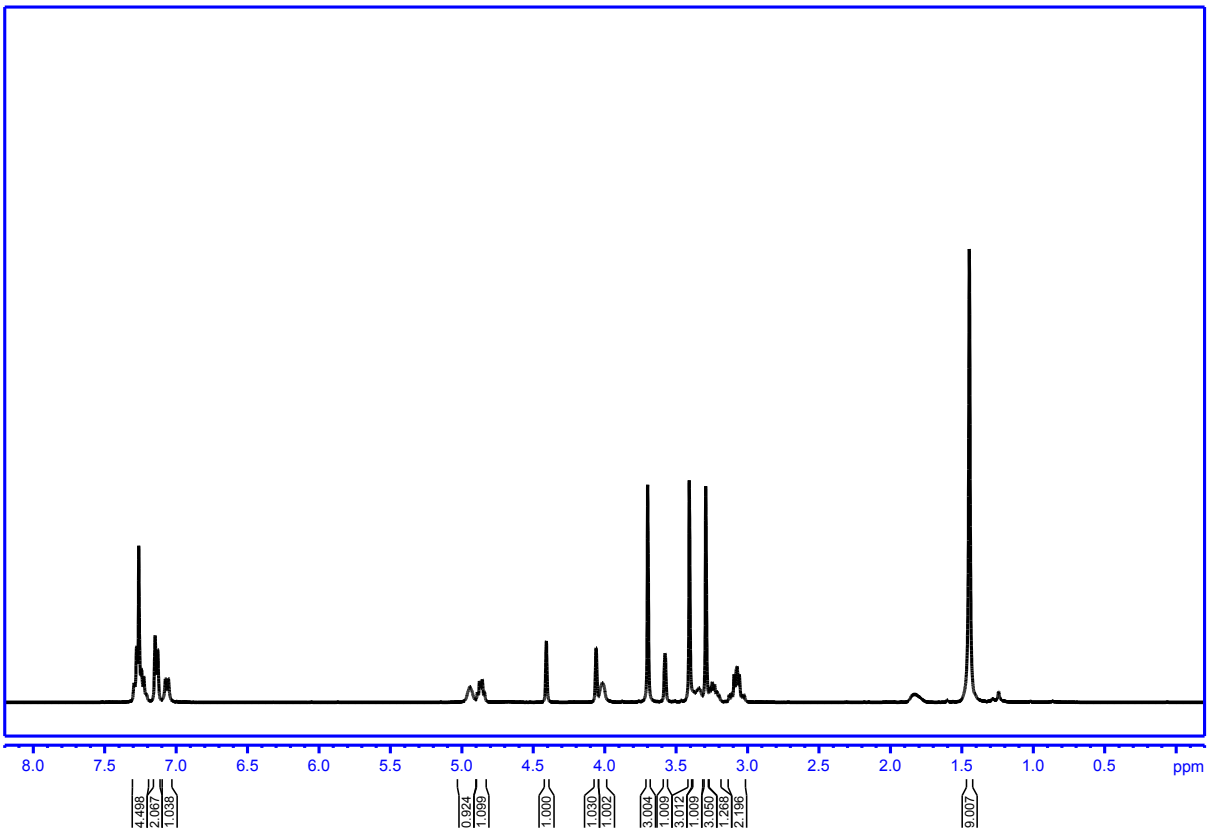
- **^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of compound 8.**



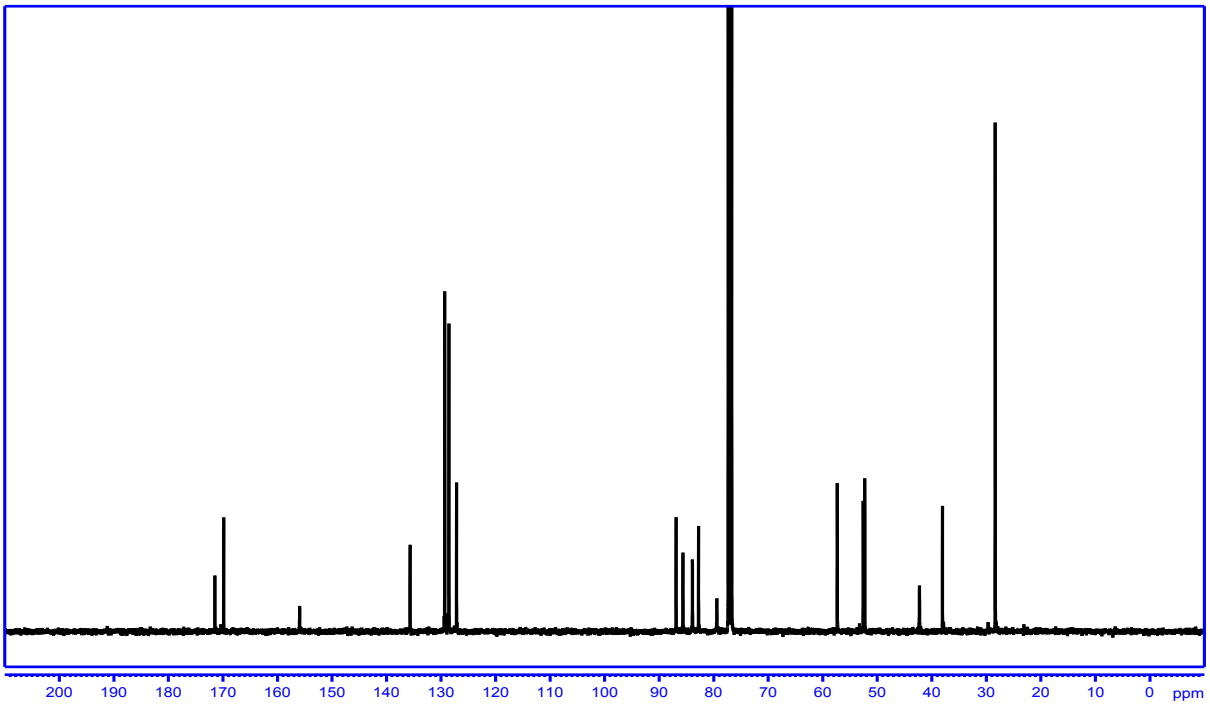
- **^{13}C NMR spectrum ($CDCl_3$, 100 MHz) of compound 8.**



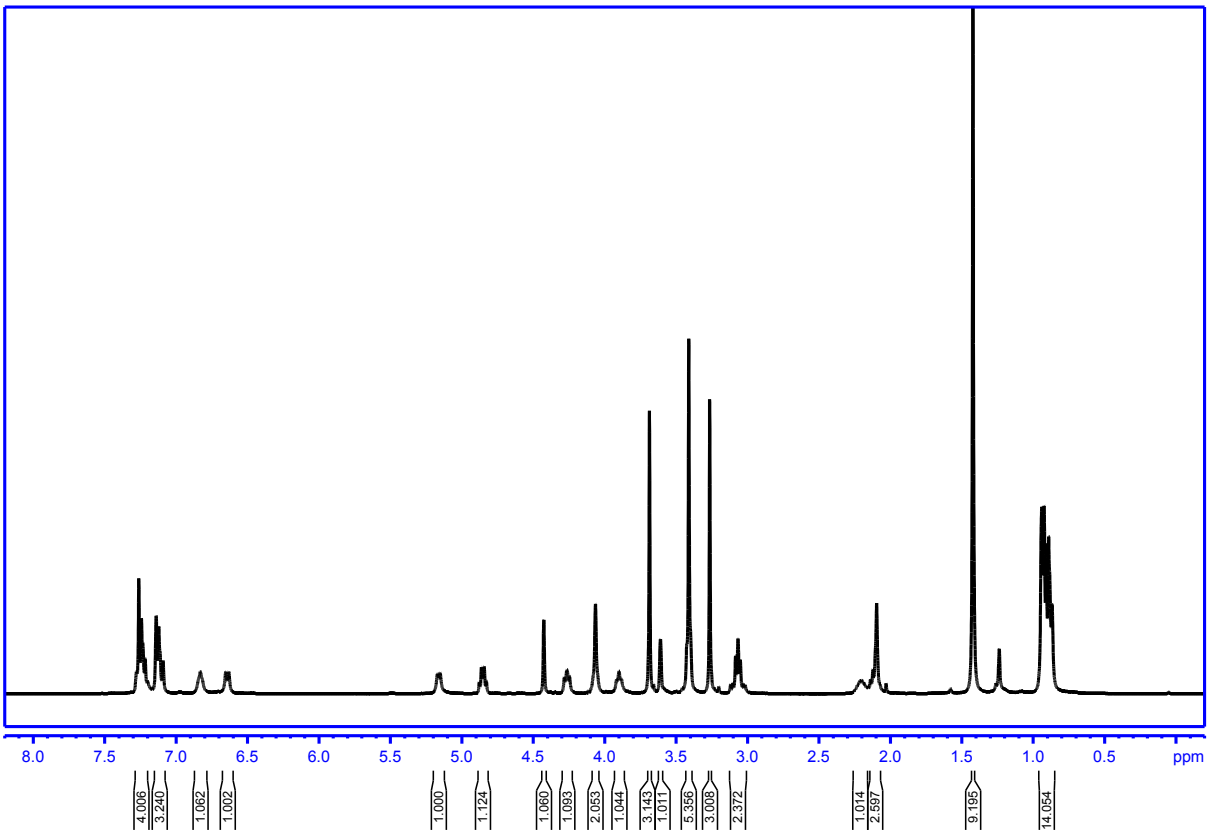
- **^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of compound 11.**



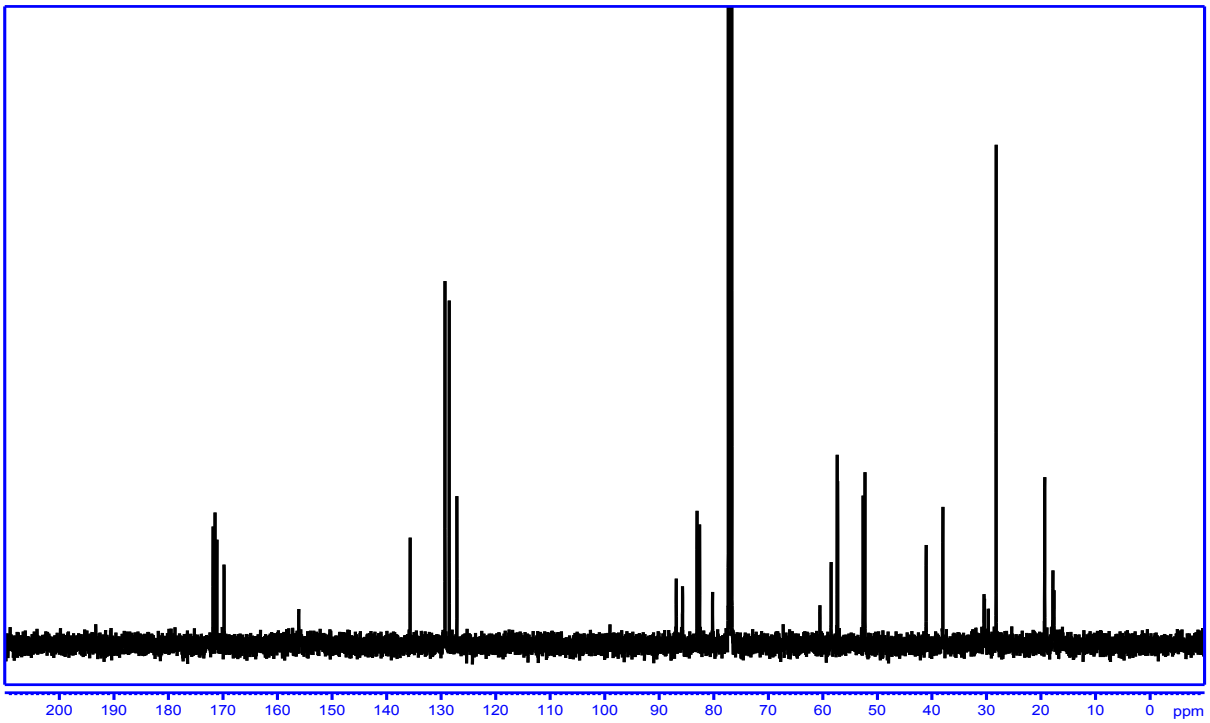
- **^{13}C NMR spectrum ($CDCl_3$, 100 MHz) of compound 11.**



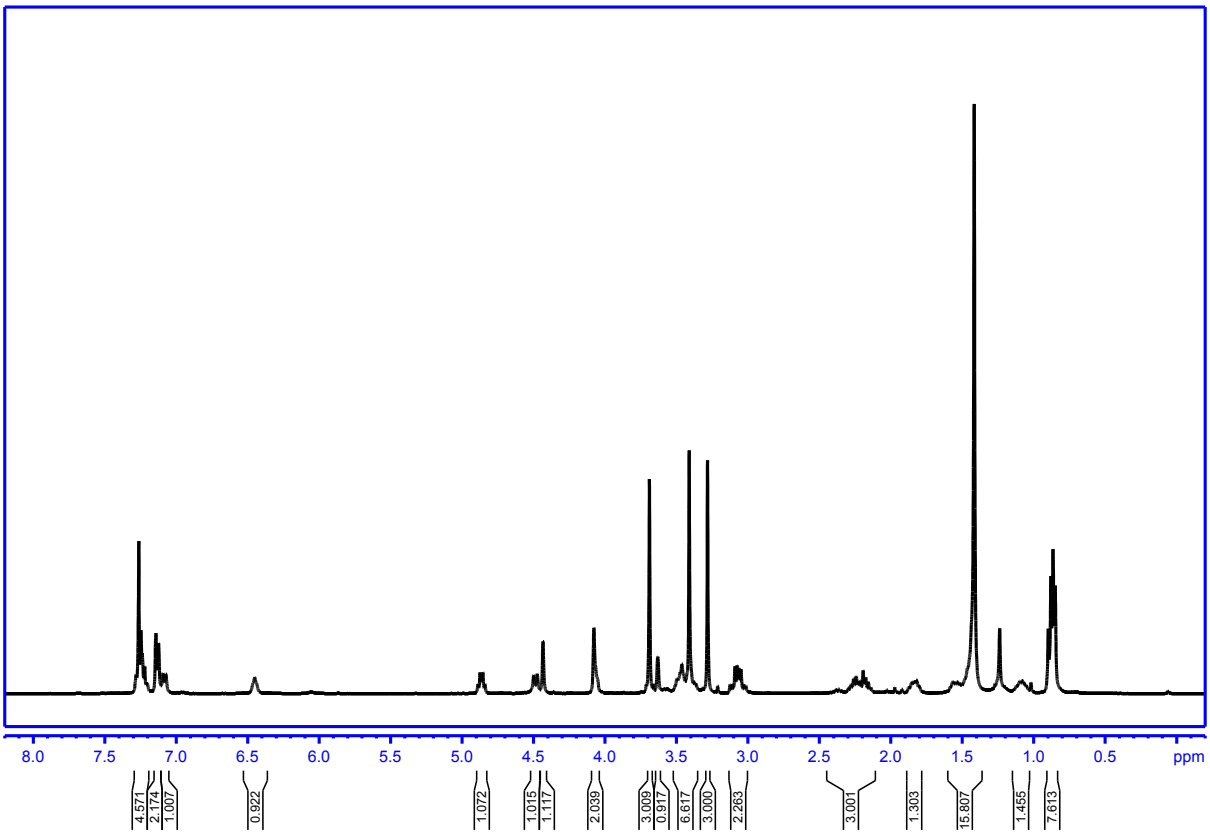
- **^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of compound 14.**



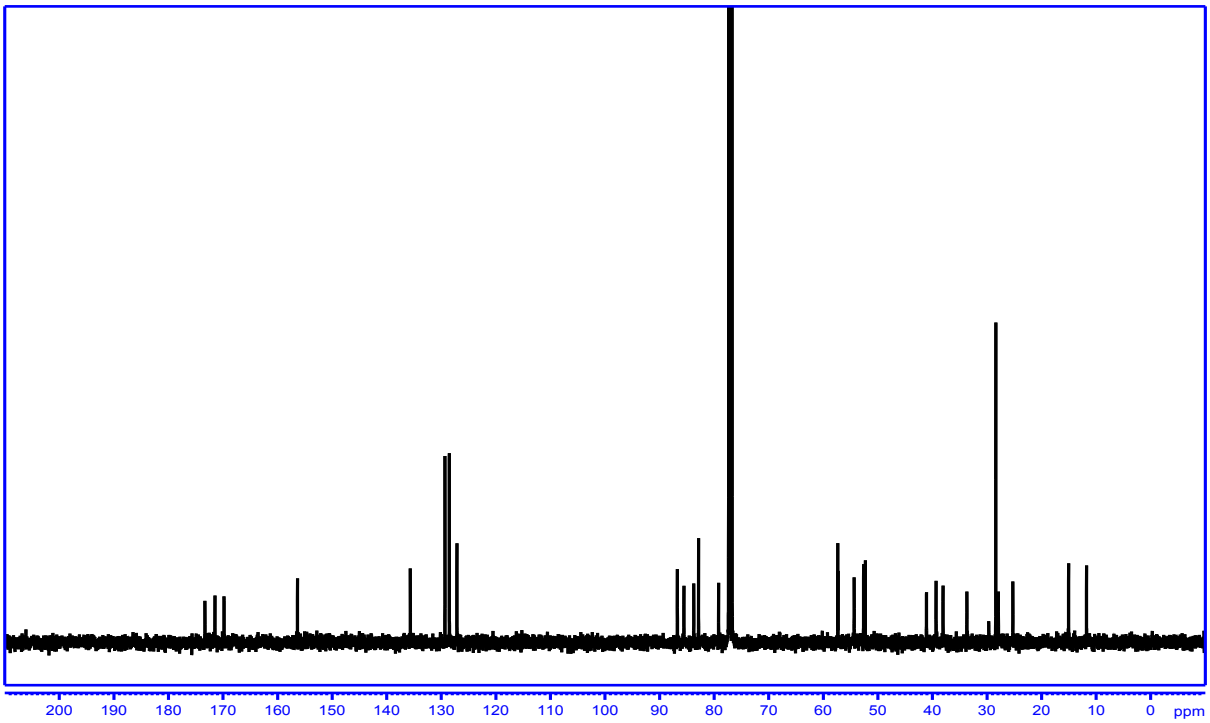
- **^{13}C NMR spectrum ($CDCl_3$, 100 MHz) of compound 14.**



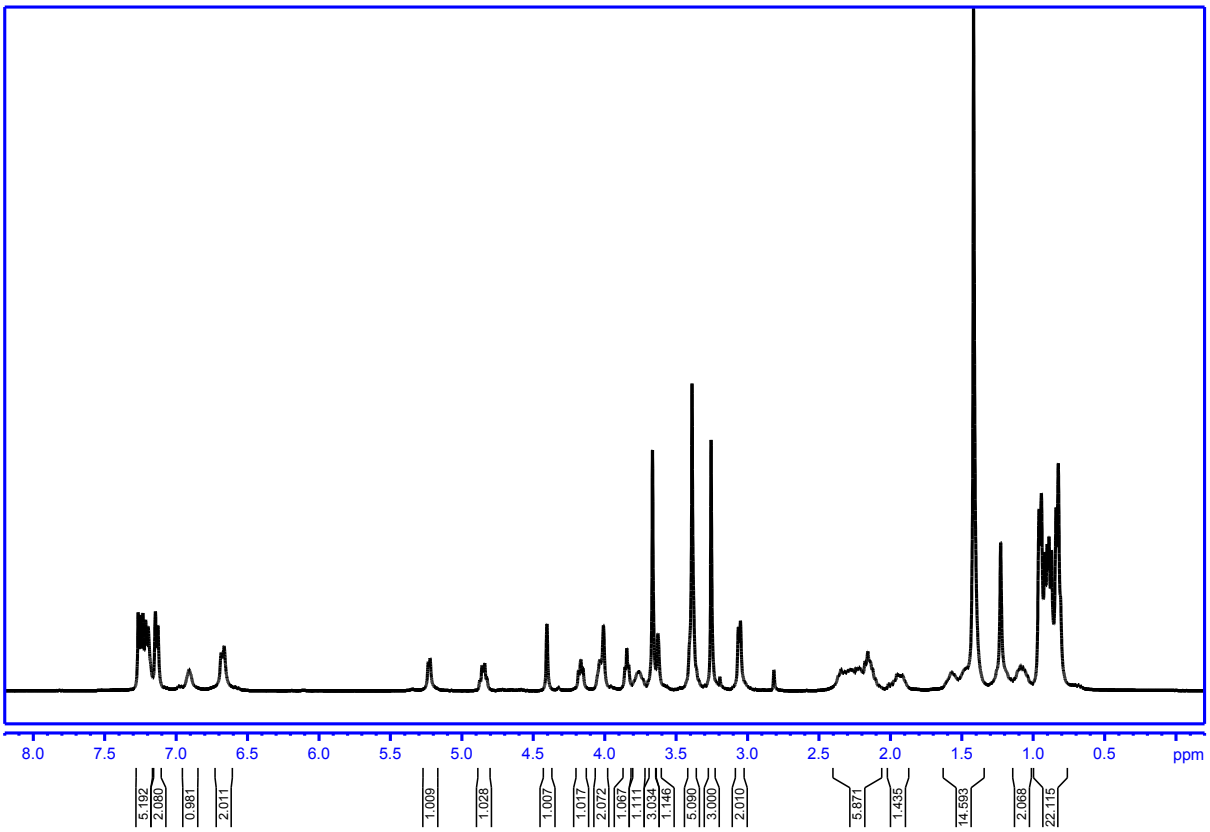
- **^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of compound 19.**



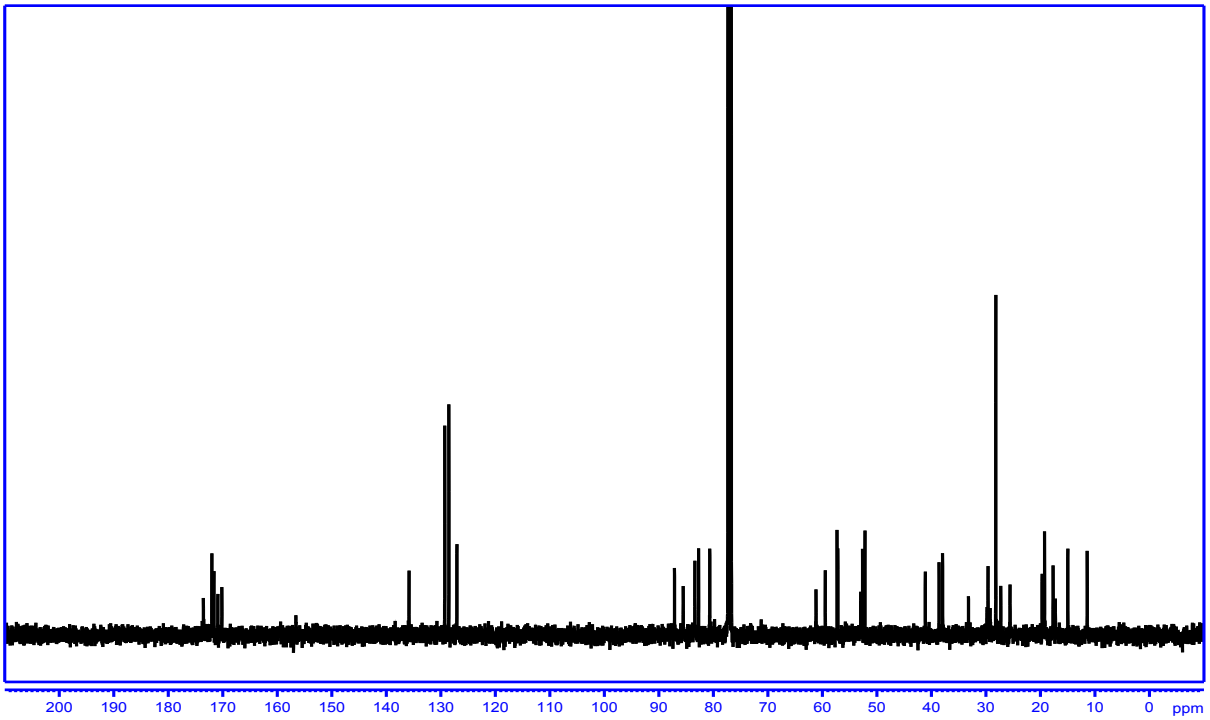
- **^{13}C NMR spectrum ($CDCl_3$, 100 MHz) of compound 19.**



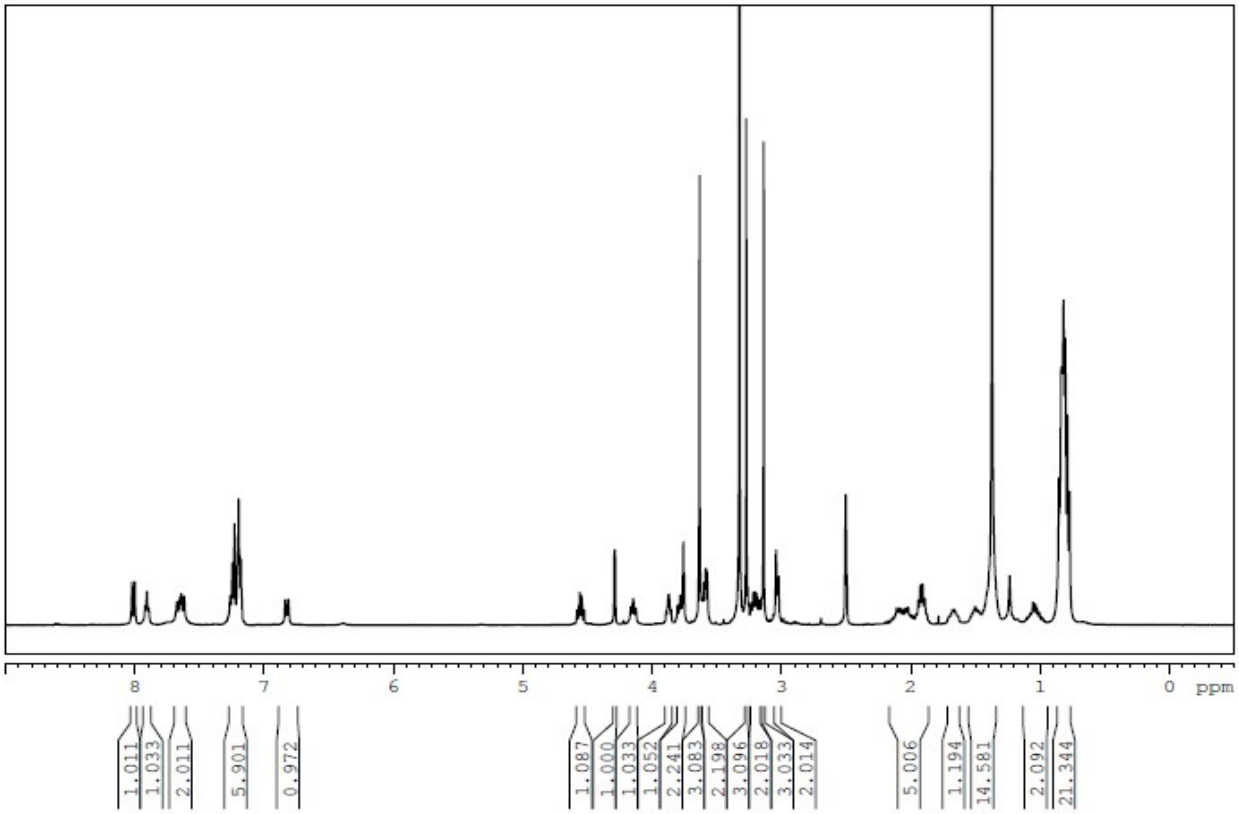
- **^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of compound 20.**



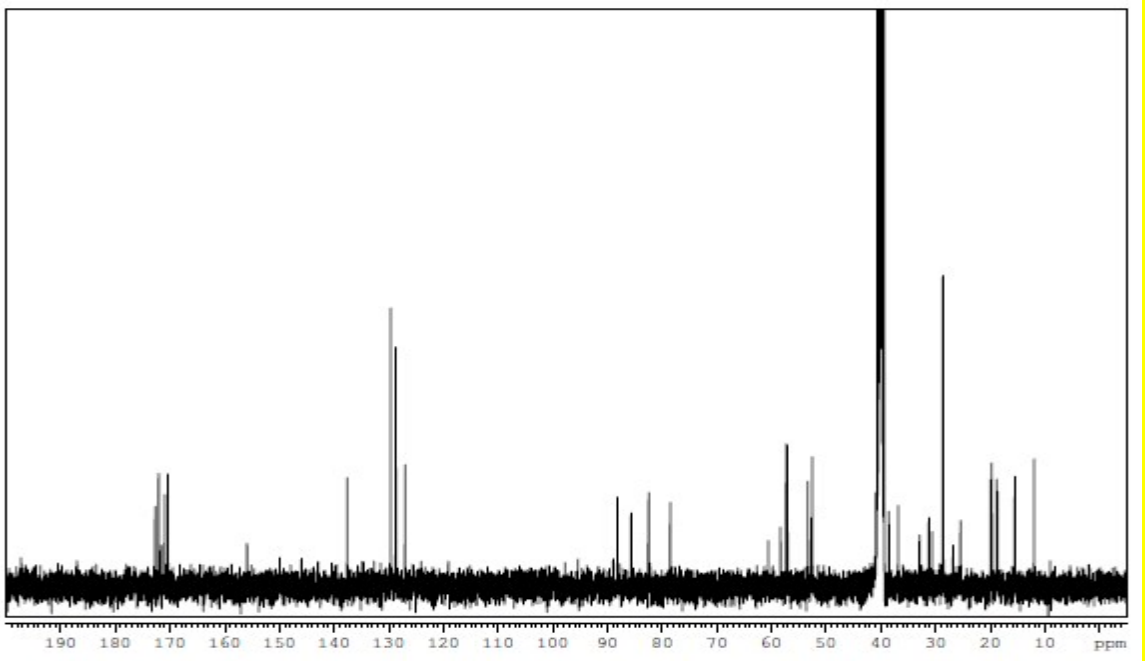
- **^{13}C NMR spectrum ($CDCl_3$, 100 MHz) of compound 20.**



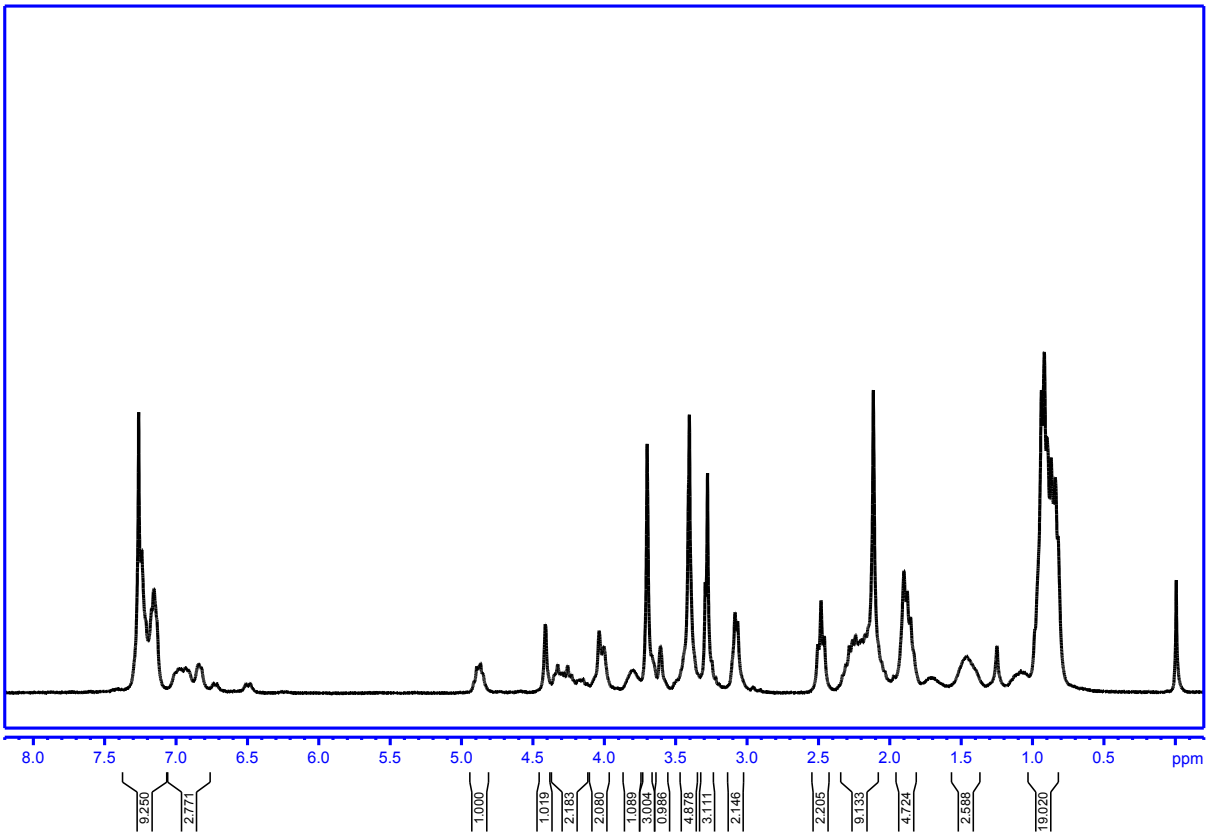
- **^{1}H NMR spectrum (DMSO-d_6, 400 MHz) of compound 20.**



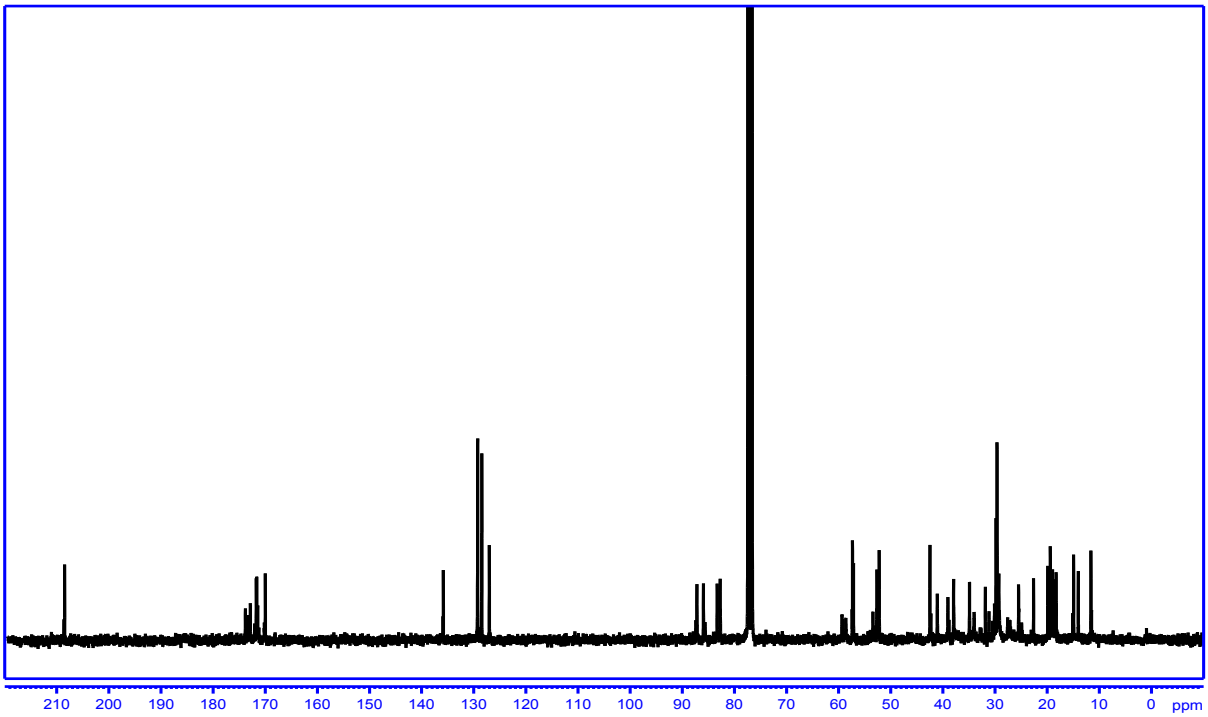
- **^{13}C NMR spectrum (DMSO-d_6, 100 MHz) of compound 20.**



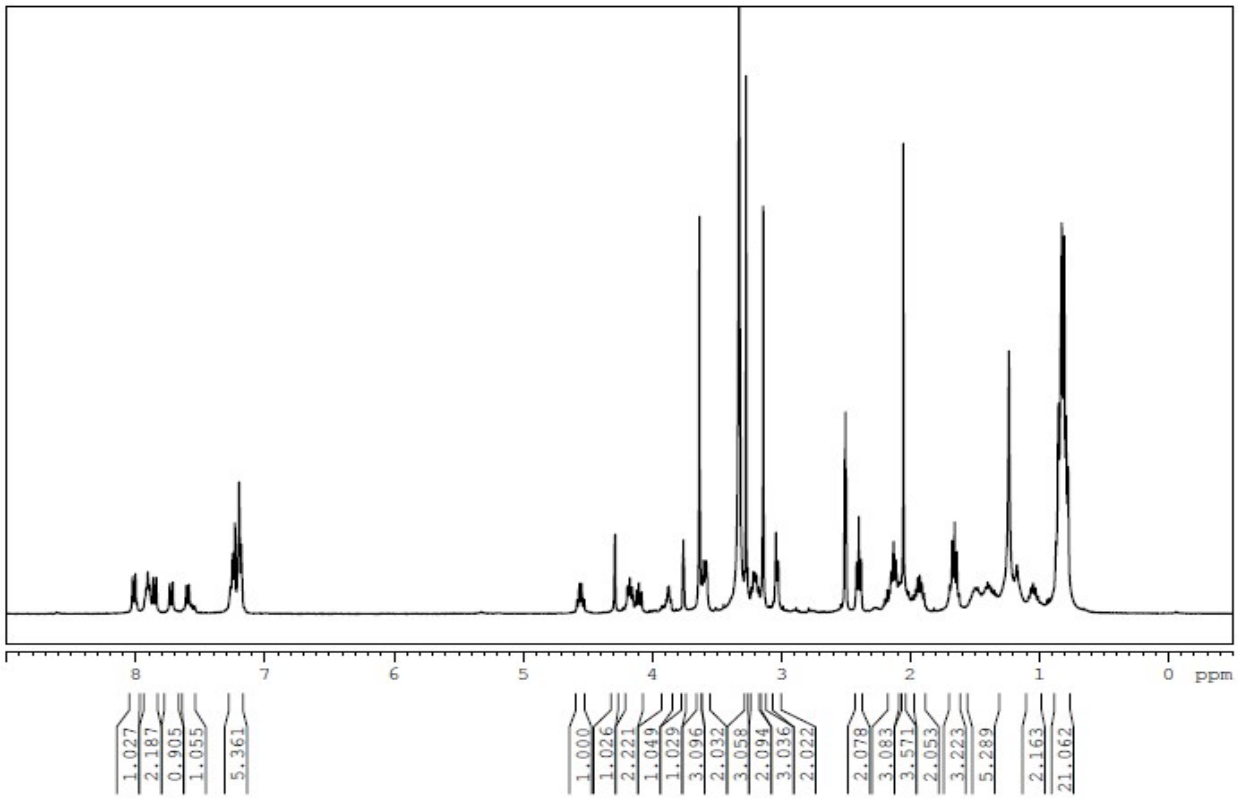
- **^{1}H NMR spectrum ($CDCl_3$, 300 MHz) of compound 4A.**



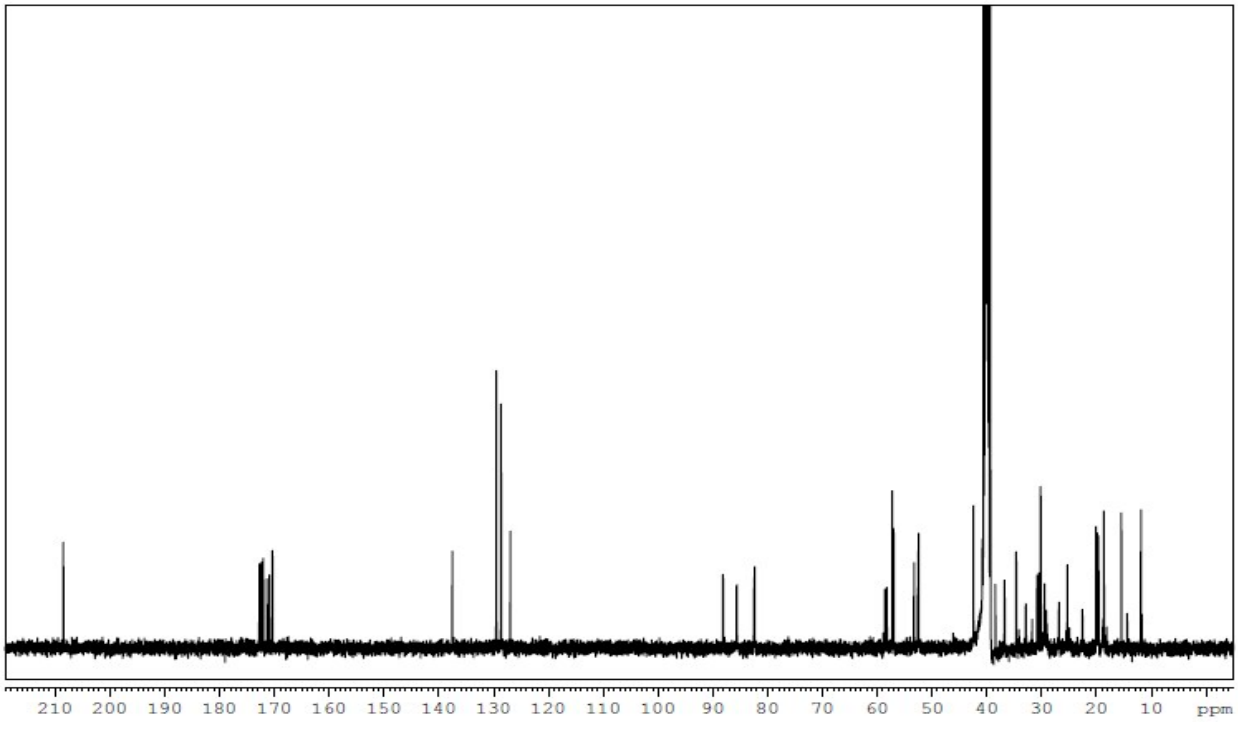
- **^{13}C NMR spectrum ($CDCl_3$, 75 MHz) of compound 4A.**



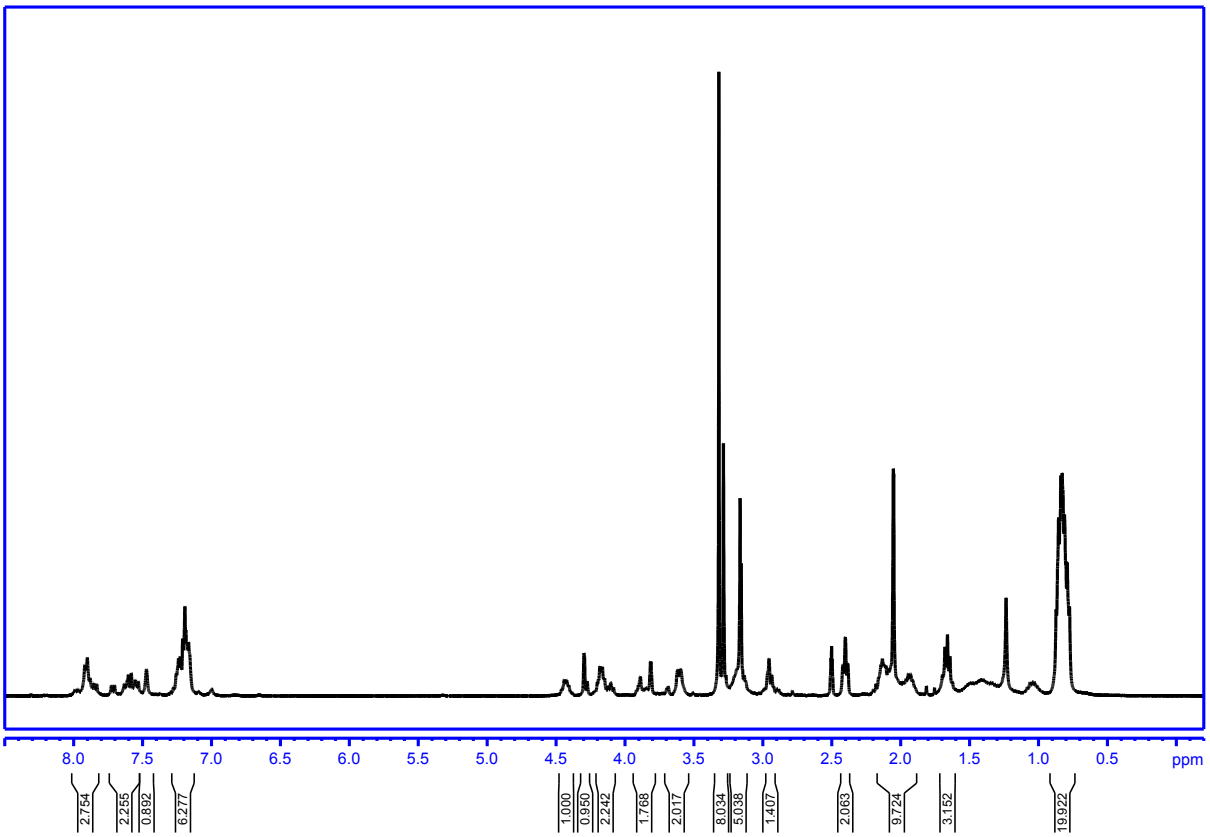
- **^{1}H NMR spectrum (DMSO-d_6, 400 MHz) of compound 4A.**



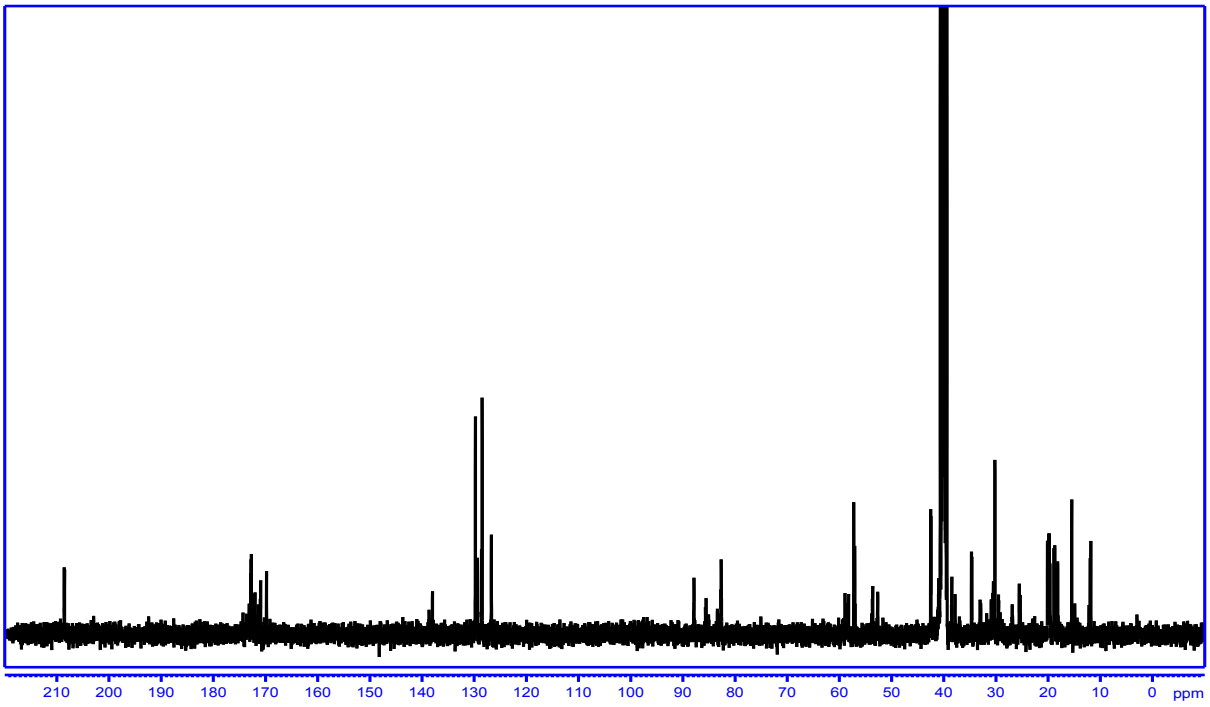
- **^{13}C NMR spectrum (DMSO-d_6, 100 MHz) of compound 4A.**



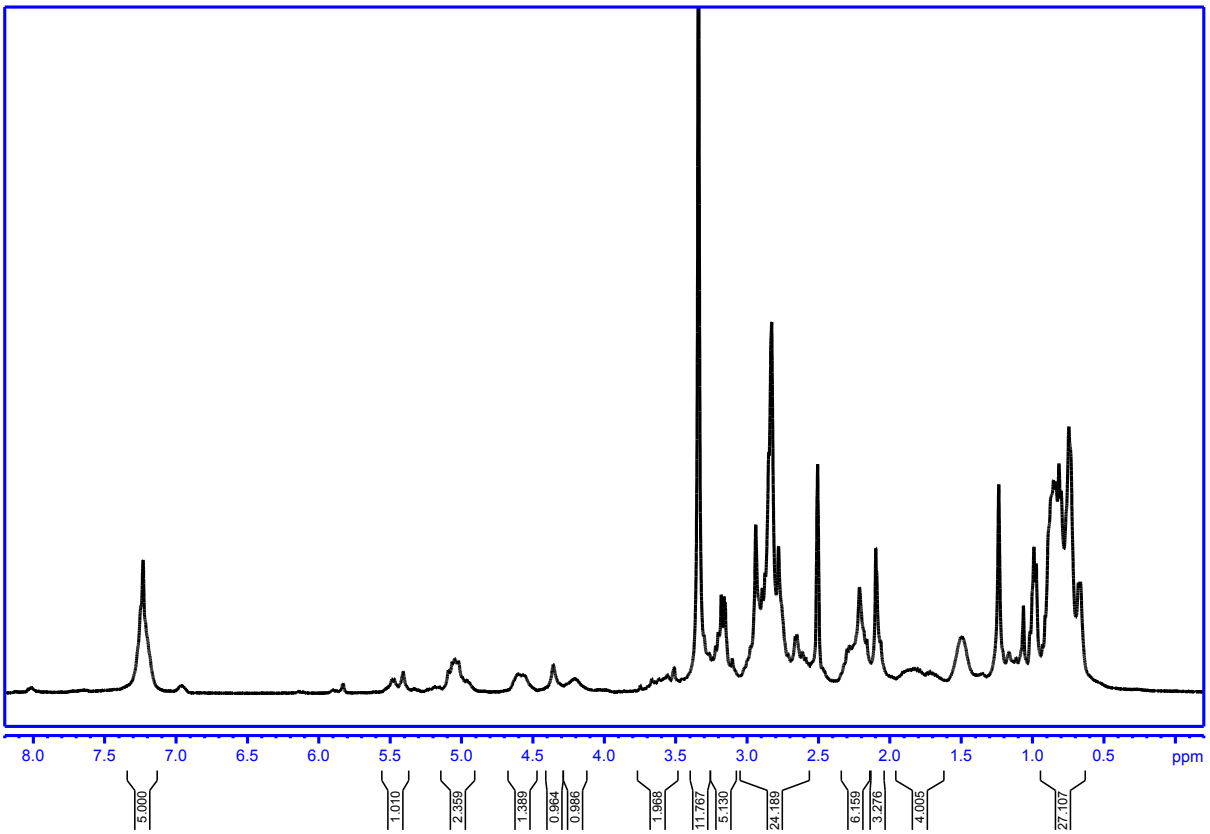
- **^{1}H NMR spectrum (DMSO-d_6, 400 MHz) of compound 4B.**



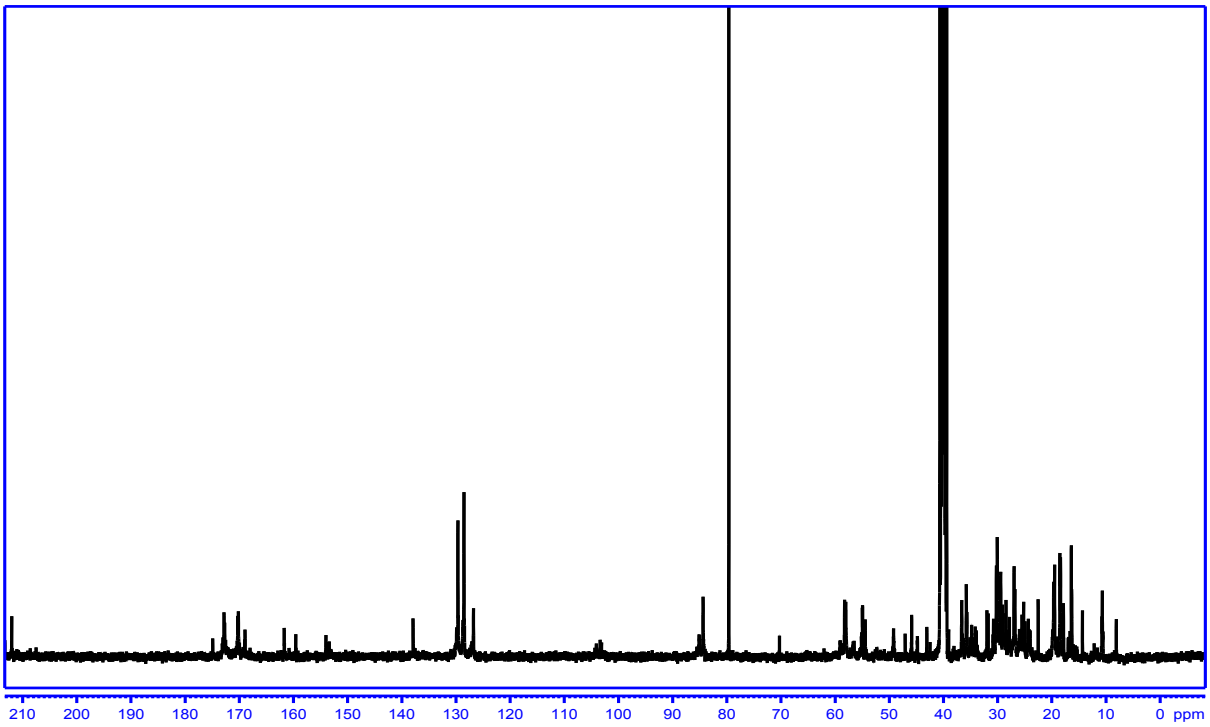
- **^{13}C NMR spectrum (DMSO-d_6, 100 MHz) of compound 4B.**



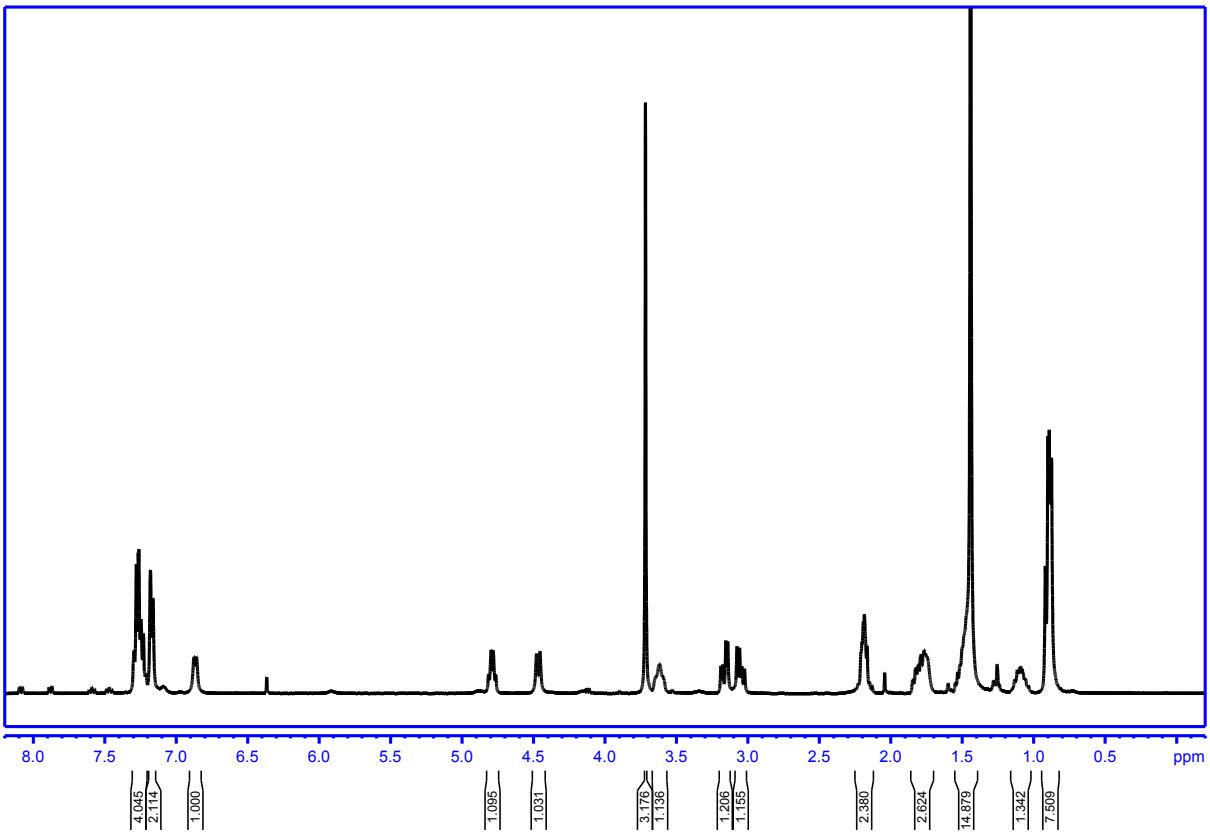
- **^{1}H NMR spectrum (DMSO-d_6, 400 MHz) of compound 4C.**



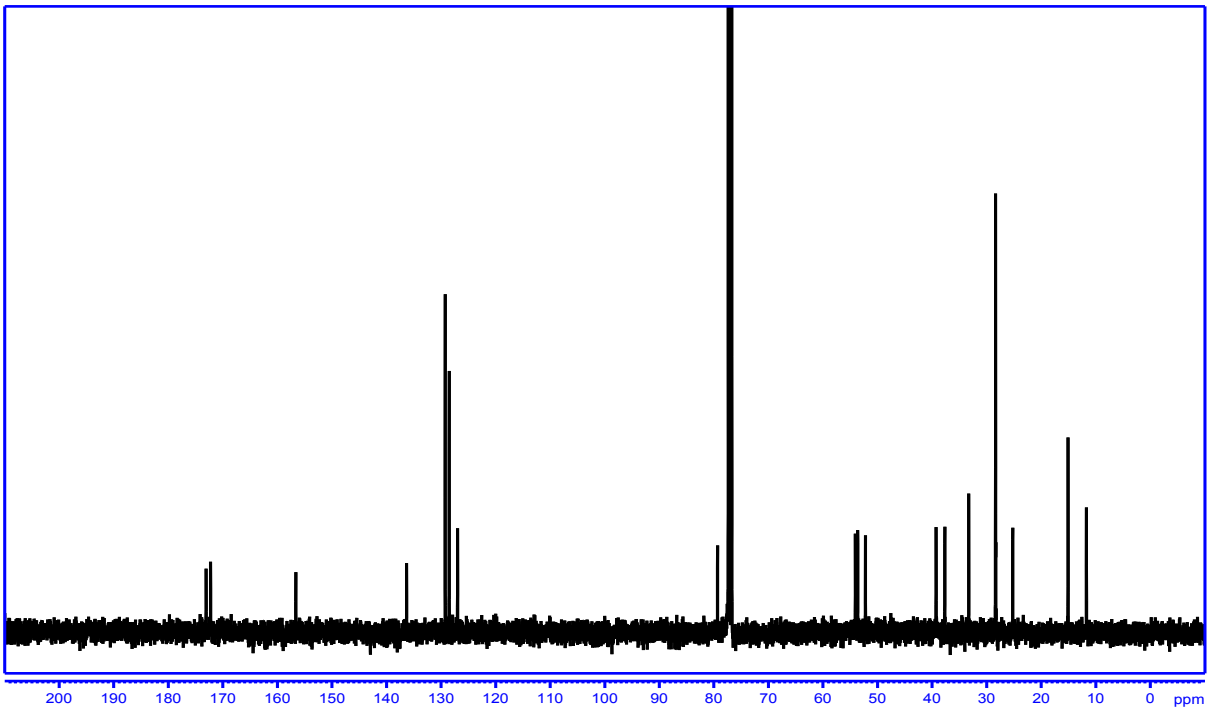
- **^{1}H NMR spectrum (DMSO-d_6, 400 MHz) of compound 4C.**



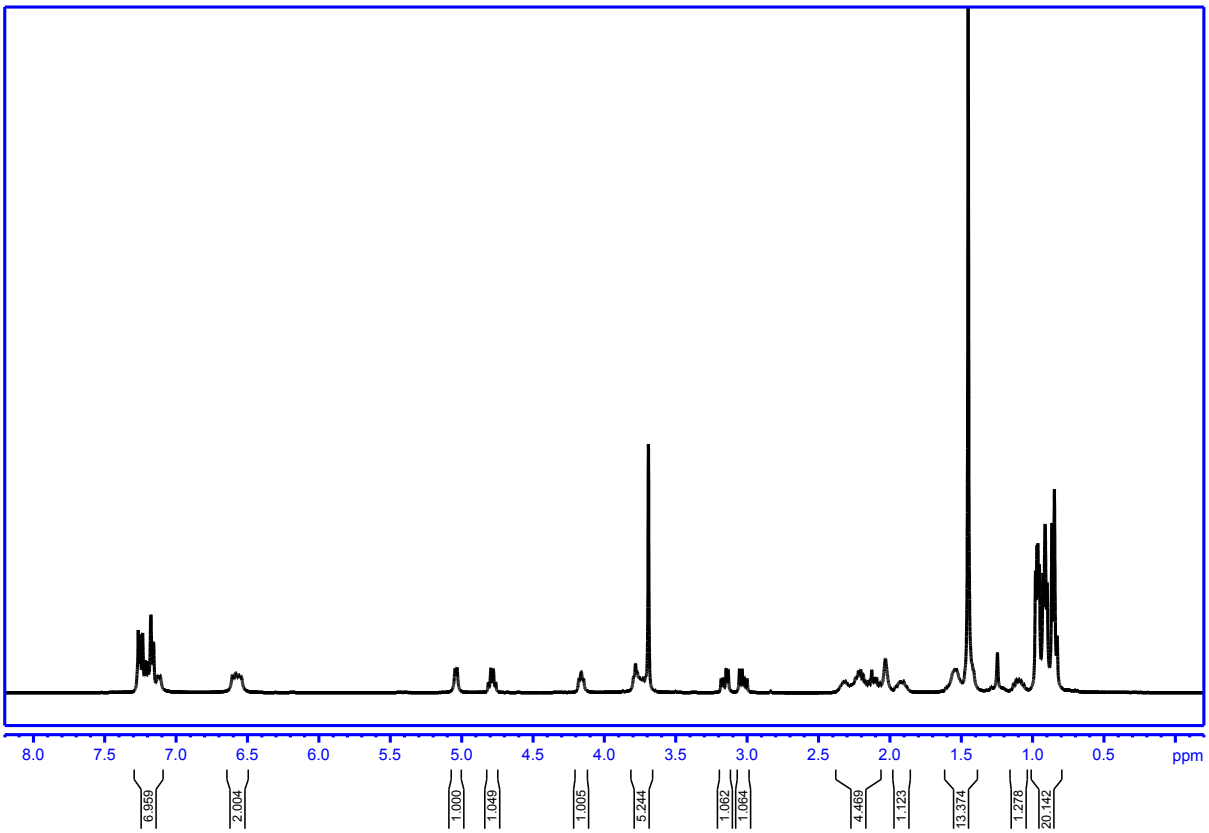
- **^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of compound 21.**



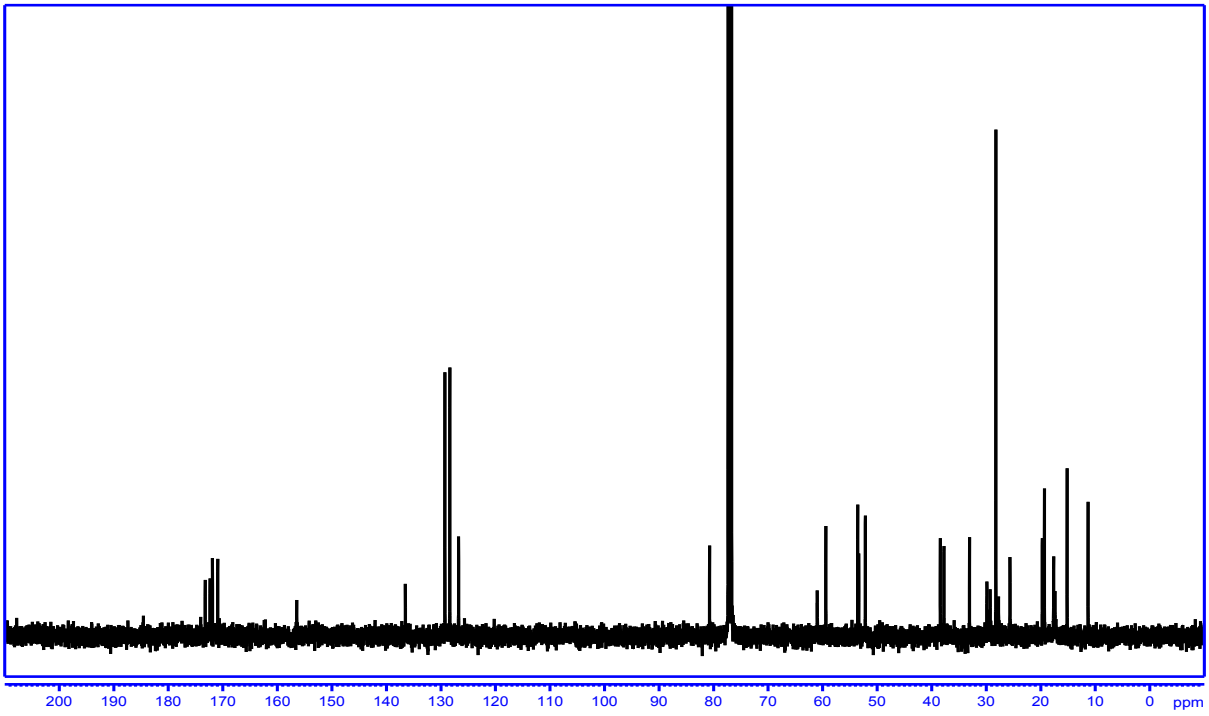
- **^{13}C NMR spectrum ($CDCl_3$, 100 MHz) of compound 21.**



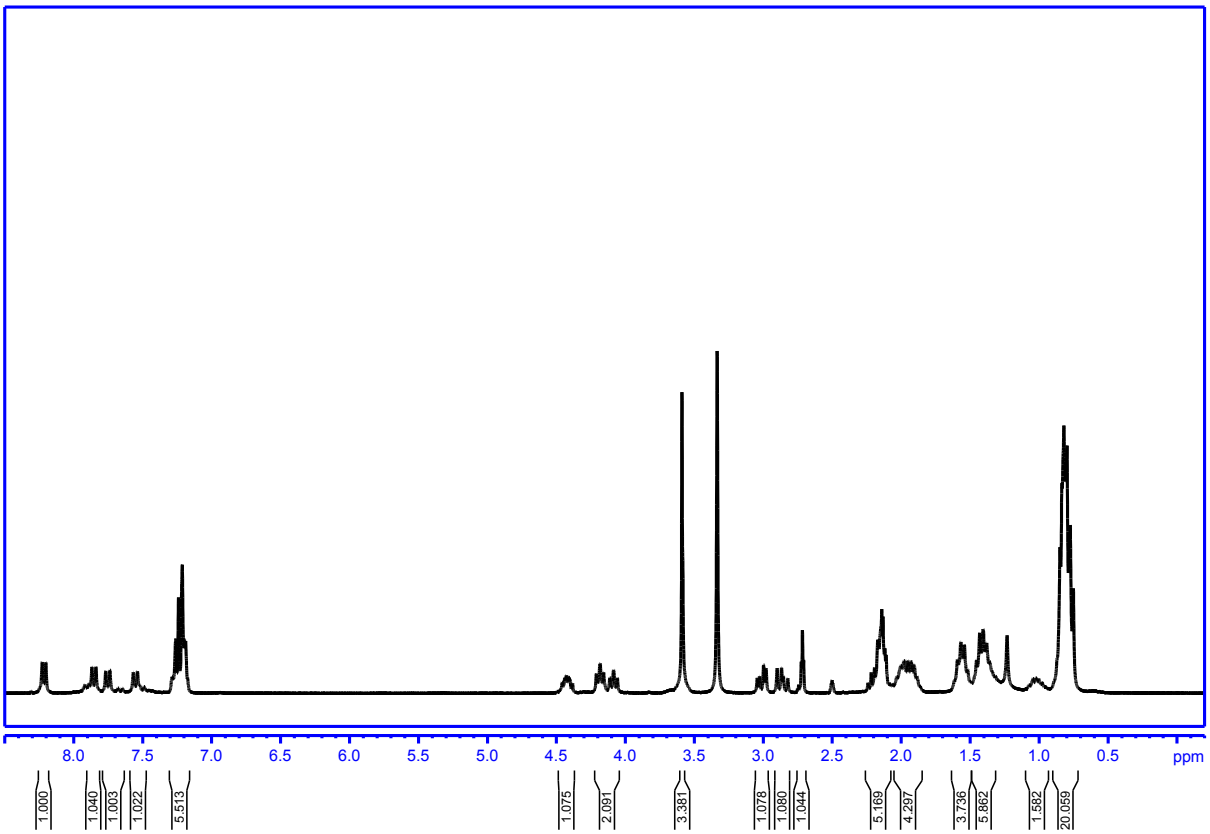
- **^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of compound 22.**



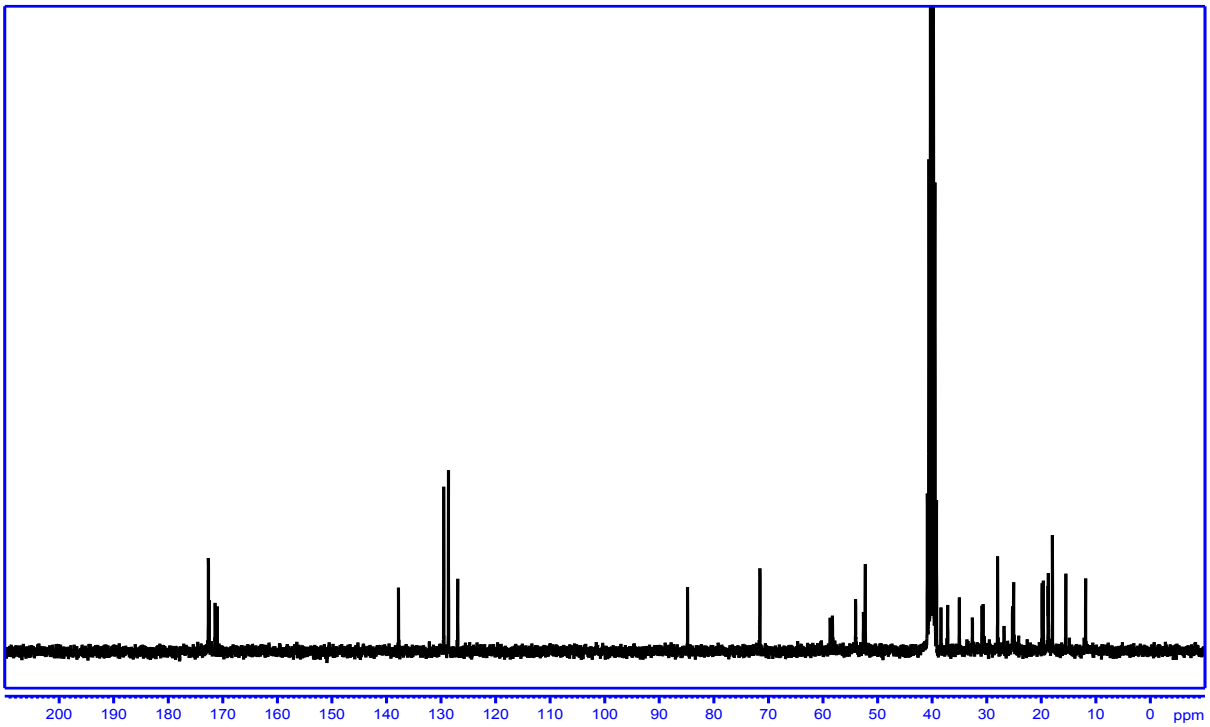
- **^{13}C NMR spectrum ($CDCl_3$, 100 MHz) of compound 22.**



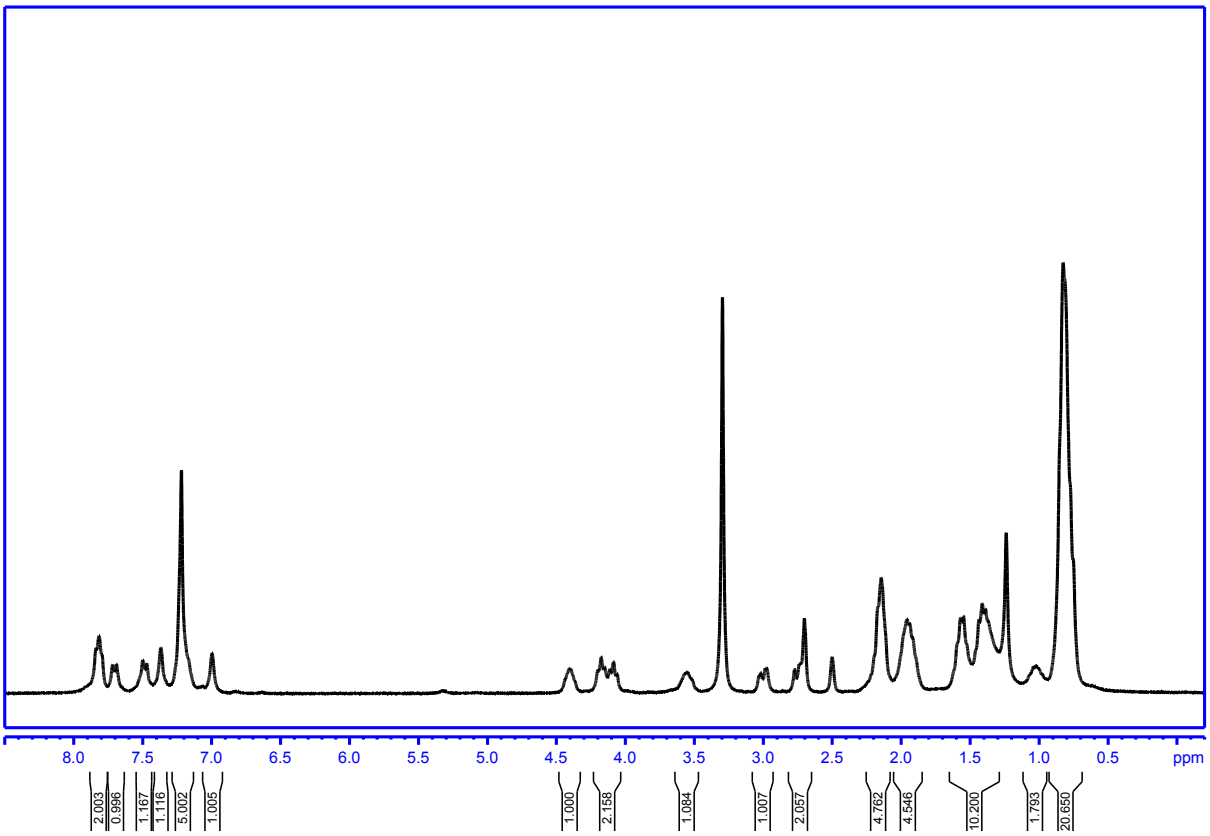
- **^{1}H NMR spectrum (DMSO-d_6, 300 MHz) of compound 4D.**



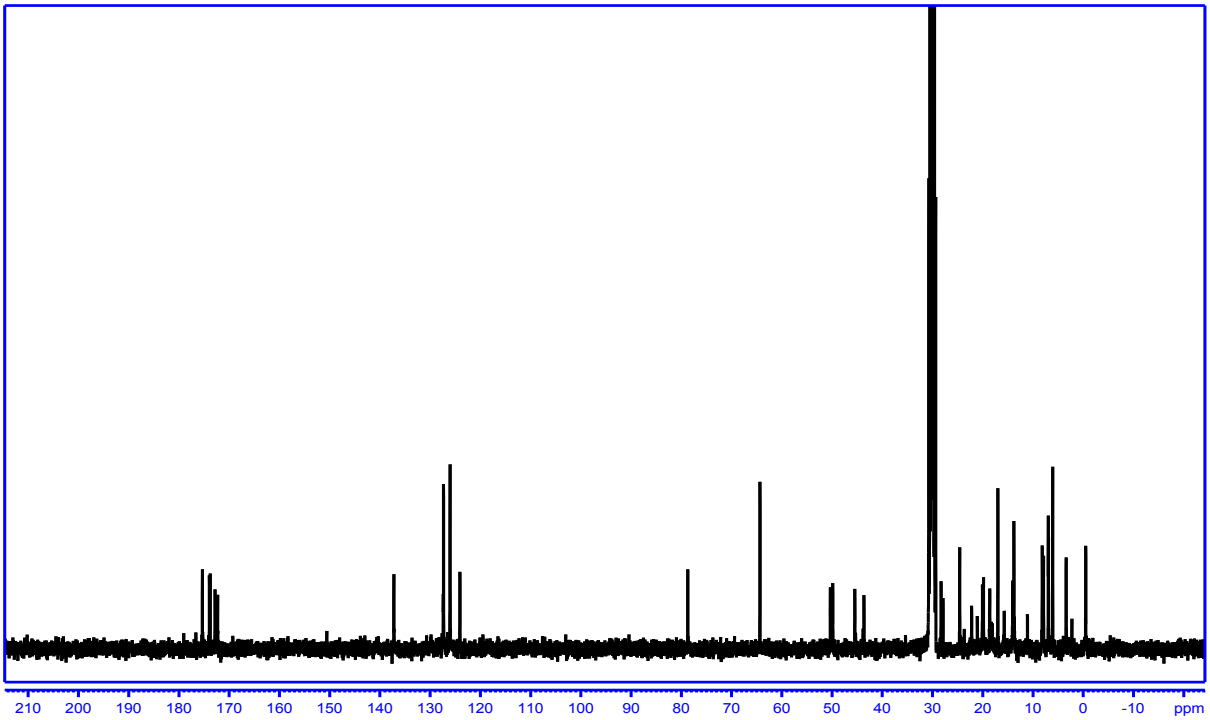
- **^{13}C NMR spectrum (DMSO-d_6, 75 MHz) of compound 4D.**



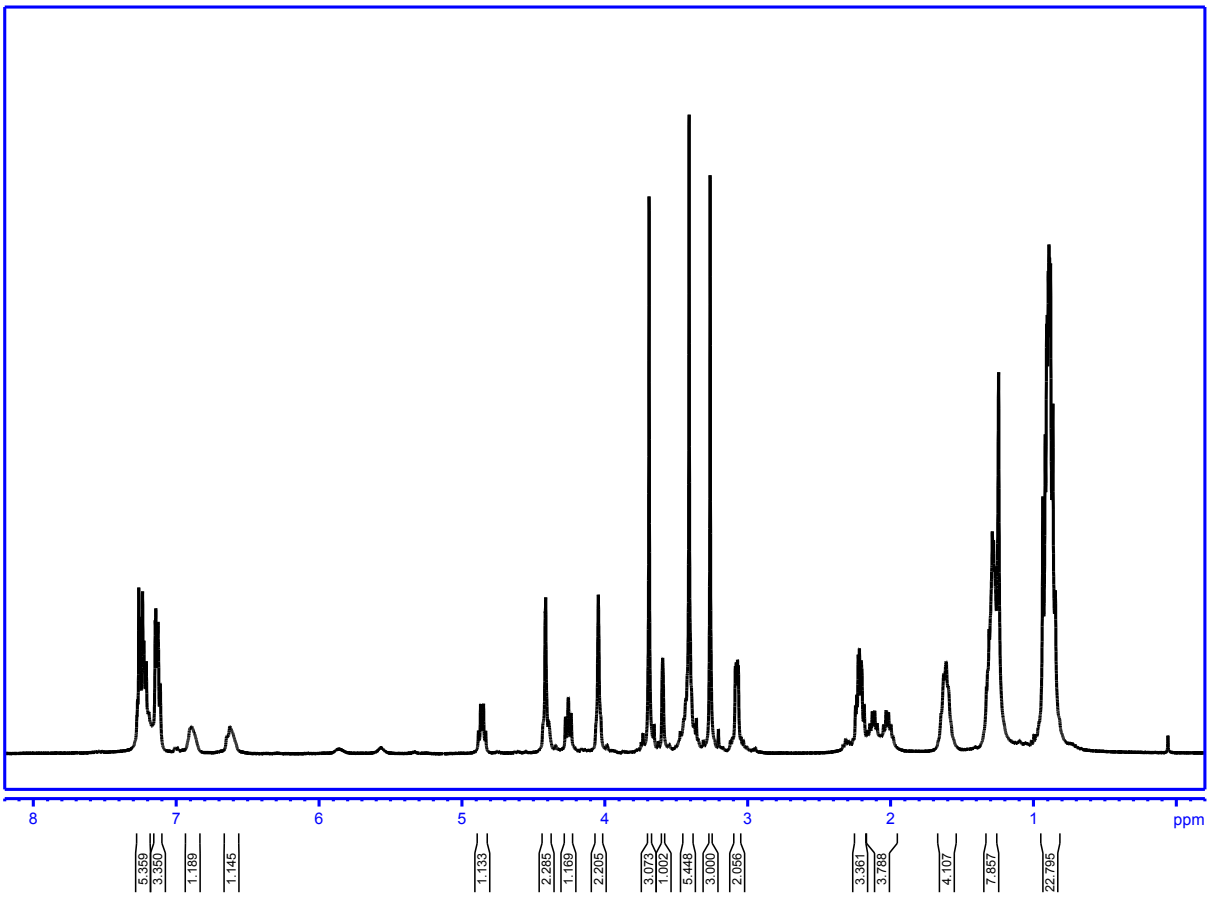
- **^{1}H NMR spectrum (DMSO-d_6, 300 MHz) of compound 4E.**



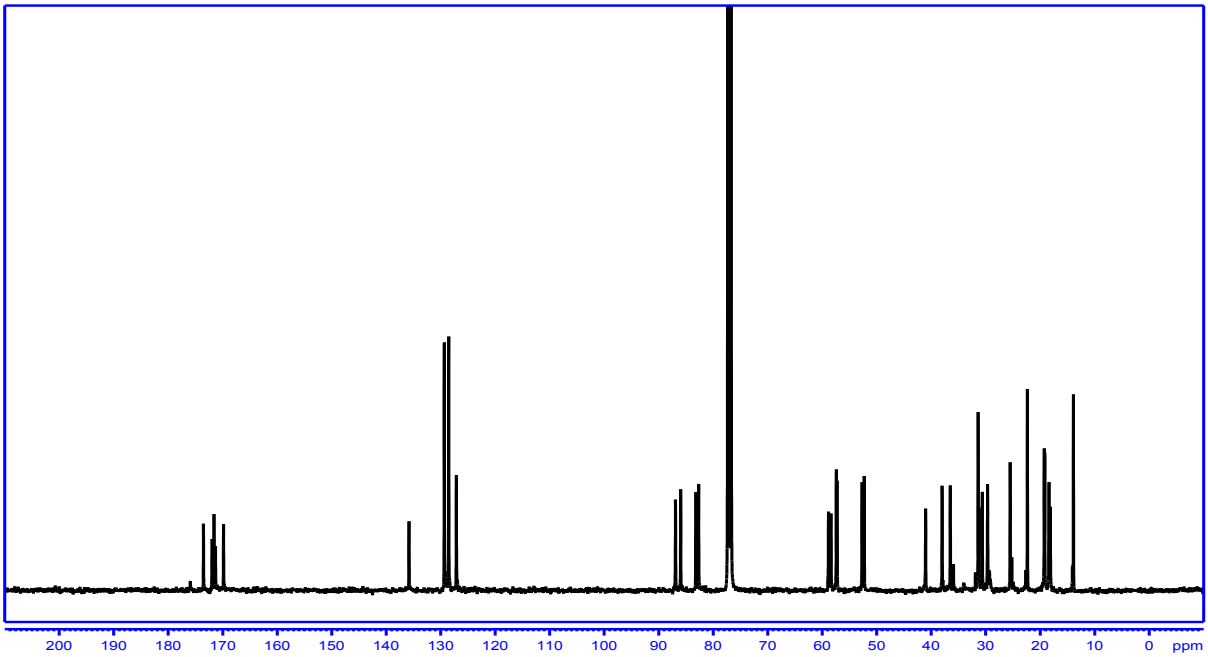
- **^{13}C NMR spectrum (DMSO-d_6, 100 MHz) of compound 4E.**



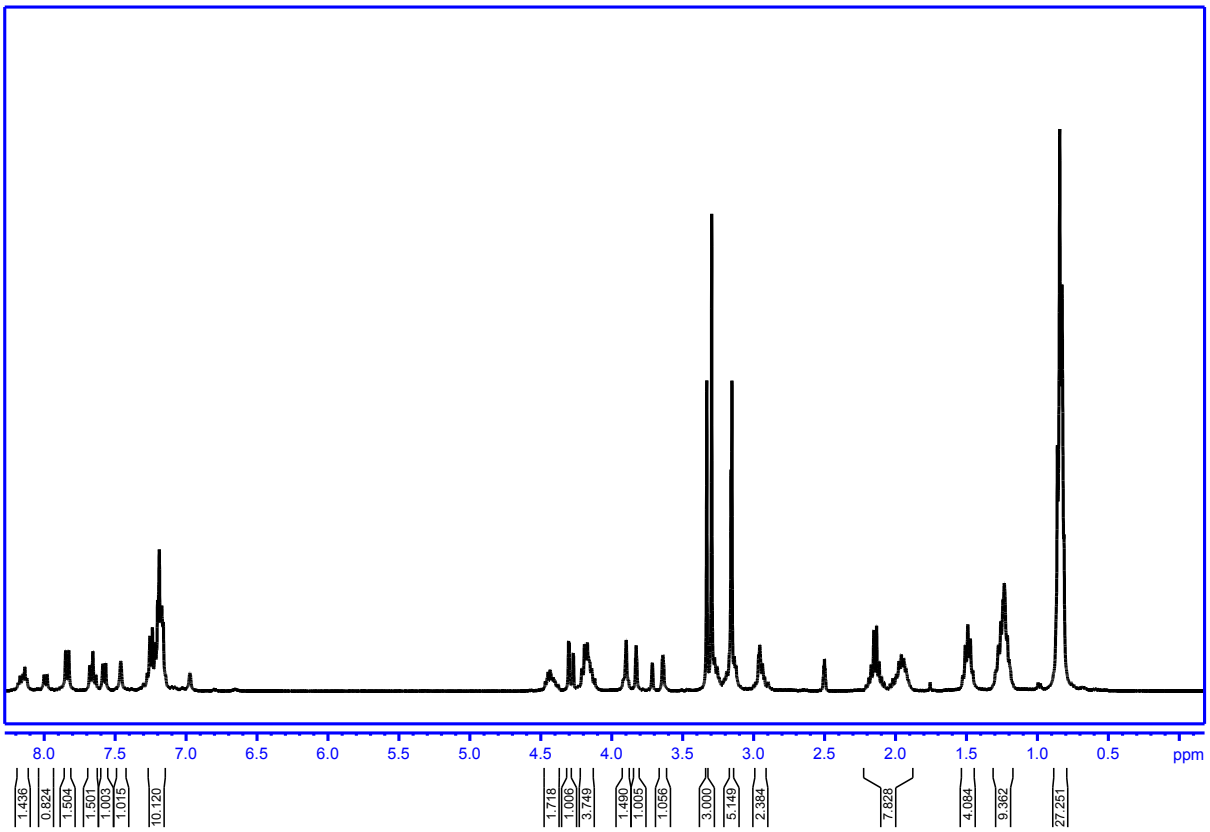
- **^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of compound 4F.**



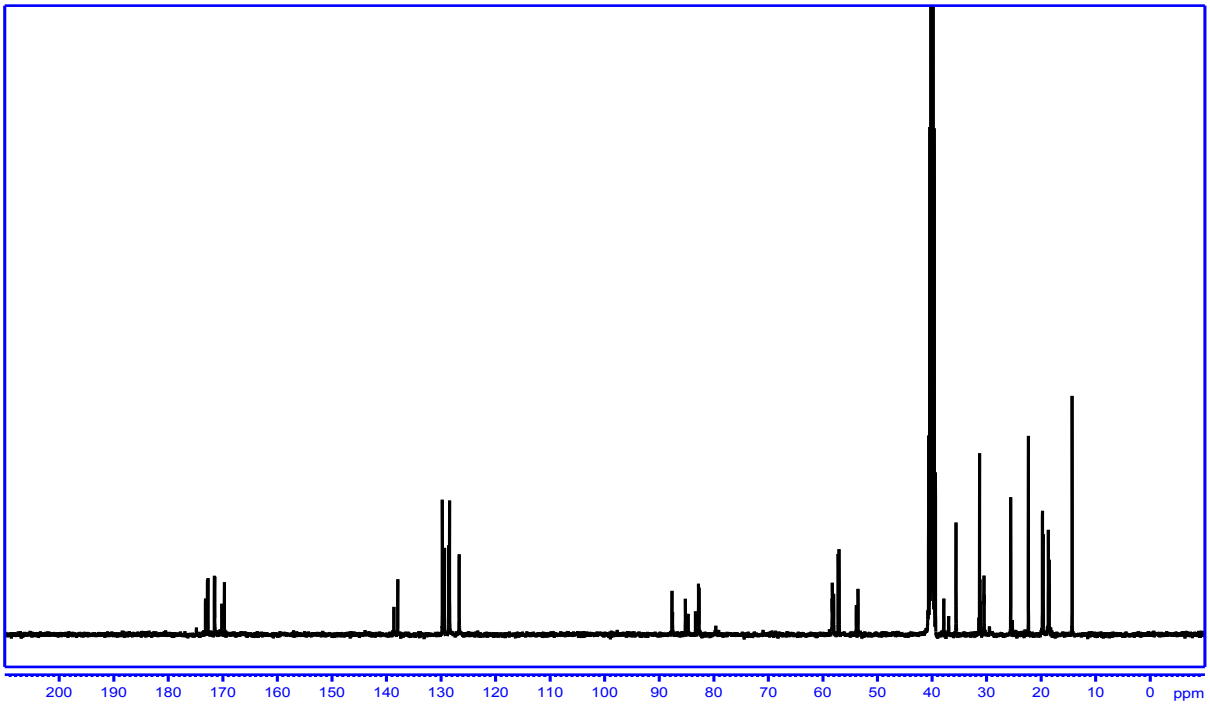
- **^{13}C NMR spectrum ($CDCl_3$, 100 MHz) of compound 4F.**



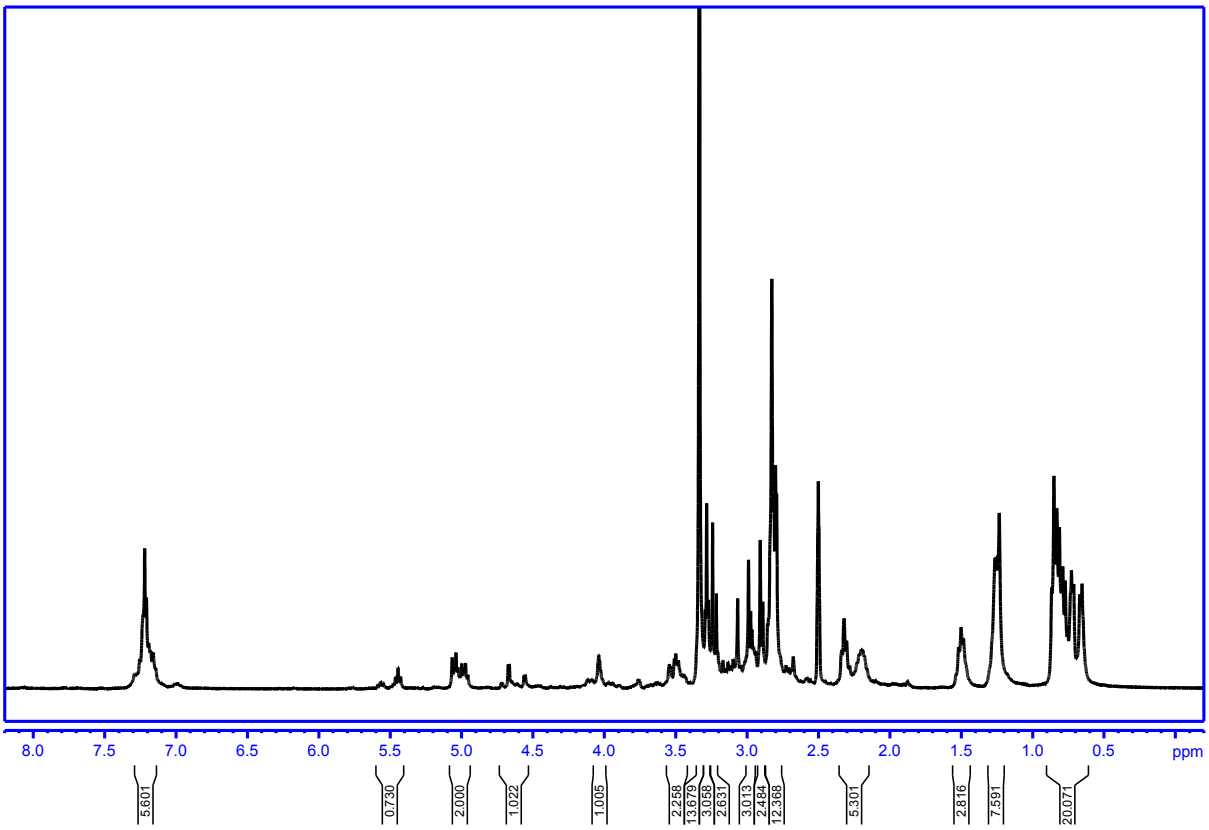
- **^{1}H NMR spectrum (DMSO-d_6, 400 MHz) of compound 4G.**



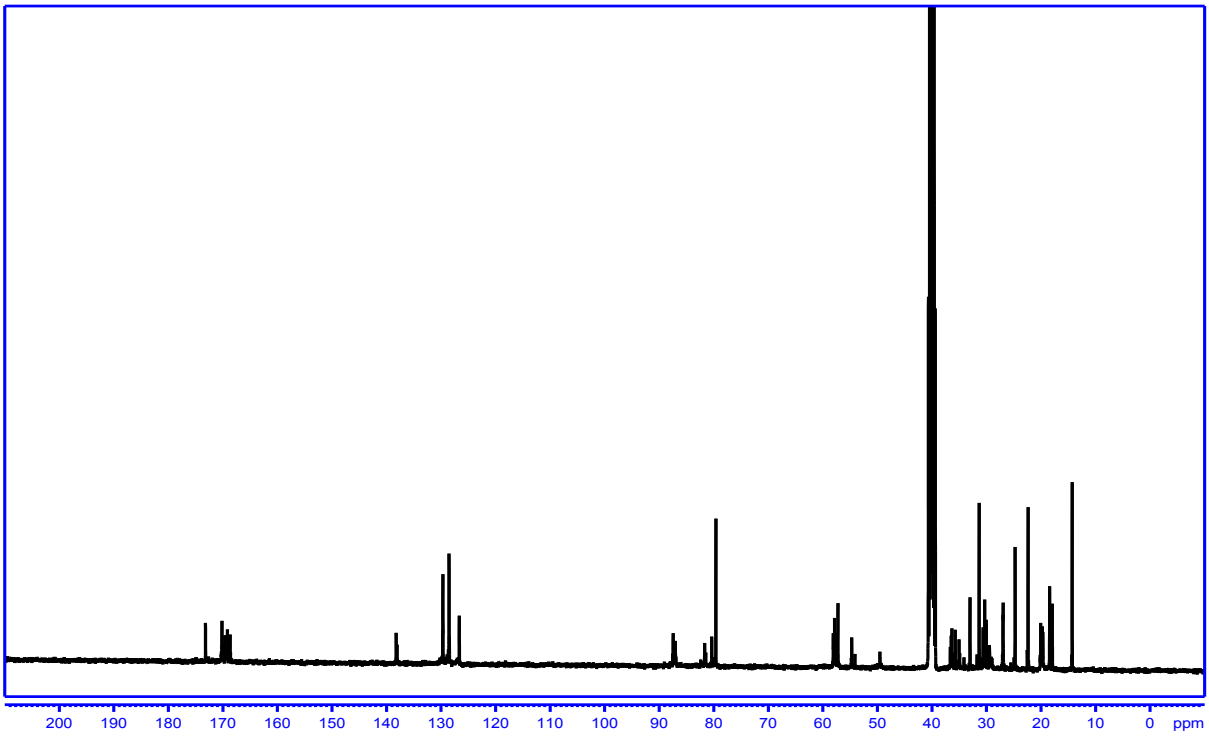
- **^{13}C NMR spectrum (DMSO-d_6, 100 MHz) of compound 4G.**



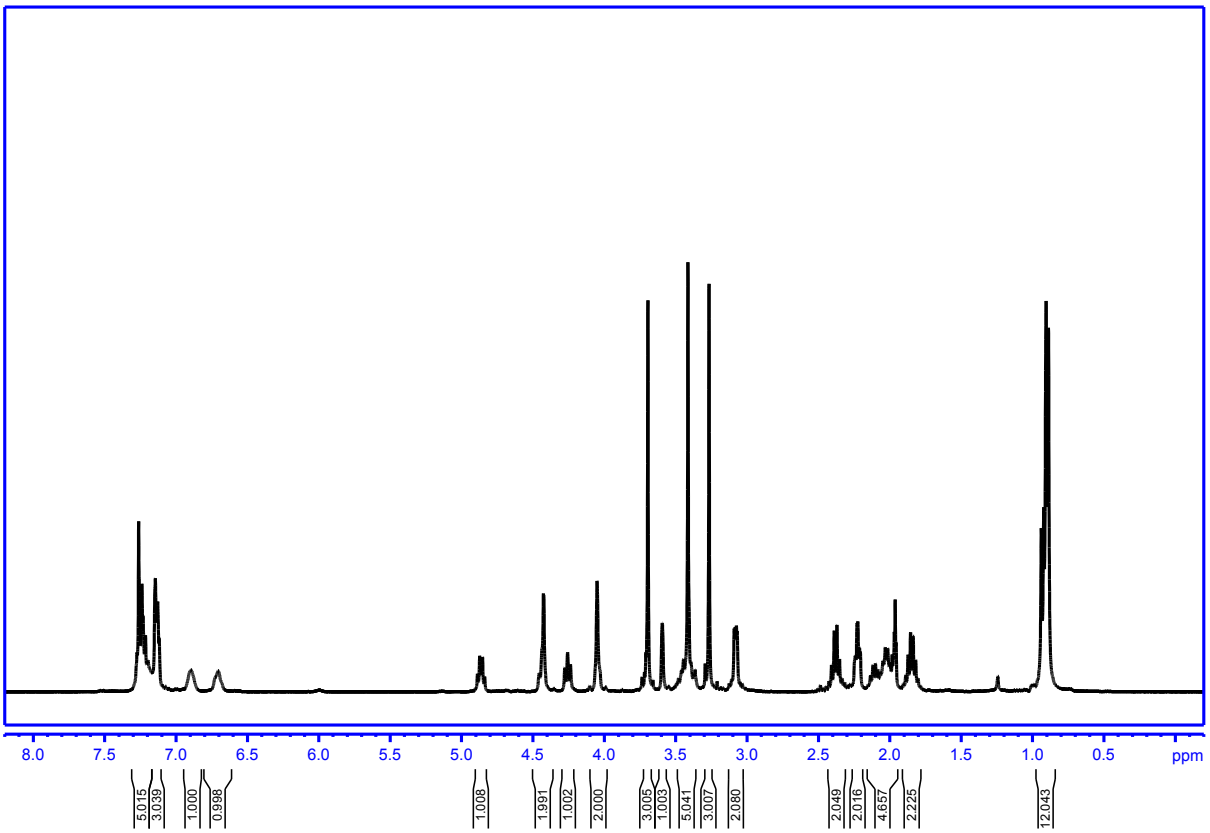
- **^{1}H NMR spectrum (DMSO-d_6, 400 MHz) of compound 4H.**



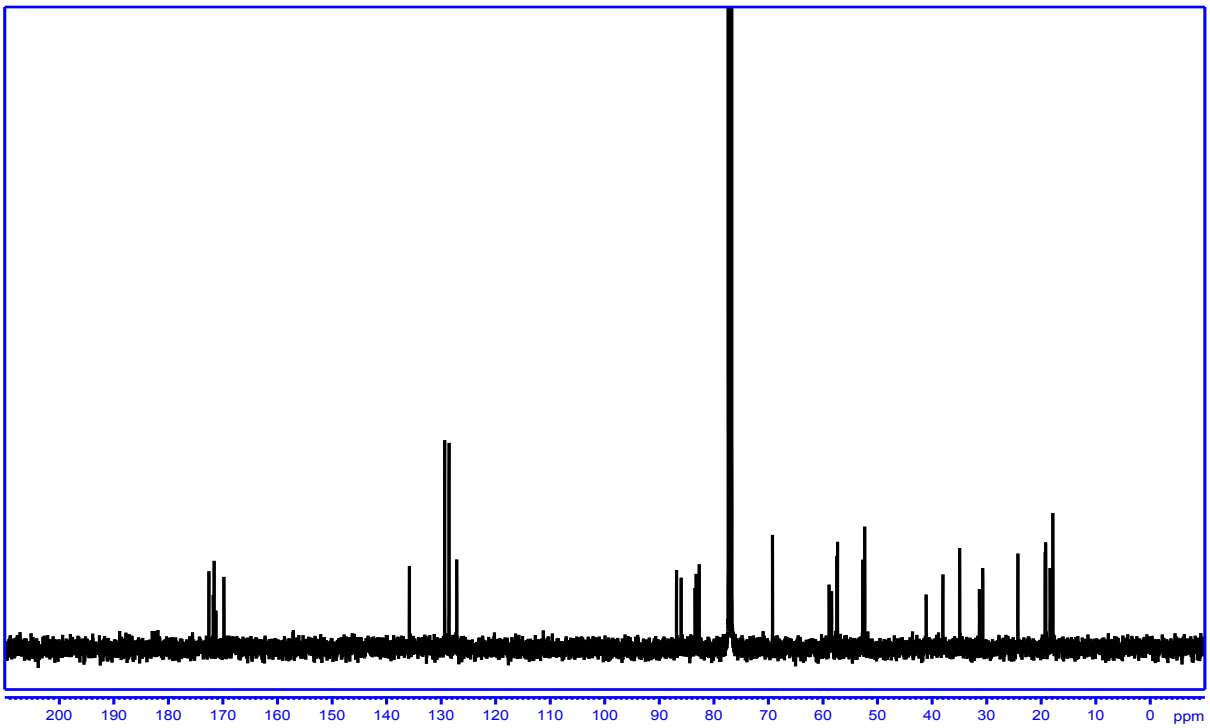
- **^{13}C NMR spectrum (DMSO-d_6, 100 MHz) of compound 4H.**



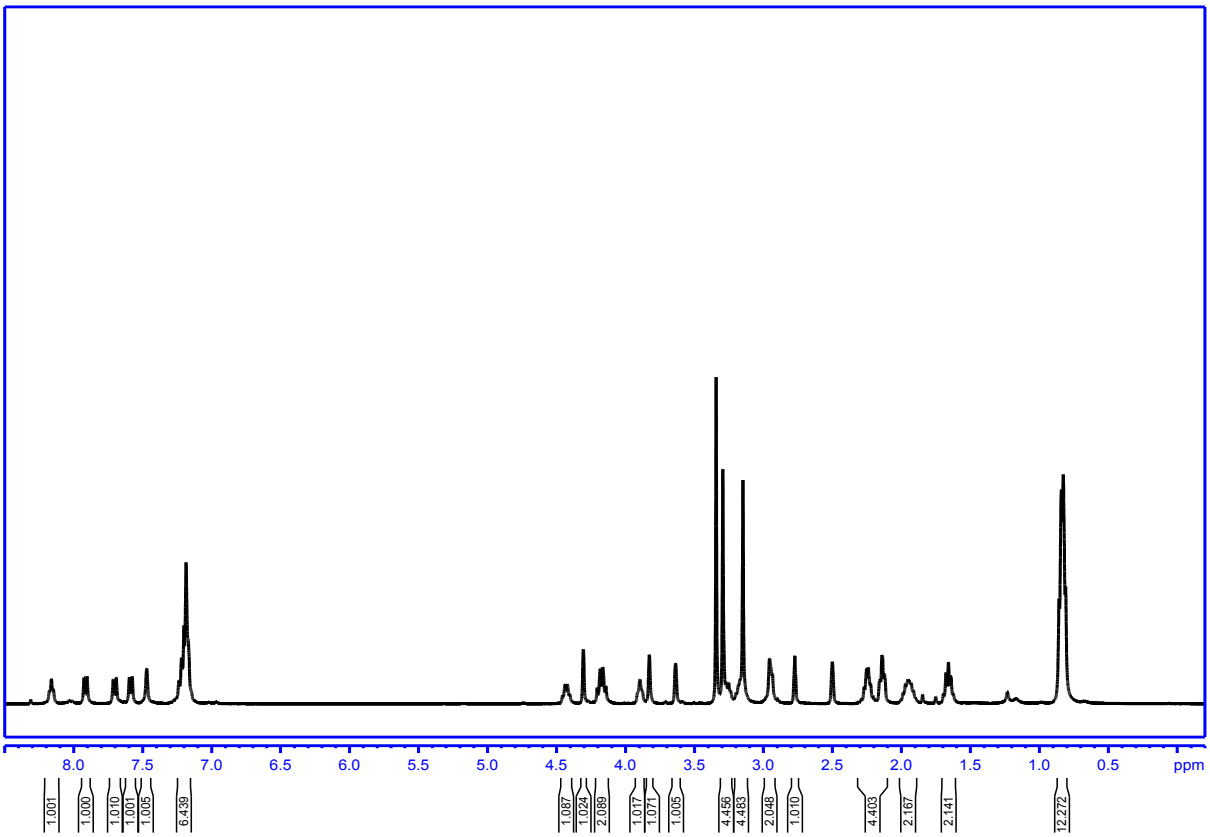
- **^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of compound 4I.**



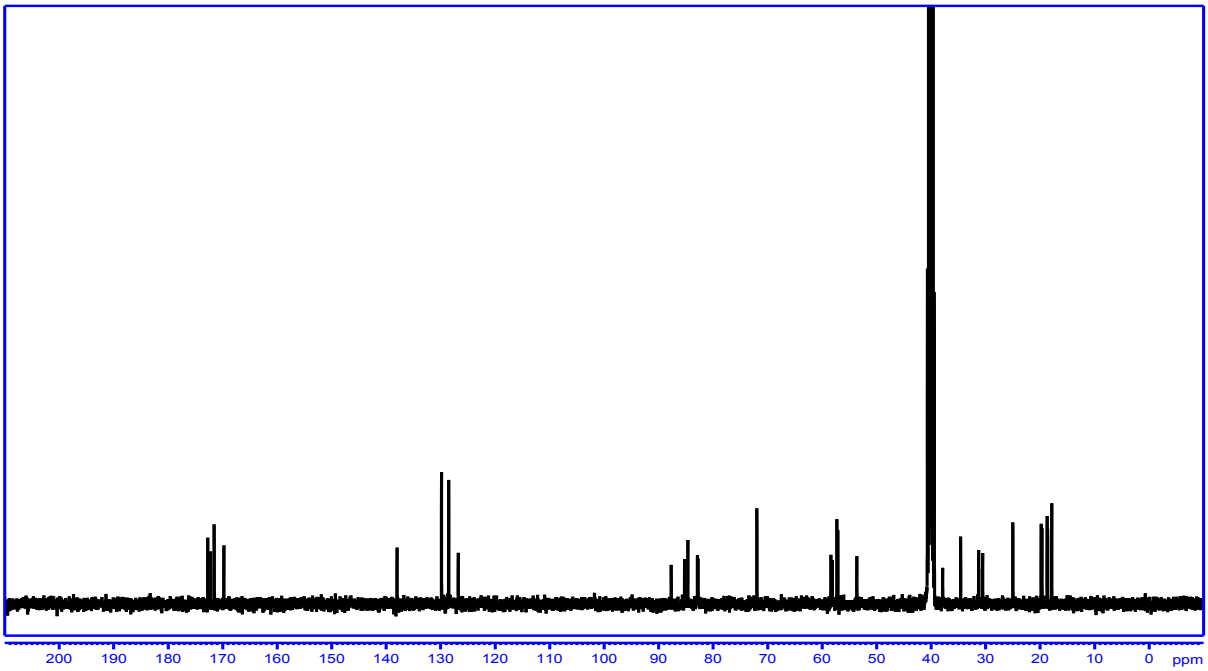
- **^{13}C NMR spectrum ($CDCl_3$, 100 MHz) of compound 4I.**



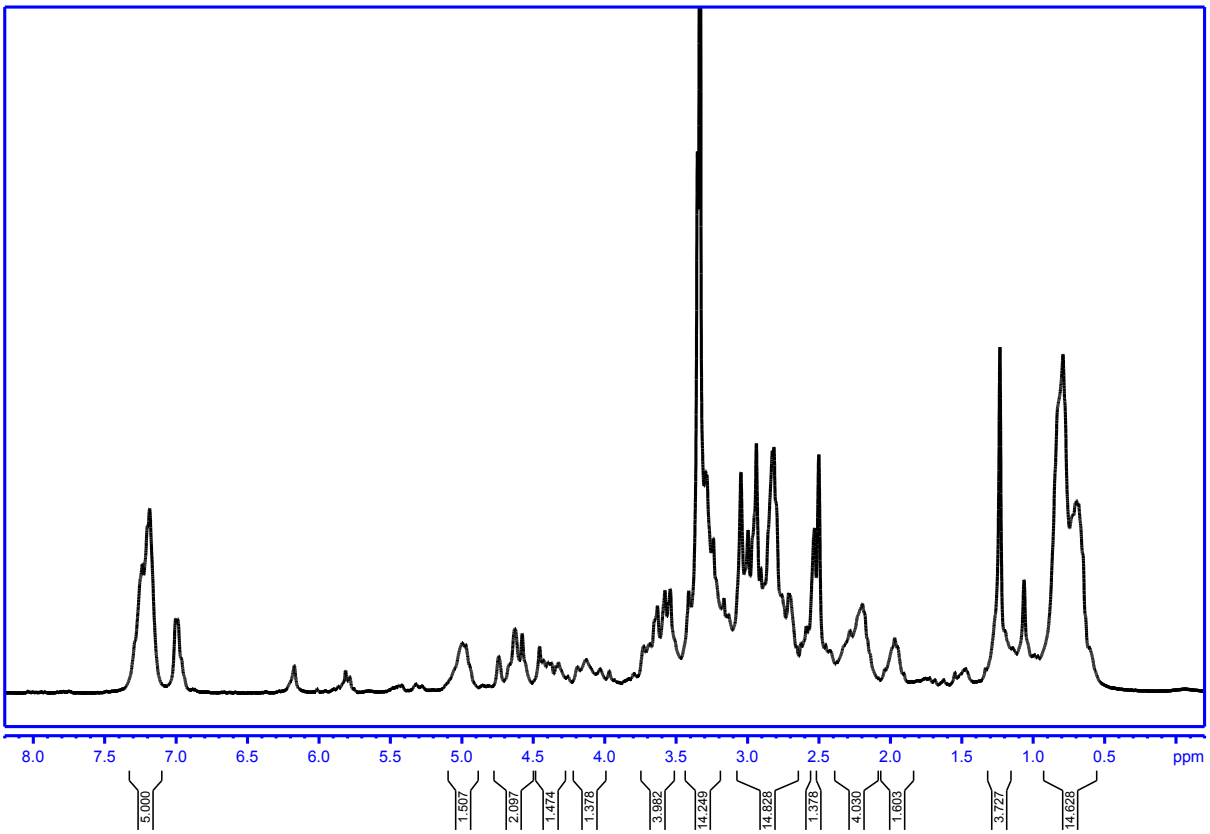
- **^{1}H NMR spectrum (DMSO-d_6, 400 MHz) of compound 4J.**



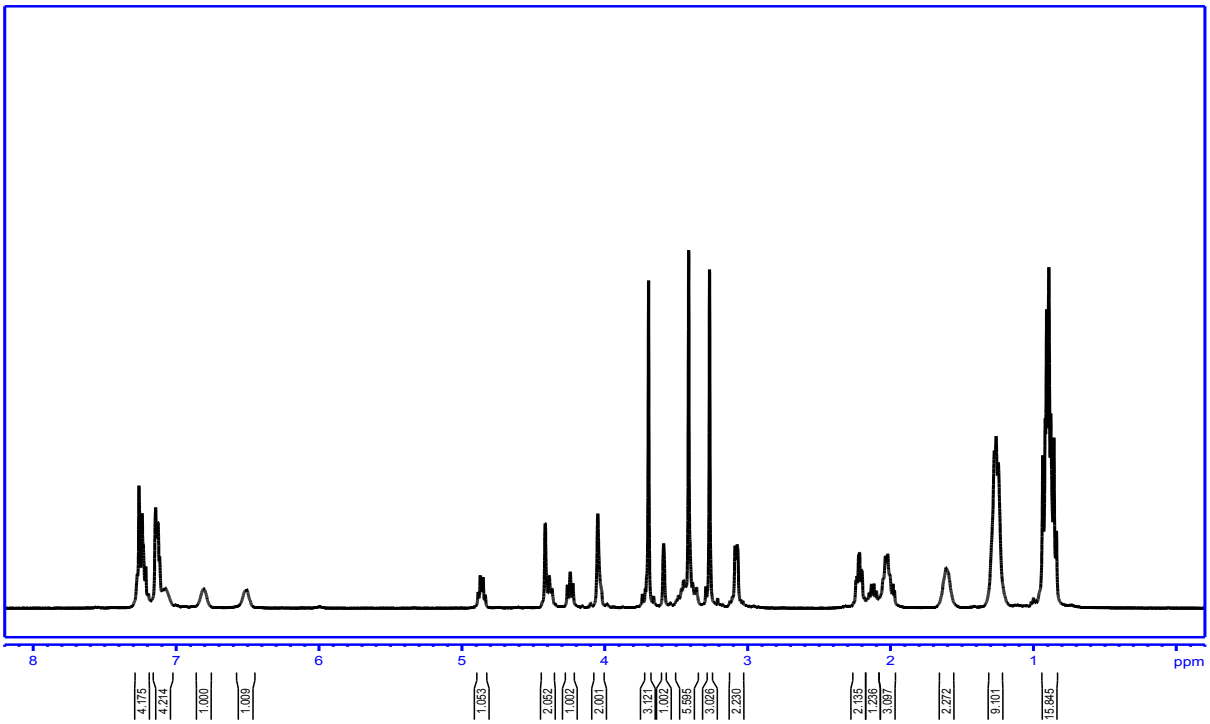
- **^{13}C NMR spectrum (DMSO-d_6, 100 MHz) of compound 4J.**



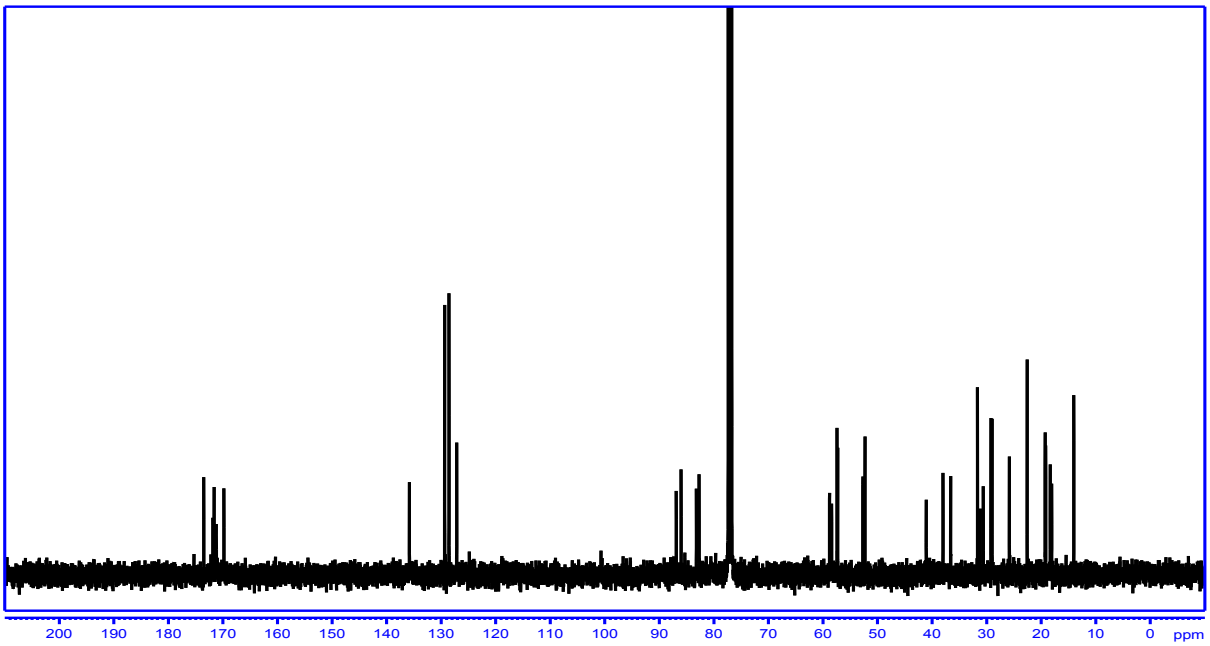
- **^{1}H NMR spectrum (DMSO-d_6, 400 MHz) of compound 4K.**



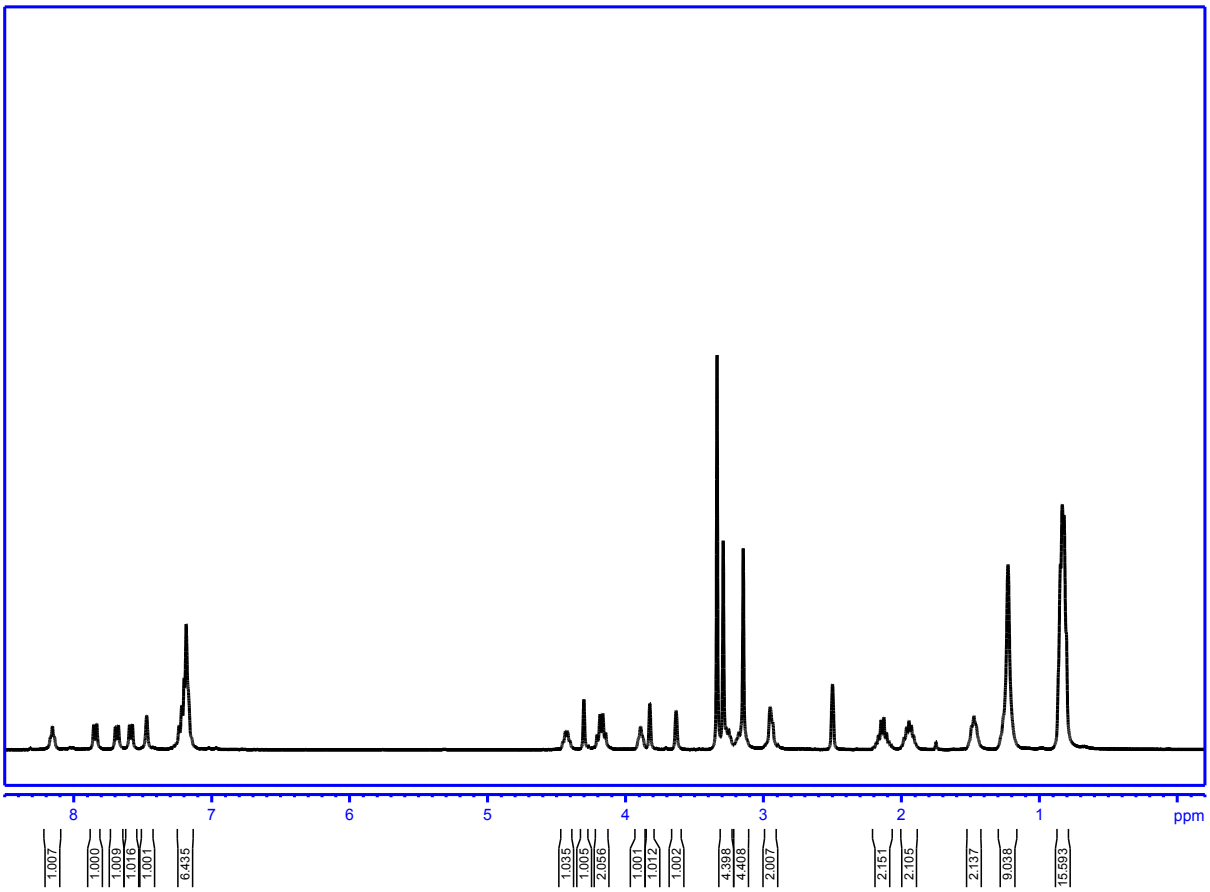
- **^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of compound 4L.**



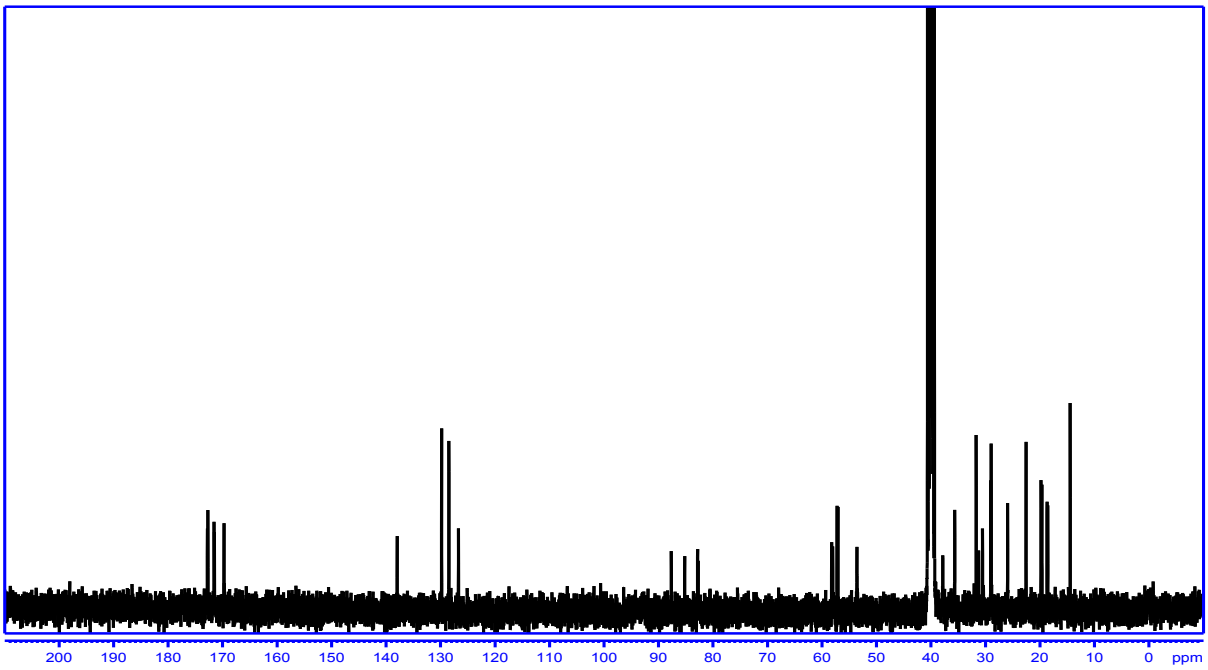
- **^{13}C NMR spectrum ($CDCl_3$, 100 MHz) of compound 4L.**



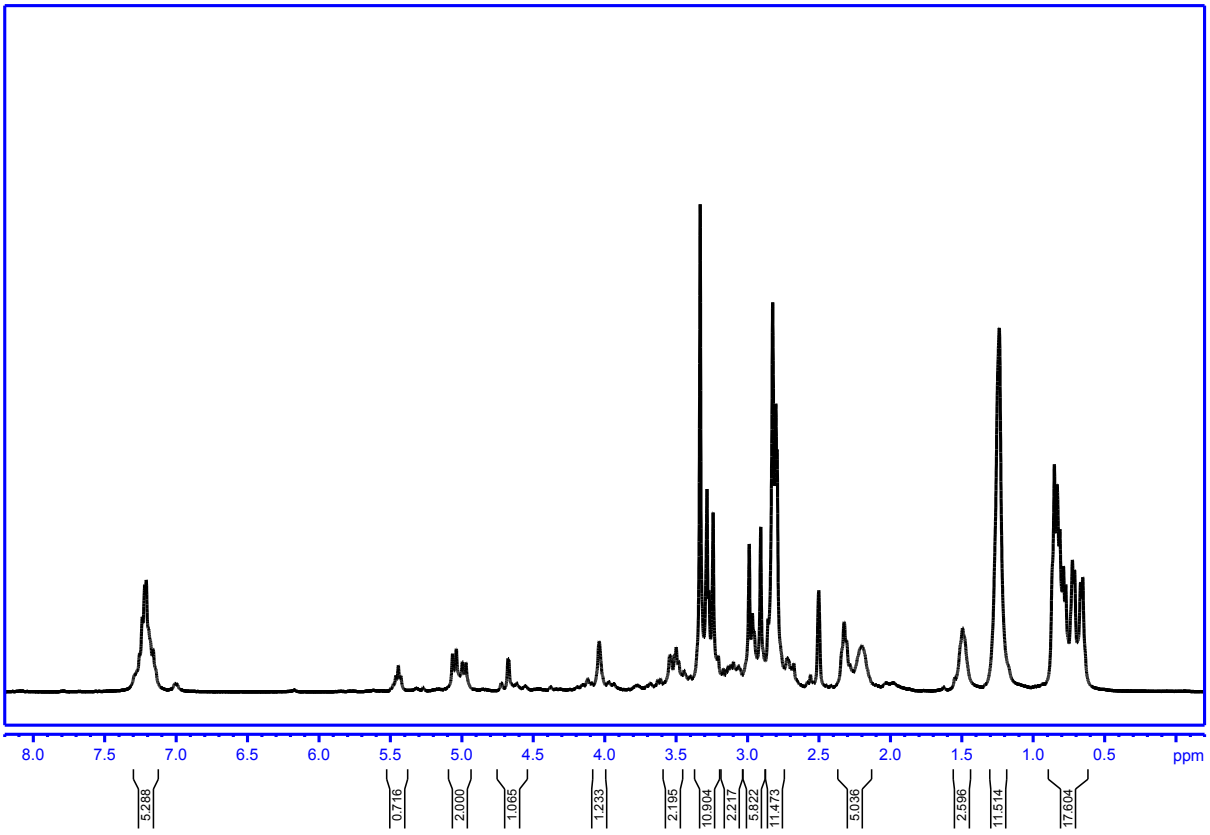
- **^{1}H NMR spectrum (DMSO-d_6, 400 MHz) of compound 4M.**



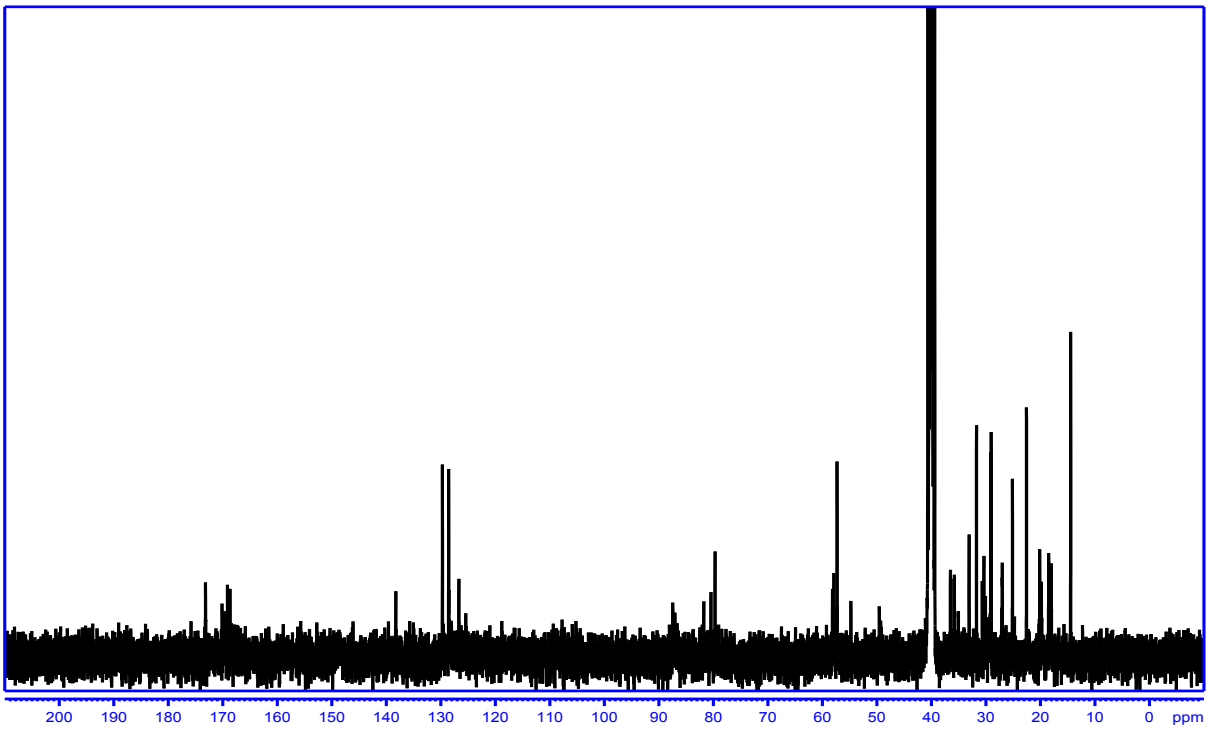
- **^{13}C NMR spectrum (DMSO-d_6, 100 MHz) of compound 4M.**



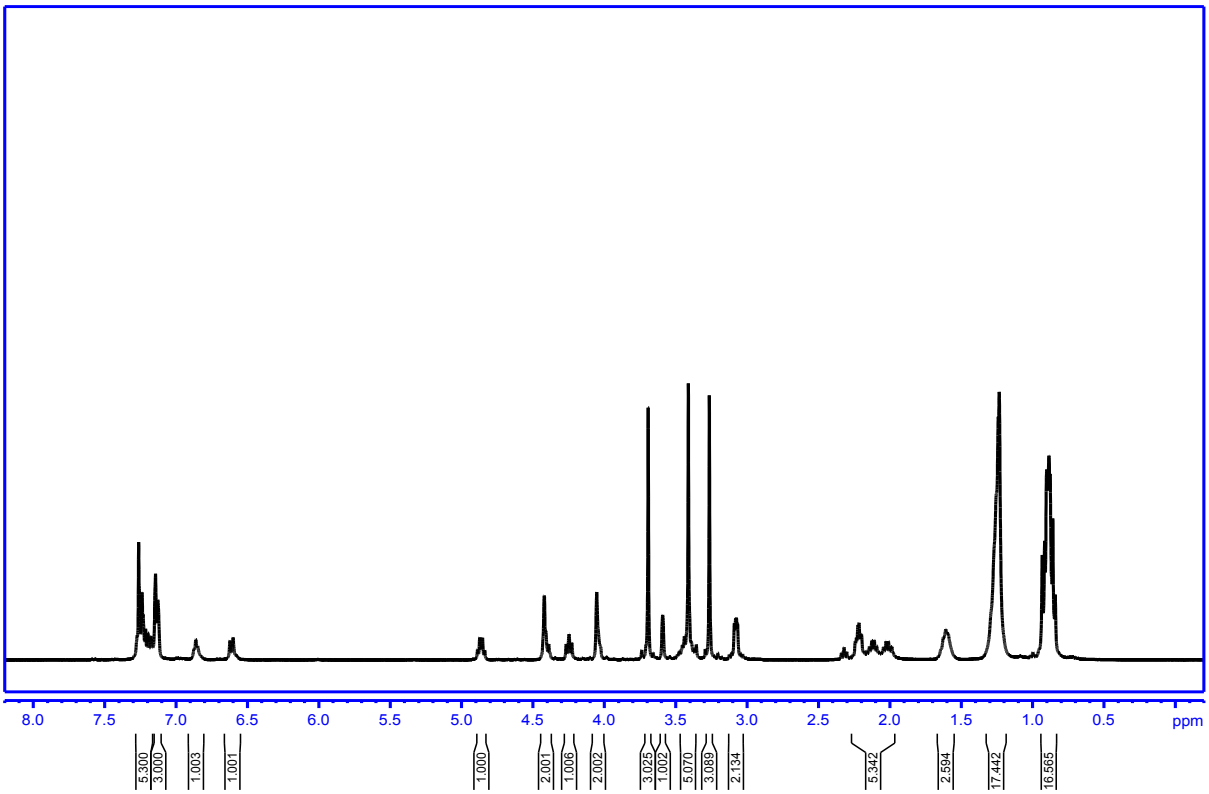
- **^{1}H NMR spectrum (DMSO-d_6, 400 MHz) of compound 4N.**



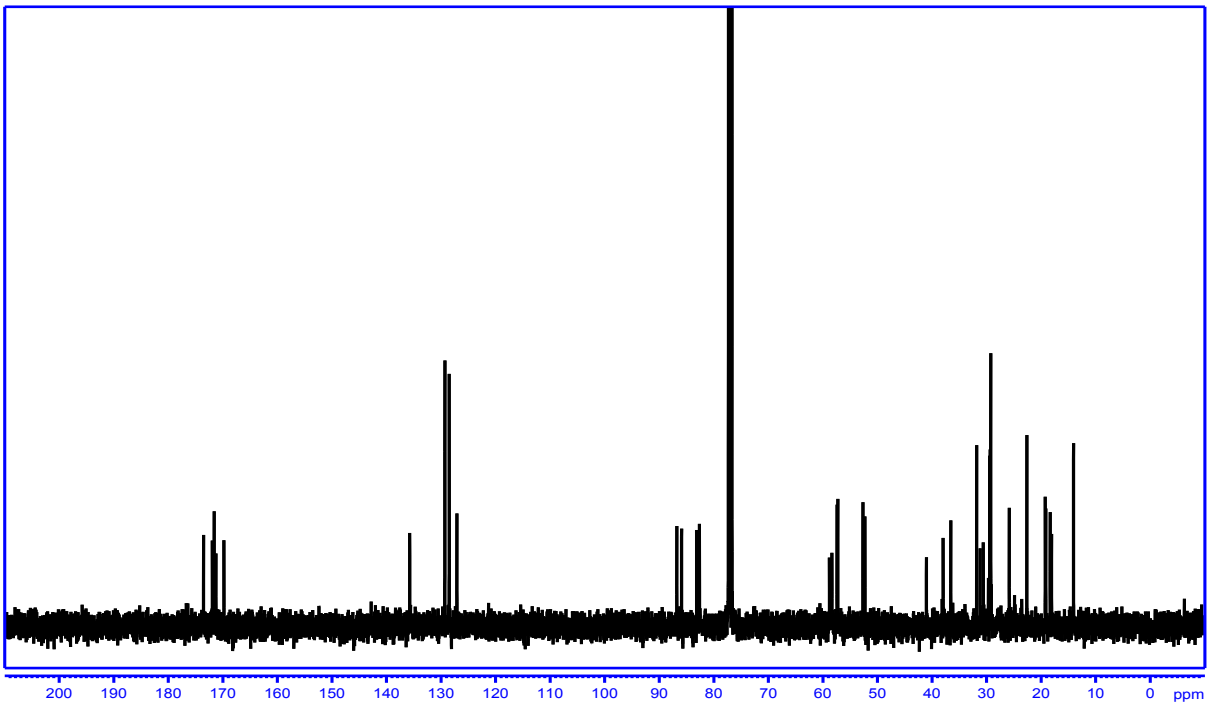
- **^{13}C NMR spectrum (DMSO-d_6, 100 MHz) of compound 4N.**



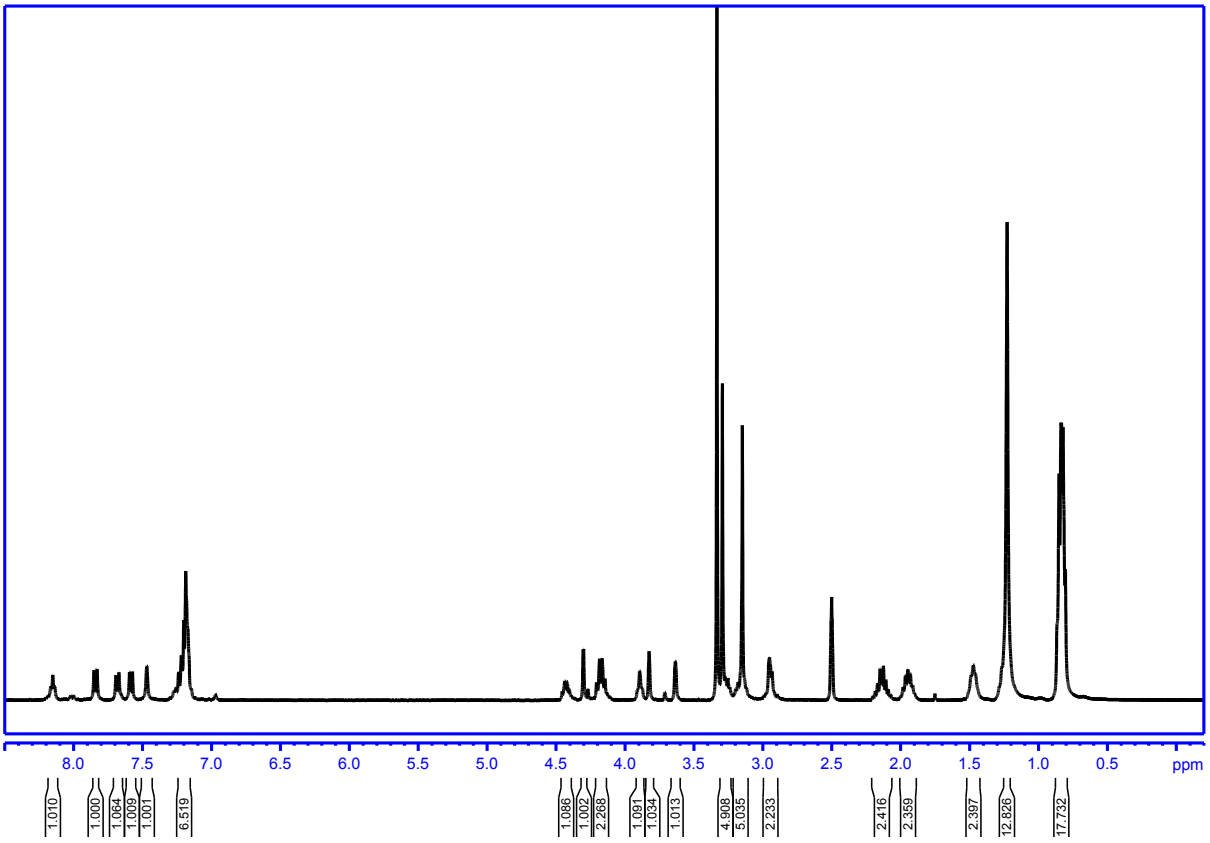
- **^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of compound 4O.**



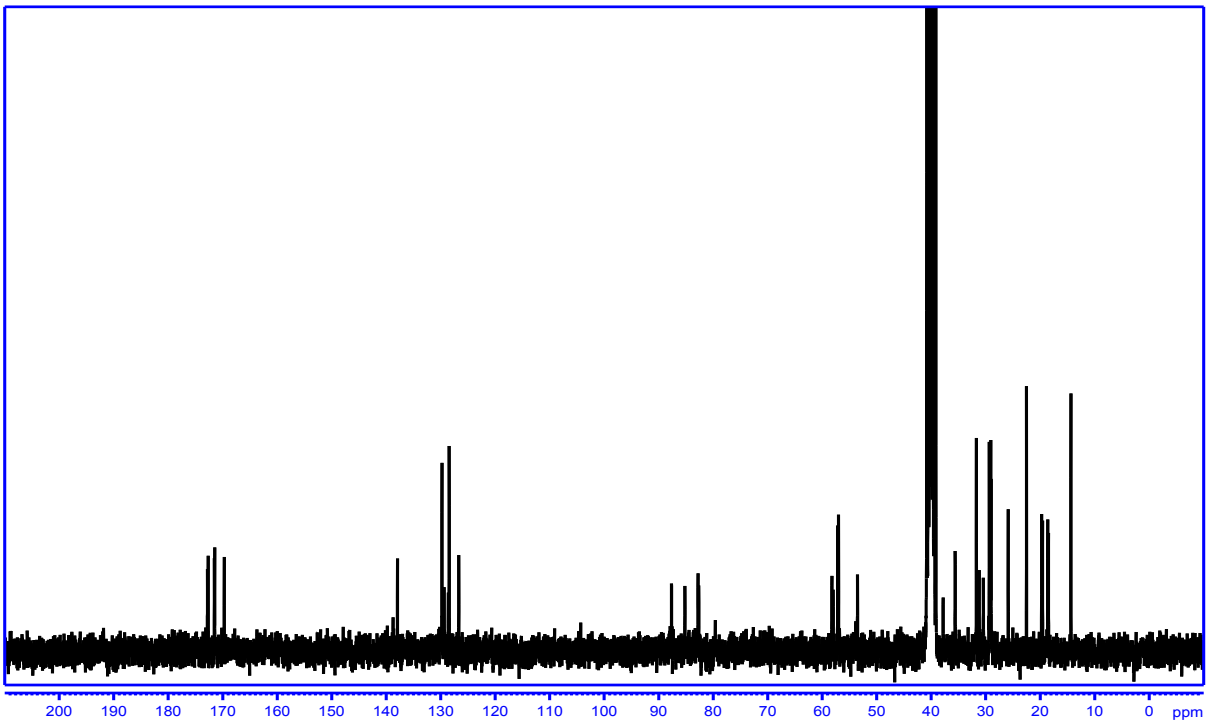
- **^{13}C NMR spectrum ($CDCl_3$, 100 MHz) of compound 4O.**



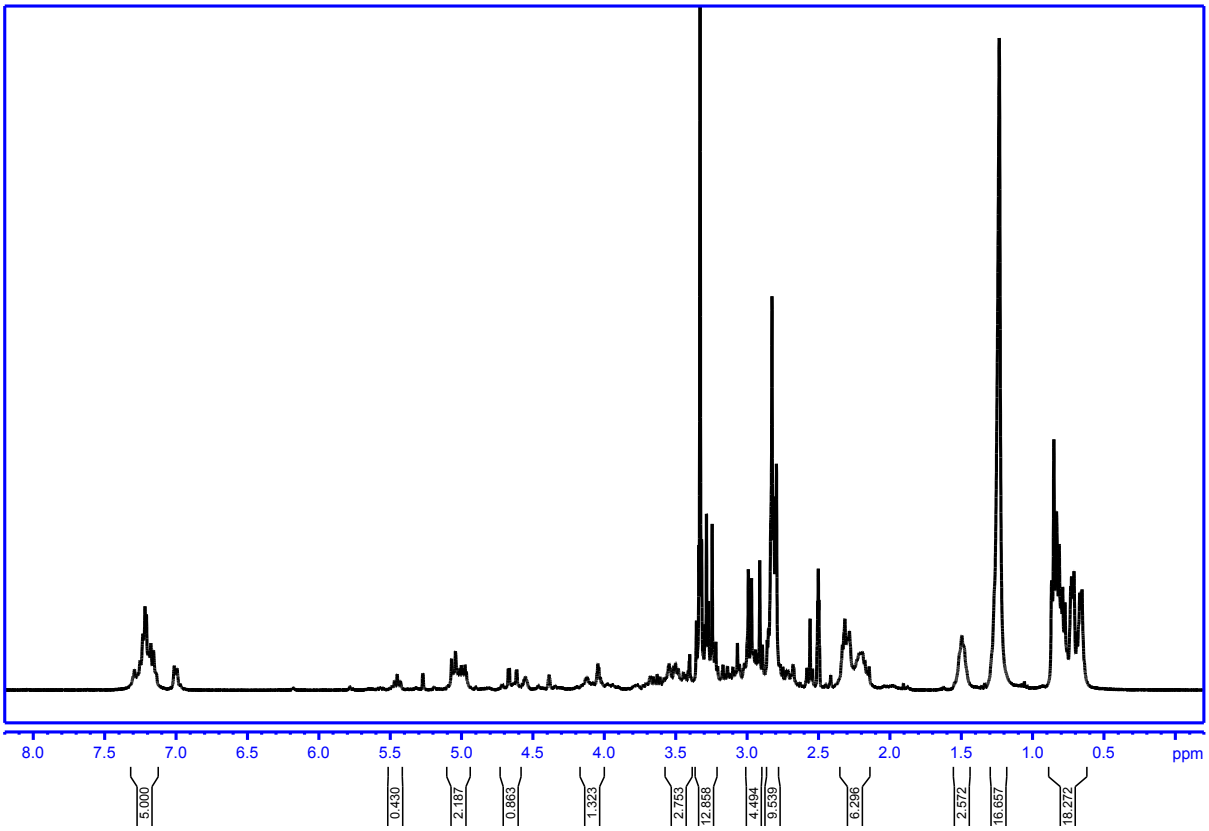
- **^{1}H NMR spectrum (DMSO-d_6, 400 MHz) of compound 4P.**



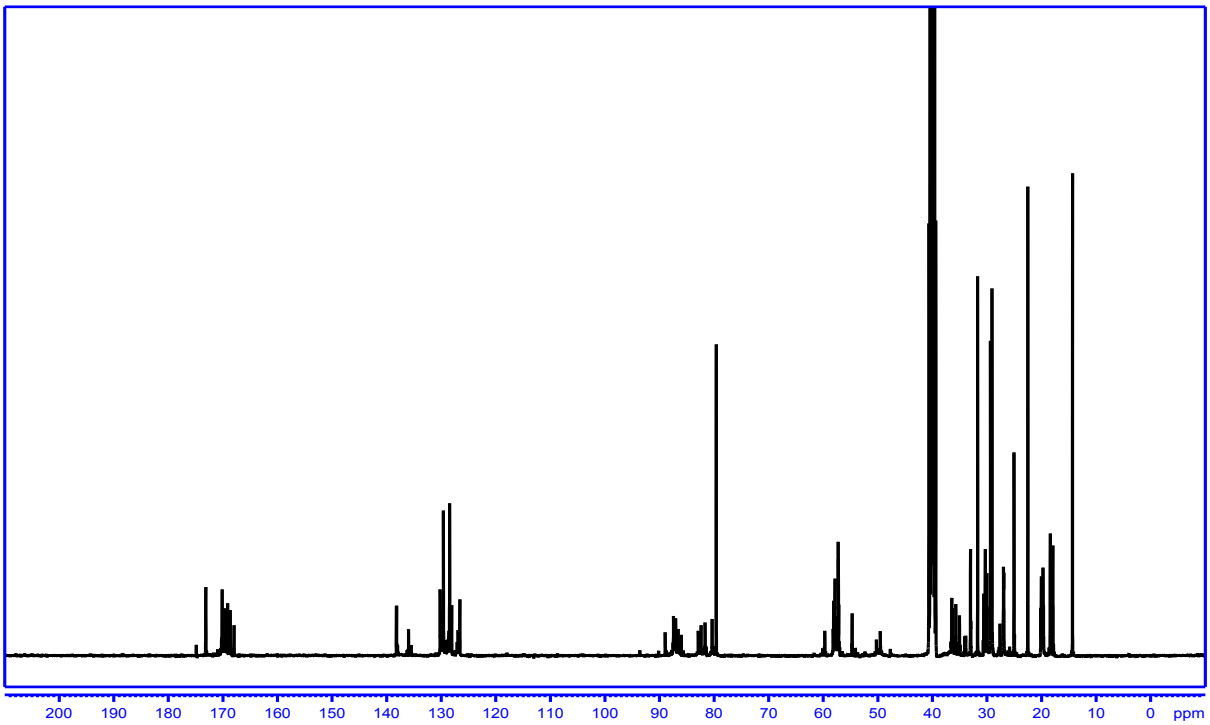
- **^{13}C NMR spectrum (DMSO-d_6, 75 MHz) of compound 4P.**



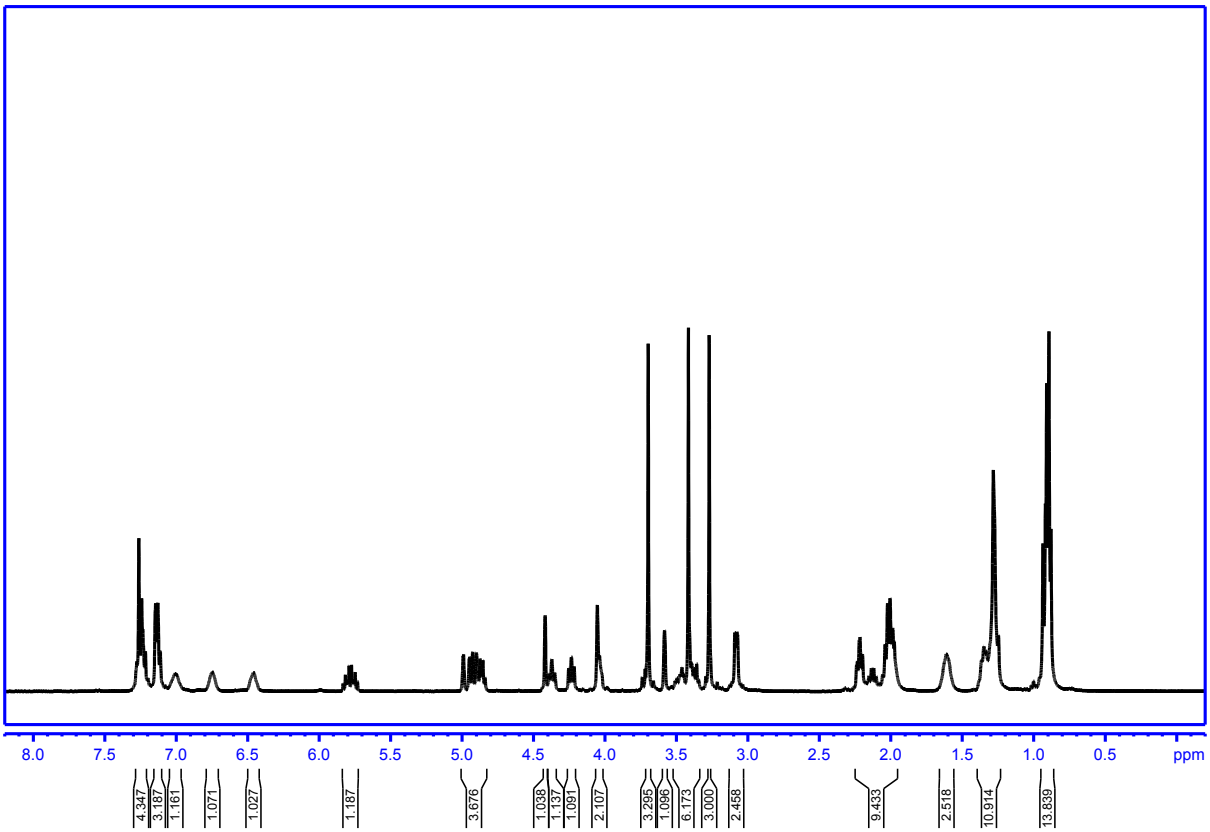
- **^{1}H NMR spectrum (DMSO-d_6, 400 MHz) of compound 4Q.**



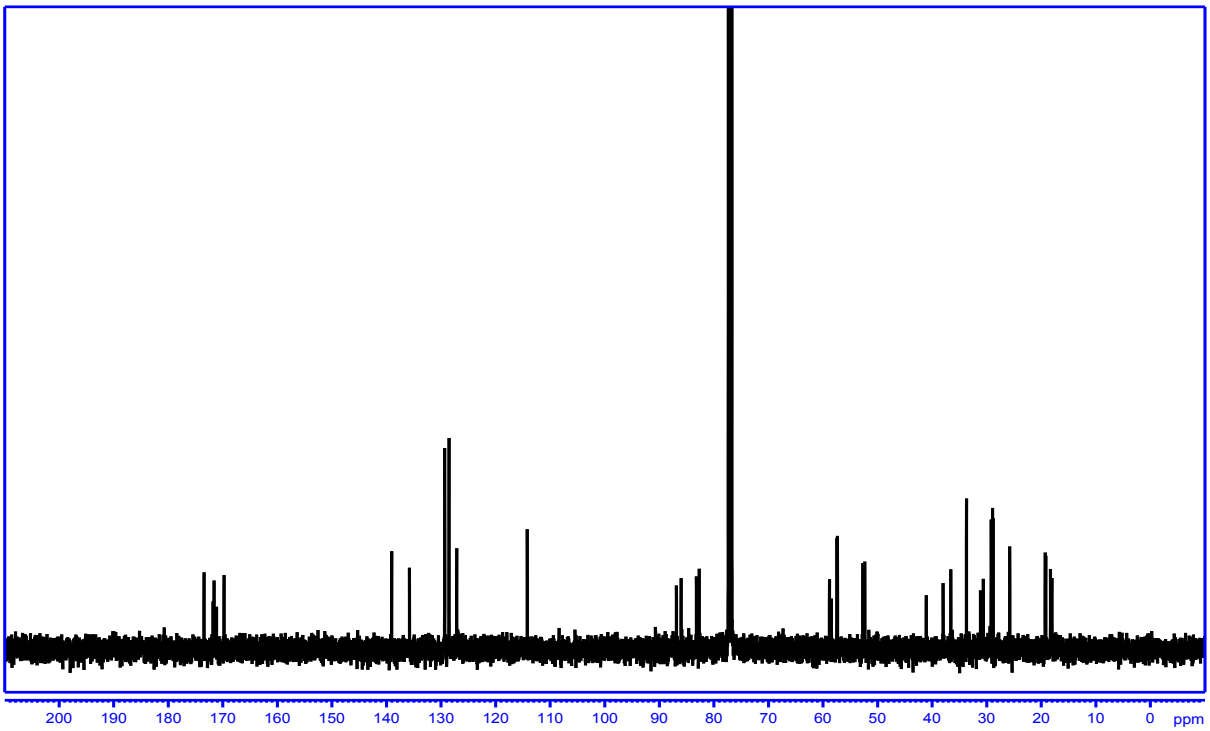
- **^{13}C NMR spectrum (DMSO-d_6, 100 MHz) of compound 4Q.**



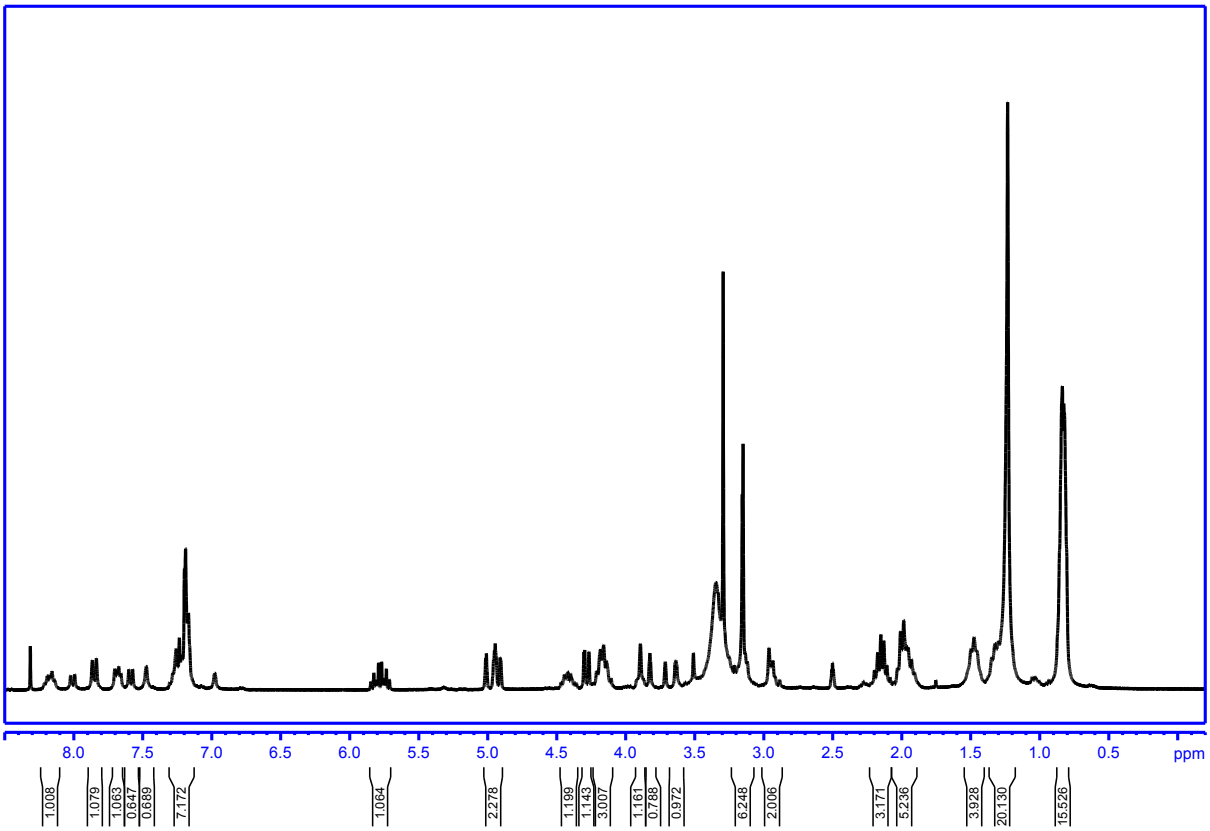
- **^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of compound 4R.**



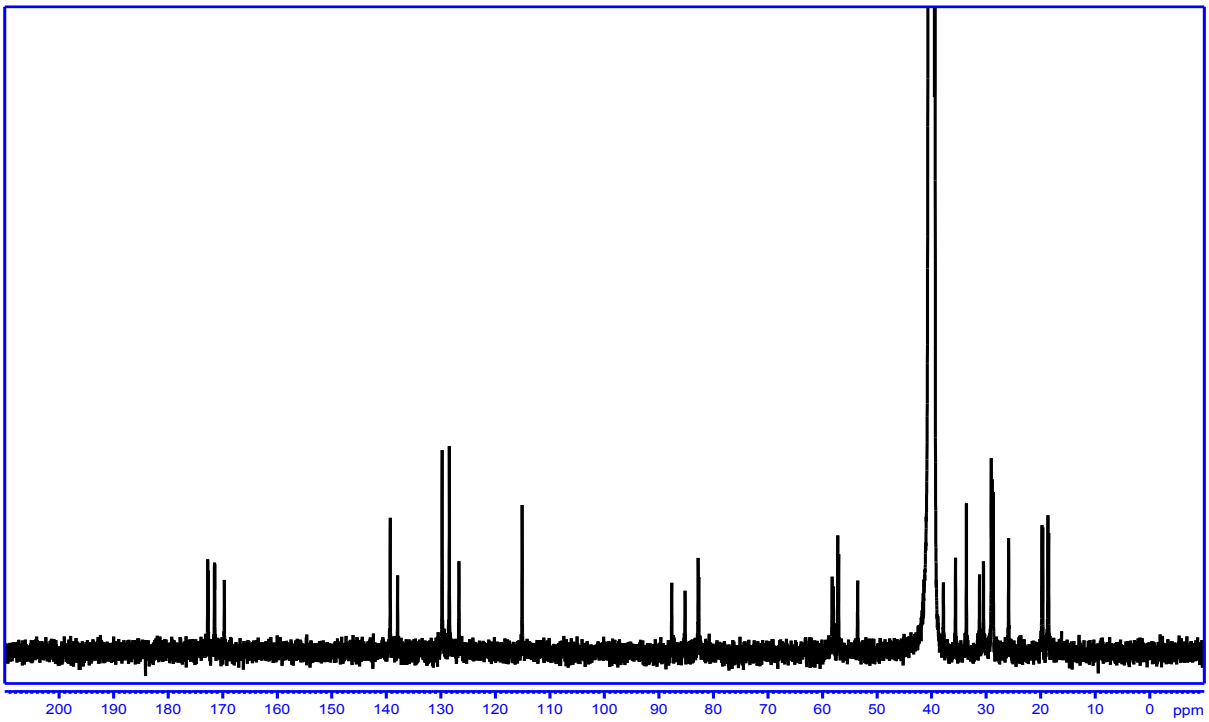
- **^{13}C NMR spectrum ($CDCl_3$, 100 MHz) of compound 4R.**



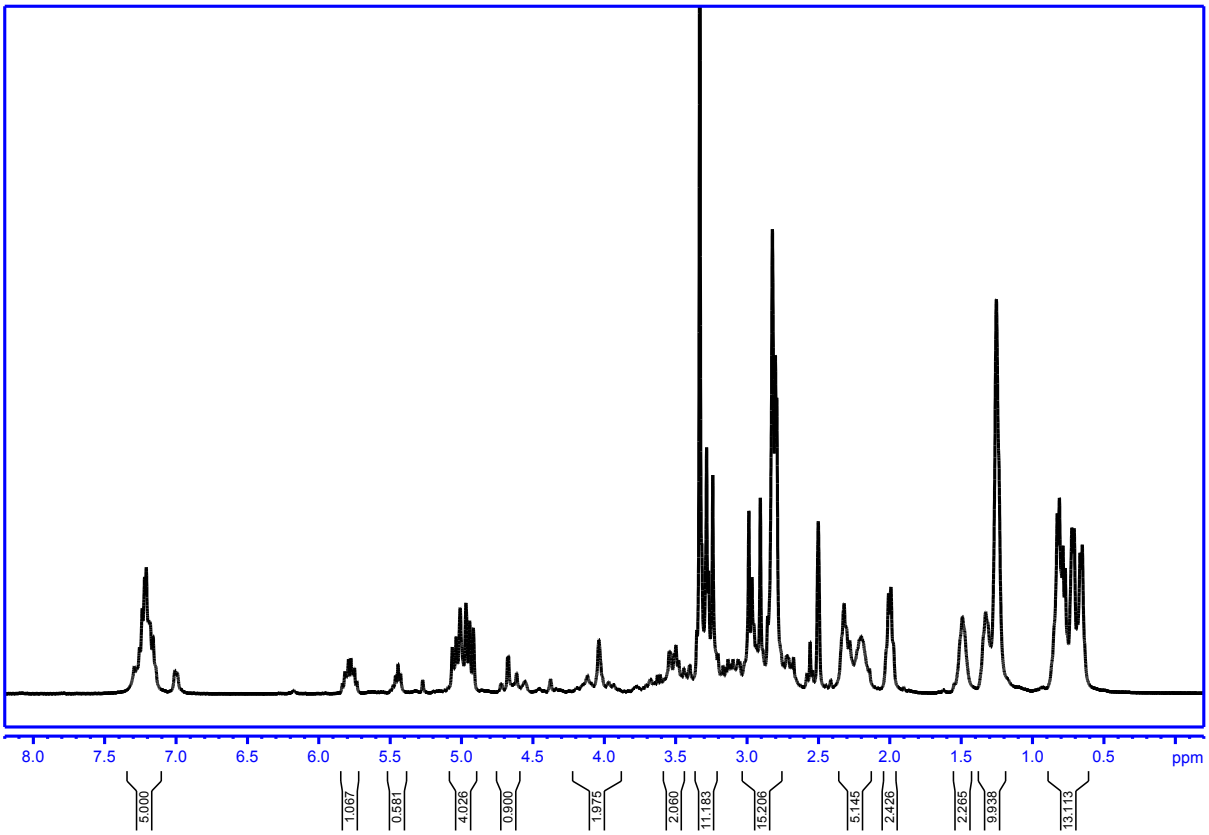
- **^{1}H NMR spectrum (DMSO-d_6, 300 MHz) of compound 4S.**



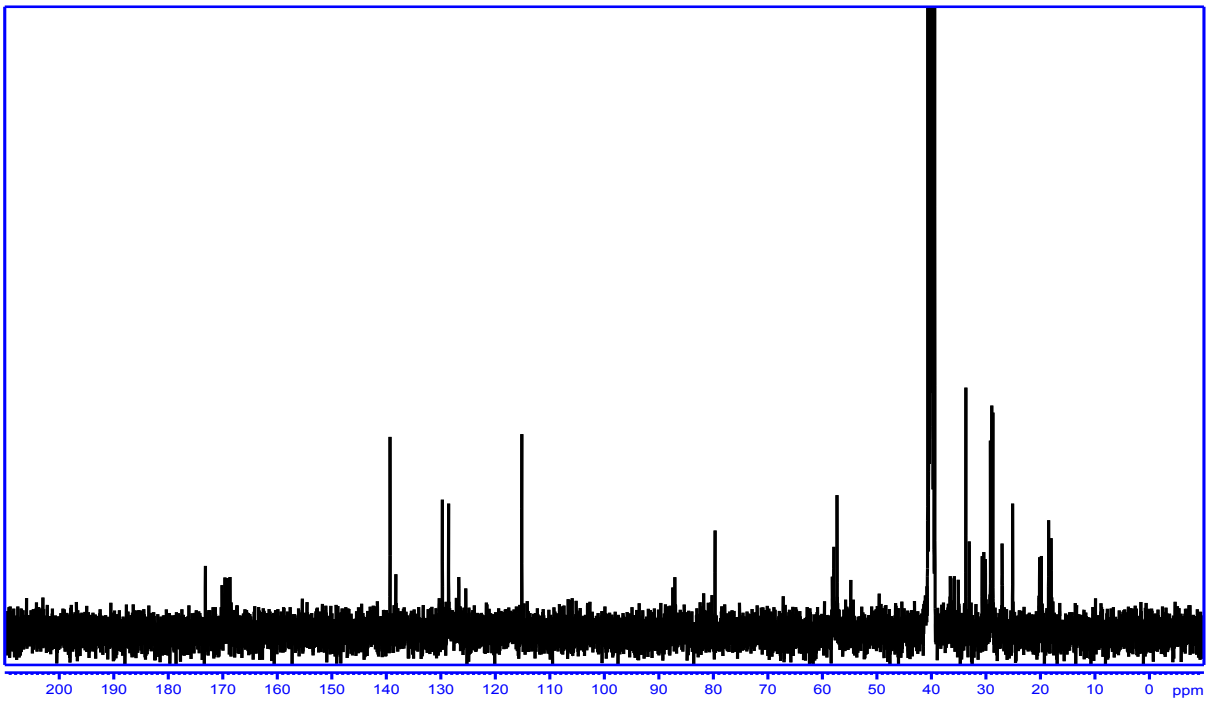
- **^{13}C NMR spectrum (DMSO-d_6, 100 MHz) of compound 4S.**



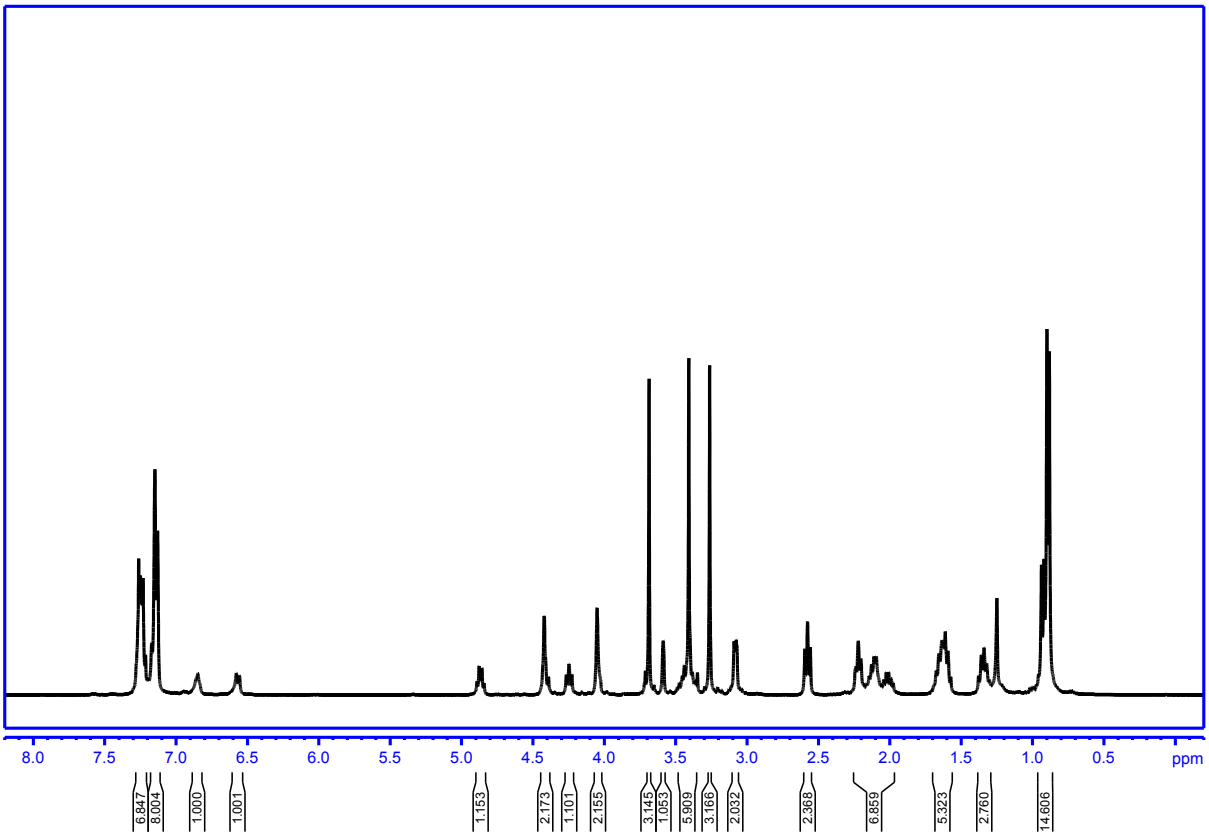
- **^{1}H NMR spectrum (DMSO-d_6, 400 MHz) of compound 4T.**



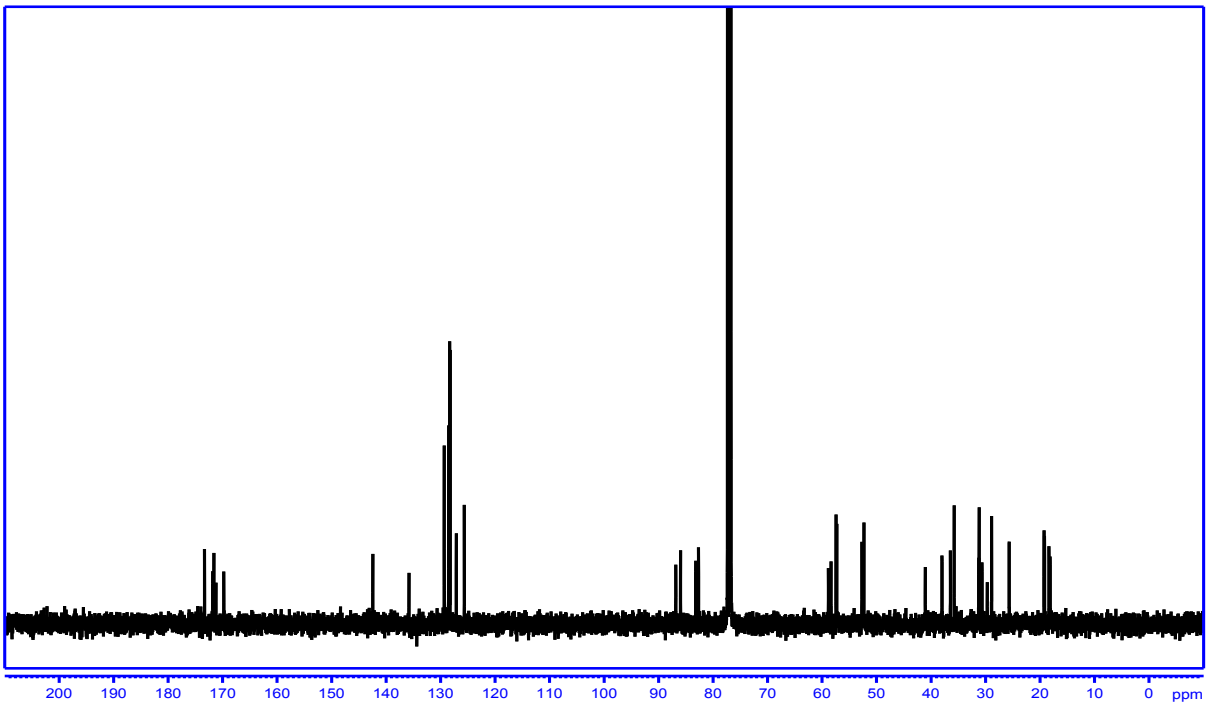
- **^{13}C NMR spectrum (DMSO-d_6, 100 MHz) of compound 4T.**



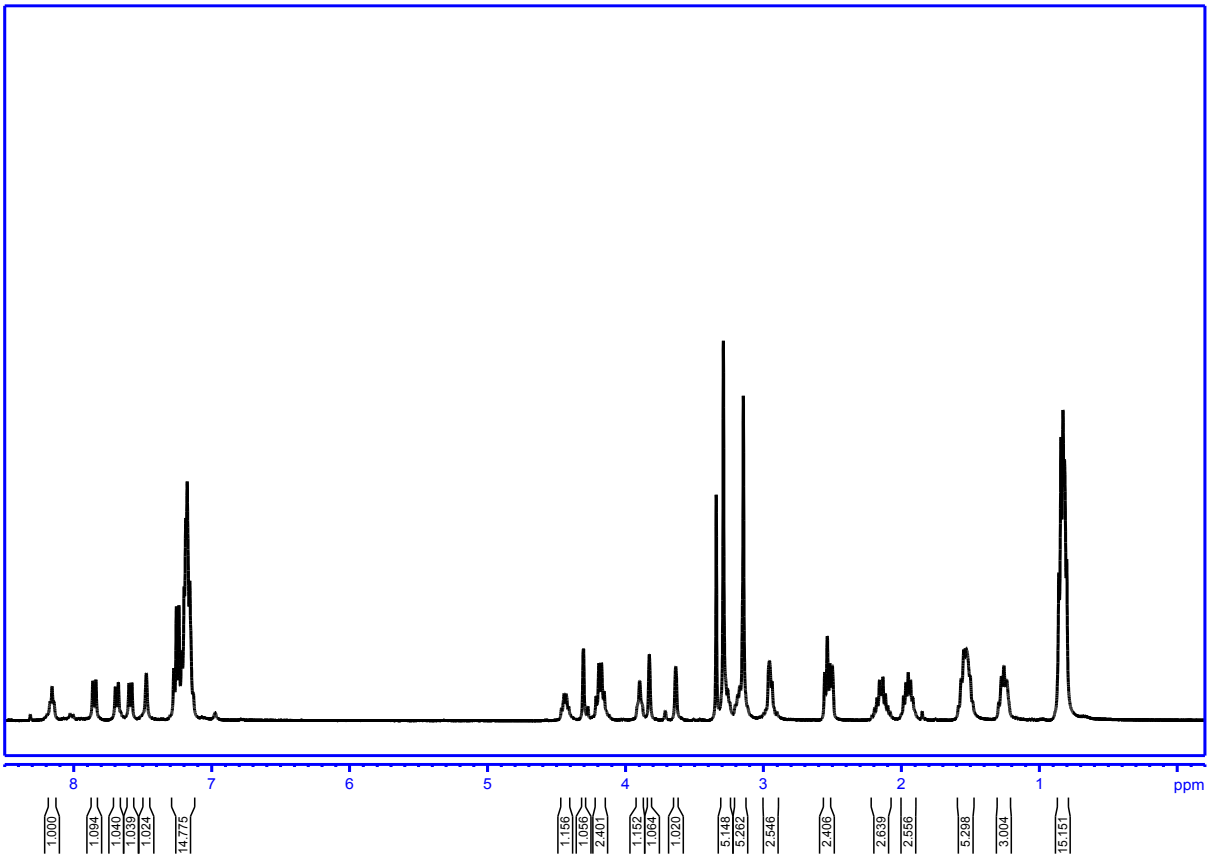
- **^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of compound 4U.**



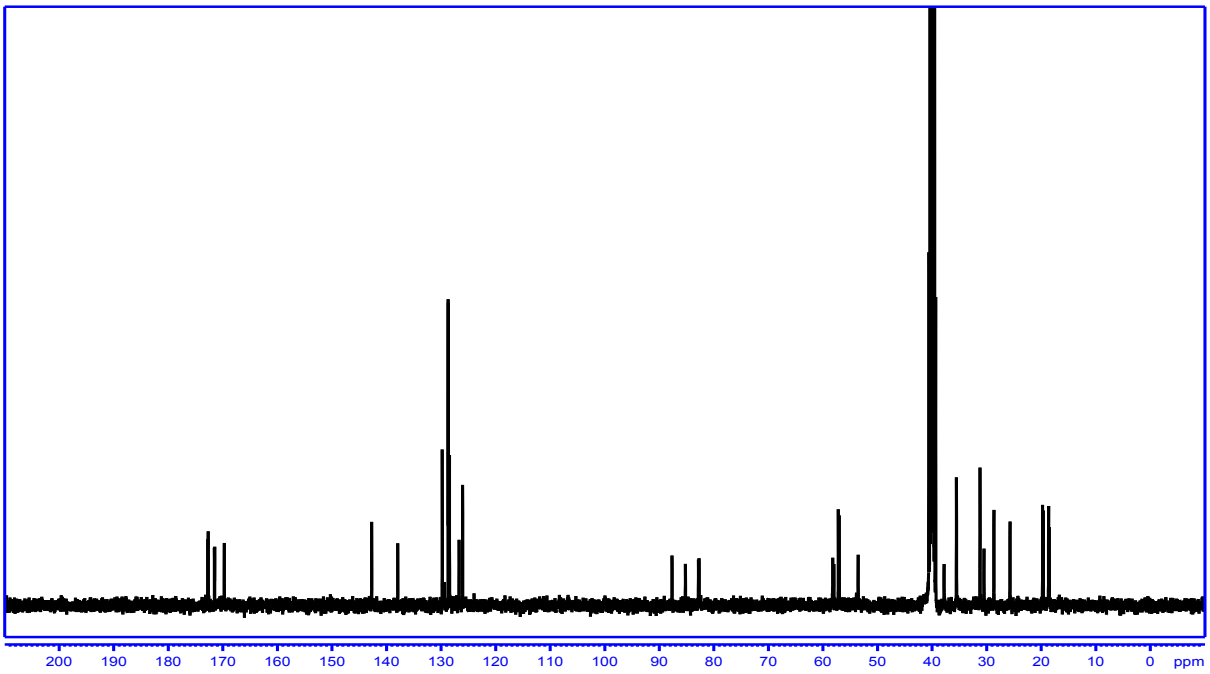
- **^{13}C NMR spectrum ($CDCl_3$, 100 MHz) of compound 4U.**



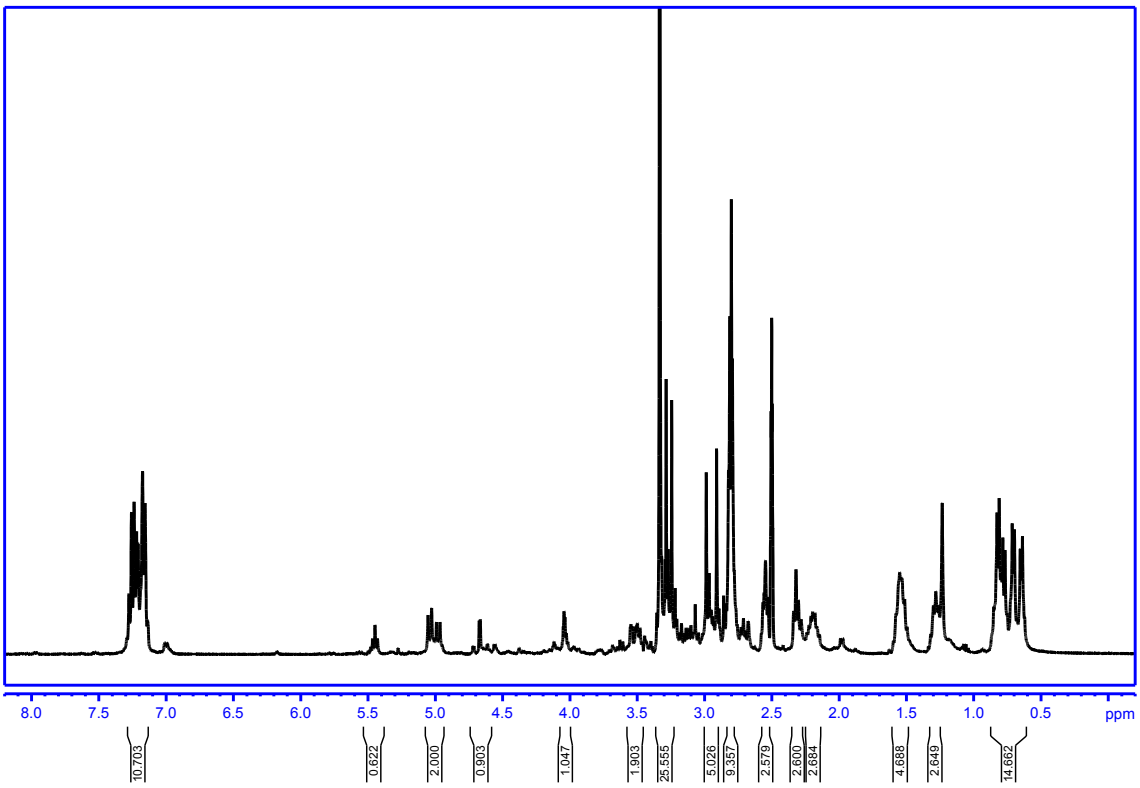
- **^{1}H NMR spectrum (DMSO-d_6, 400 MHz) of compound 4V.**



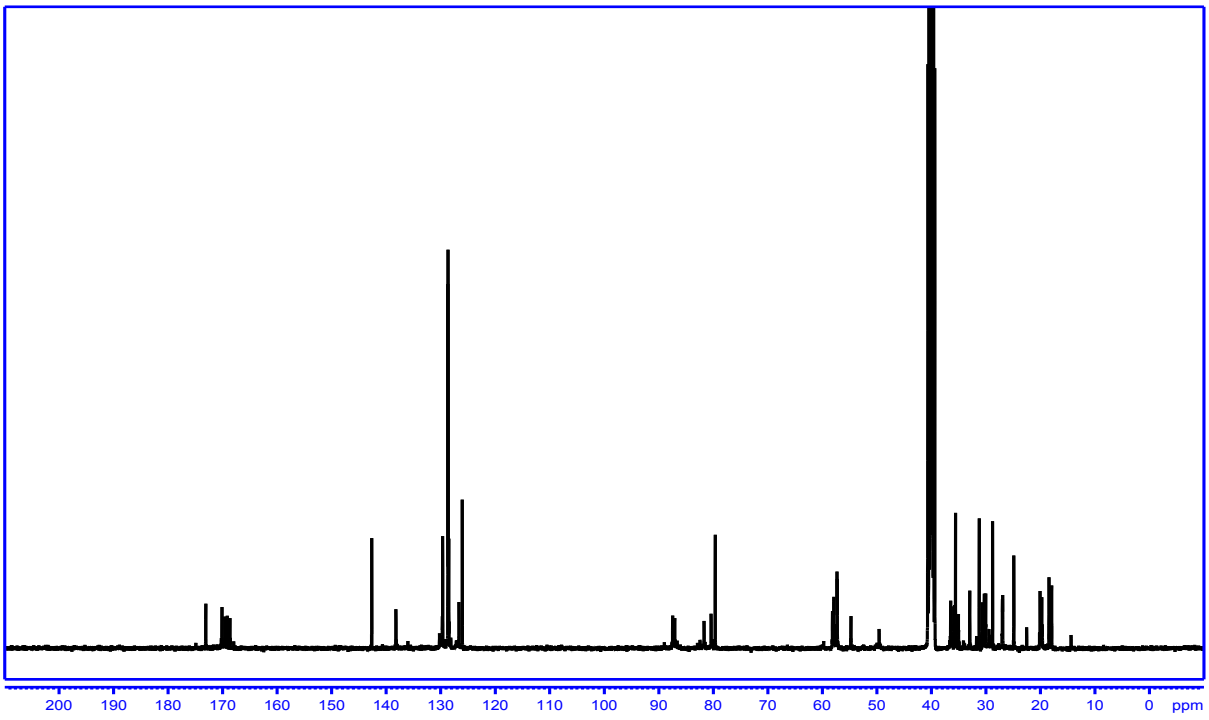
- **^{13}C NMR spectrum (DMSO-d_6, 100 MHz) of compound 4V.**



- **^{1}H NMR spectrum (DMSO-d_6, 400 MHz) of compound 4W.**



- **^{13}C NMR spectrum (DMSO-d_6, 100 MHz) of compound 4W.**



SAR studies:

- **Method:**

Molecules were drawn and minimized in MOE followed by partial charge calculation using AMBER99. Structures were subsequently subjected to molecular dynamics simulation at 300 K and AMBER99 force field in vacuum with 100 ps of equilibrium run followed by production run for 500 ps. Resulting structures were analyzed in Chimera.

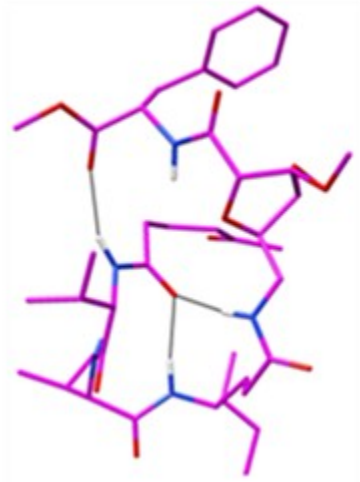
- **Table S1. Listing the phi and psi values for compounds with their corresponding activities:**

Compound	Antiamastigote activity (IC_{50},μM) (MQ/amast. model)	phi1	psi1
4A	>100	-61.755	-0.71
4B	>100	-134.198	-1.212
4C	26.41	49.707	59.072
4D	>100	-59.787	-16.771
4E	>25	-59.901	10.461
4F	92.18	-65.788	-30.967
4G	>100	-75.104	-4.855
4H	56.48	113.958	-46.977
4I	>100	-59.891	-14.16
4J	>100	-46.942	-25.482
4K	>100	-137.28	59.323

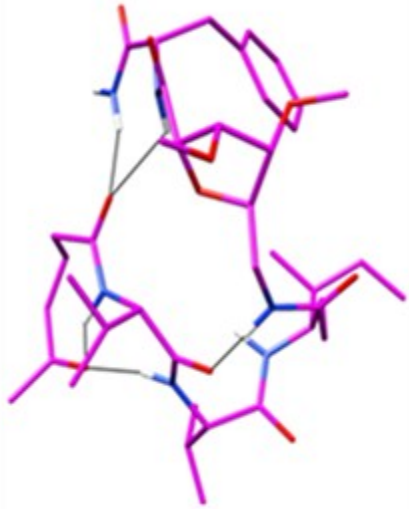
4L	60.67	-67.65	-8.03
4M	>100	-62.493	-23.785
4N	26.67	58.367	46.577
4O	68.48	-63.718	-5.054
4P	>100	-74.749	10.65
4Q	10.10	66.404	59.106
4R	>50	-44.178	-23.69
4S	>100	-68.138	-13.506
4T	10.92	50.737	53.02
4U	22.86	-50.932	-25.19
4V	>100	-53.618	-10.524
4W	13.63	66.5	61.3

- **Effect of H-bonding on the structural changes in the domain of peptides:**

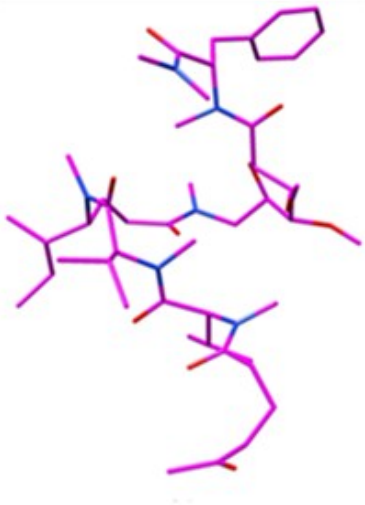
The amide proton containing molecules form the hydrogen bond between the carbonyl oxygen of the first residue and amide proton of the third residue and adopts a particular tight gamma turn resulting the *N*-terminal hydrophobic chains to turn around the backbone leading to the disruption of coiled secondary structure and also in the reduction of hydrophobic surface area.



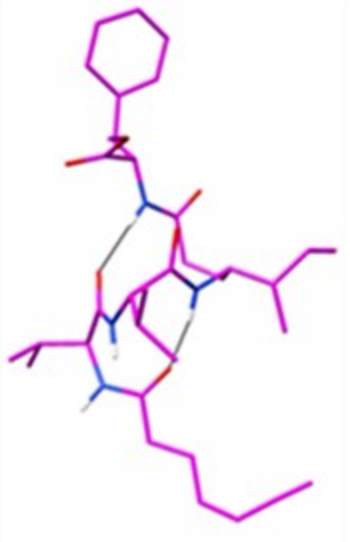
4A



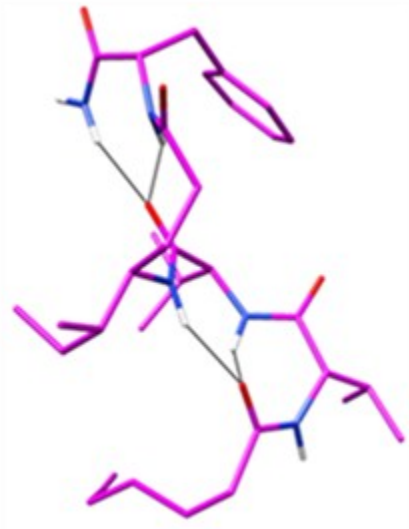
4B



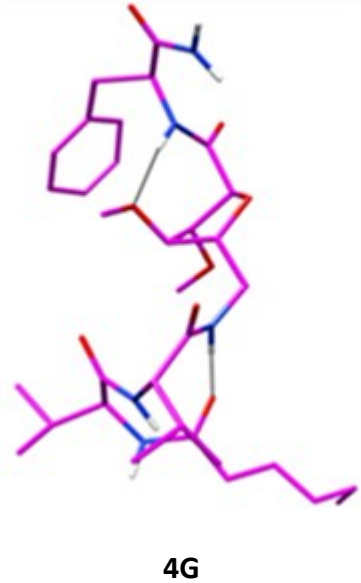
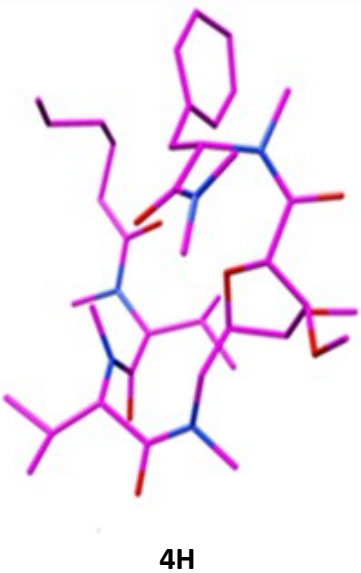
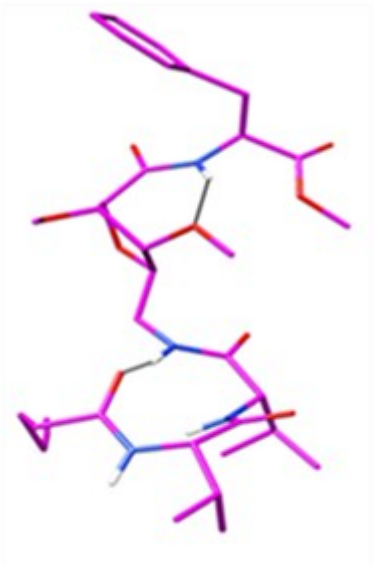
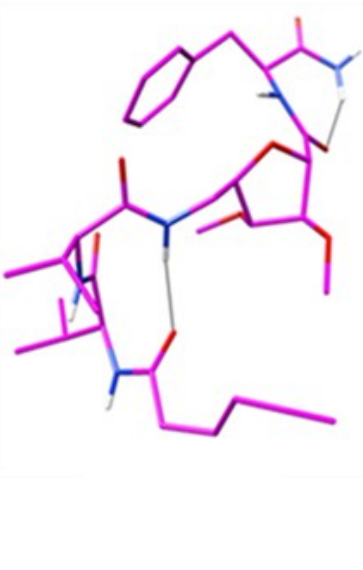
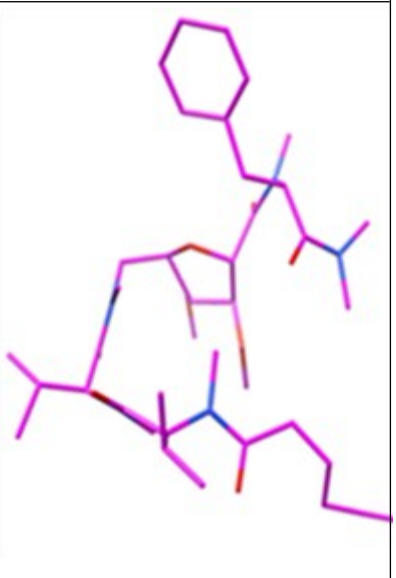
4C

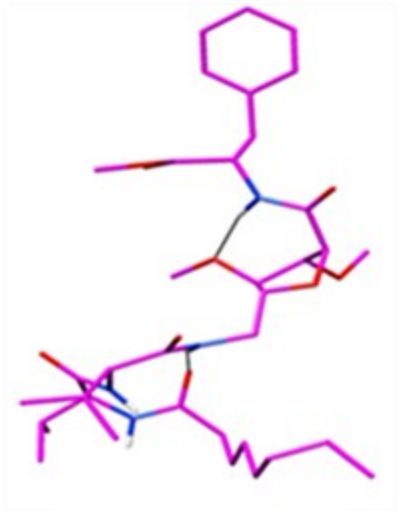
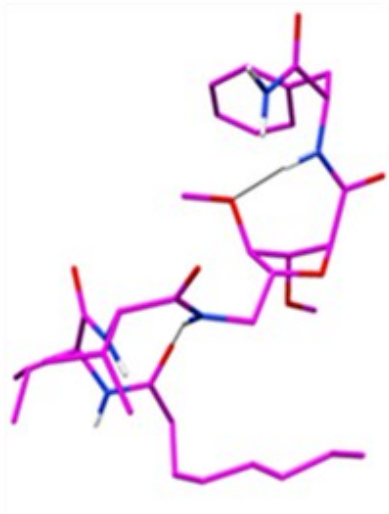
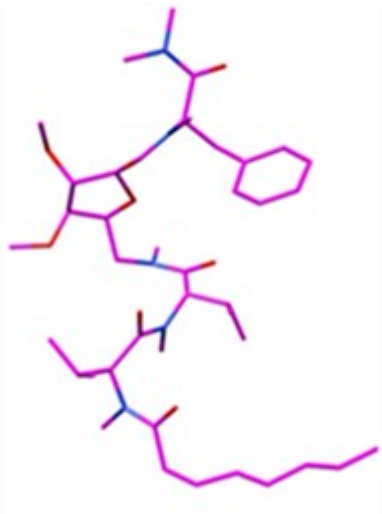
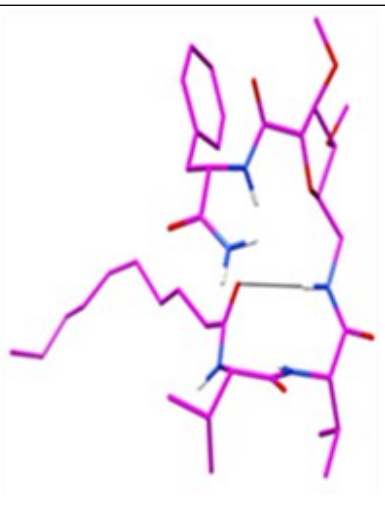
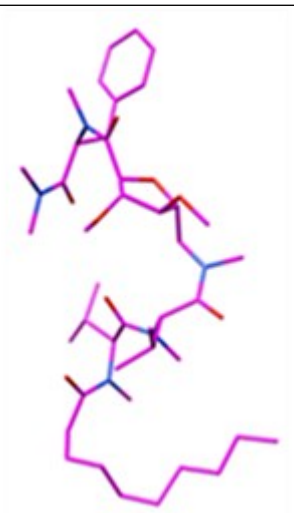


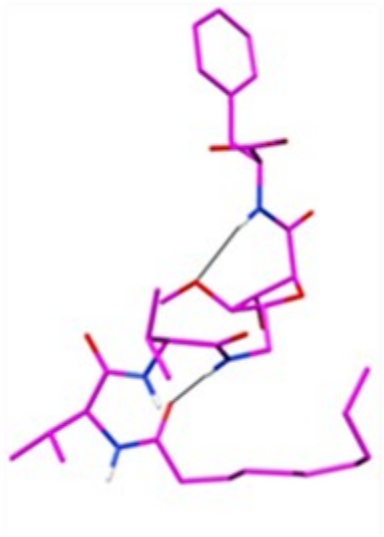
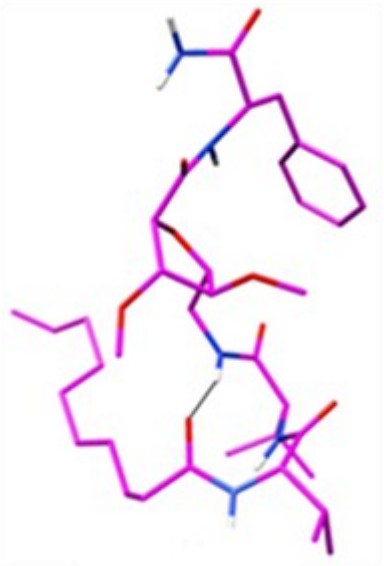
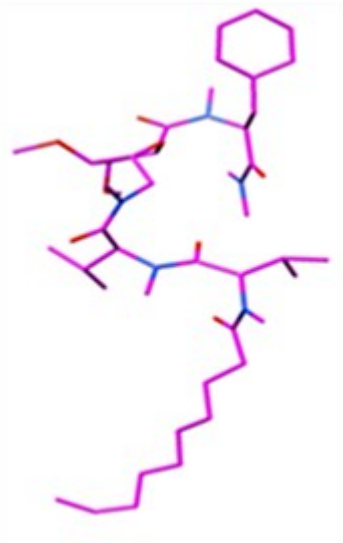
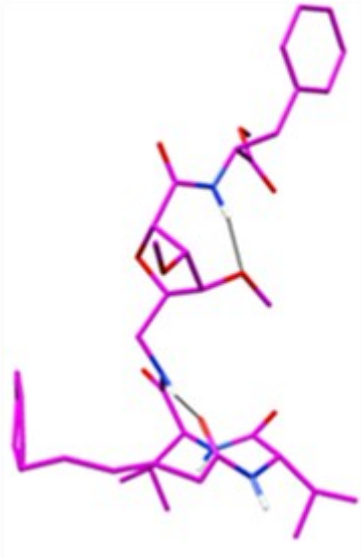
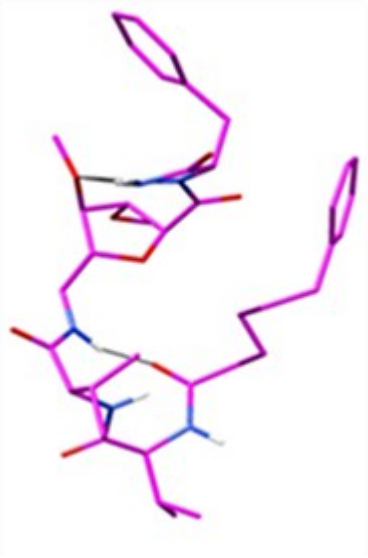
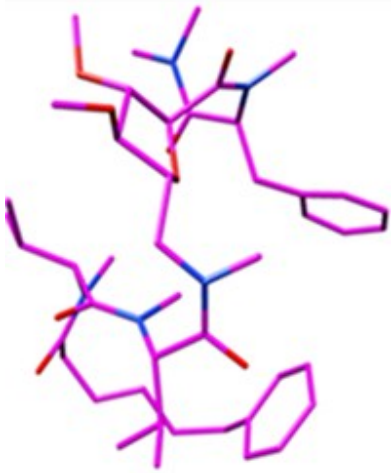
4D



4E

 **4F**	 **4G**	 **4H**
 **4I**	 **4J**	 **4K**

 **4L**	 **4M**	 **4N**
 **4O**	 **4P**	 **4Q**

 **4R**	 **4S**	 **4T**
 **4U**	 **4V**	 **4W**

NMR Studies: Solution NMR spectra were recorded on 500 MHz spectrometers at room temperature or else as mentioned using 2-10 mM concentration of peptides in appropriate solvents using TMS as internal standard or the solvent signals as secondary standards and the chemical shifts (δ) are shown in ppm scales. ^{13}C spectra were recorded at 125 MHz with complete proton decoupling. The proton resonance assignments were carried out by using ^{1}H-^{1}H Two-dimensional total correlation spectroscopy (TOCSY), and Rotating frame nuclear Overhauser effect spectroscopy (ROESY). All the experiments were carried out in the phase sensitive mode. The spectra were acquired with 1024x256 or 2048x192 free induction decays (FID) containing 8-16 transients with relaxation delay 1-2 s. The TOCSY experiments were performed with mixing time of 0.08s, and spin-locking field of 10 kHz. The two dimensional data were processed with Gaussian apodization in both the dimensions. The ROESY experiments were performed with mixing times of 0.2 to 0.3 s, and a spin locking field of about 2.5 kHz. Variable temperature (VT) studies were carried out by varying temperature by 10°C for every increment from 20°C-70°C. Small changes in amide proton chemical shifts (ppb/°K) during VT studies have been used to indicate their participation in H-bonding.

Table S2: Chemical shift (δ in ppm) and coupling constants (J in Hz) for **4P** in DMSO-d_6 (~8 mM, 500 MHz, 300 K)

Res	NH	CαH	CβH	CγH	CδH	CεH	Δδ/ΔT
^{1}PHE	7.57 (*d,* $^{3}J_{NH\text{-}C\alpha H}$=8.5 Hz)	4.425 (*ddd,* 1H, $^{3}J_{C\alpha H\text{-}C\beta H}$ = 5.3 Hz, $^{3}J_{C\alpha H\text{-}C\beta'H}$=7.9 Hz)	2.96 (*dd,* 1H, $^{3}J_{C\beta H\text{-}C\gamma H}$ = 5.3 Hz, $^{3}J_{C\beta H\text{-}C\beta'H}$ =13.2 Hz) 2.91 (*dd,* 1H, $^{3}J_{C\beta'H\text{-}C\gamma H}$= 7.9 Hz)	-	-	-	3.25
^{2}MAA	8.13 (d, 1H, $^{3}J_{NH\text{-}C\alpha H}$=6.0)	4.29 (d, 1H, $^{3}J_{C\alpha H\text{-}C\beta H}$ = 1.8 Hz)	3.813 (t, 1H, $^{3}J_{C\beta H\text{-}C\gamma H}$ = 1.8Hz)	3.63 (dd, 1H, $^{3}J_{C\gamma H\text{-}C\delta H}$ = 2.7 Hz)	3.89 (dt, 1H, $^{3}J_{C\delta H\text{-}C\varepsilon H,\ H'}$ = 6.8 Hz)	3.26 (m, 1H), 3.14 (m, 1H)	10.75

^{3}VAL	7.65 (*d*, 1H, $^{3}J_{NH\text{-}H\alpha}$=8.8 Hz)	4.15 (*dd,* 1H, $^{3}J_{C\alpha H\text{-}c\beta H}$=6.8 Hz)	1.93 (*dd,*$^{3}J_{CbH\text{-}c\gamma H}$=6.8 Hz)	0.822 (d, 6H)			5.75
^{4}VAL	7.83 (*t*, $^{3}J_{NH\text{-}H\alpha}$ =8.9	4.17 (*dd,*$^{3}J_{C\alpha H\text{-}c\beta H}$=6.8	1.95 (*dd,*$^{3}J_{C\alpha H\text{-}c\beta H}$= 6.8	0.804 (d, 6H)			4.50
Acetyl	---	2.136 (m,2H)	1.515(m,2H)	1.254 (m,2H)	1.537 (m,2H)	2.53 (m, 2H)	4.0 for 7.45

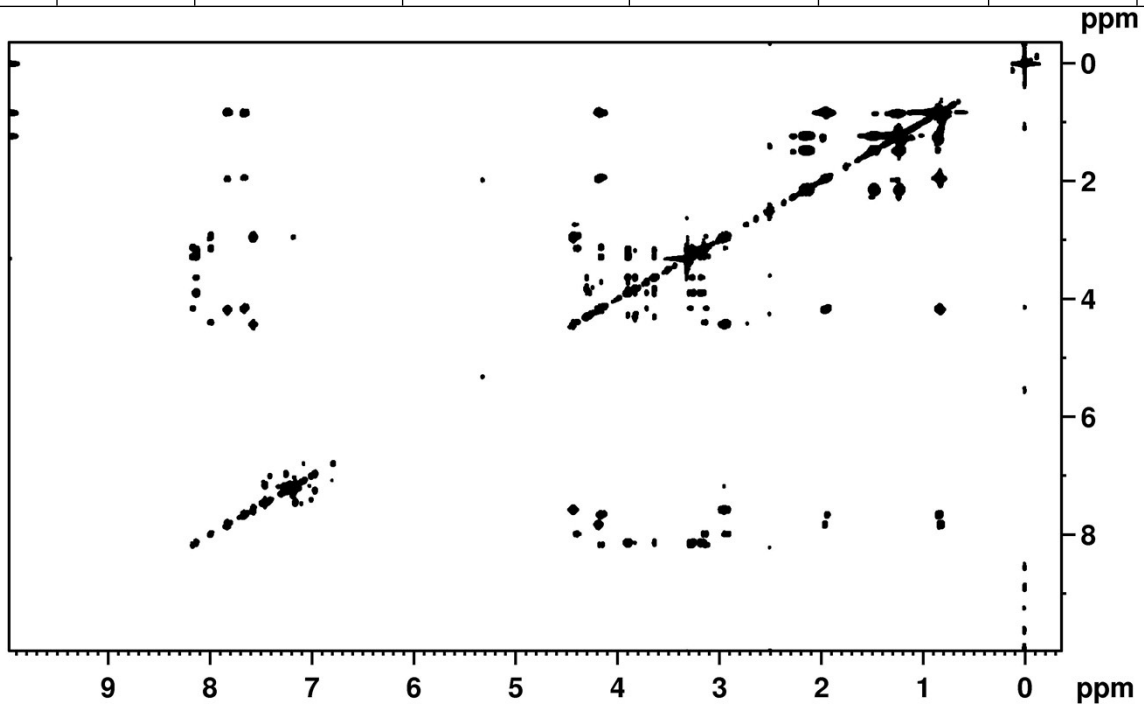


Figure S1: 2D-TOCSY NMR spectrum (DMSO-d_6, 400 MHz) of compound 4P

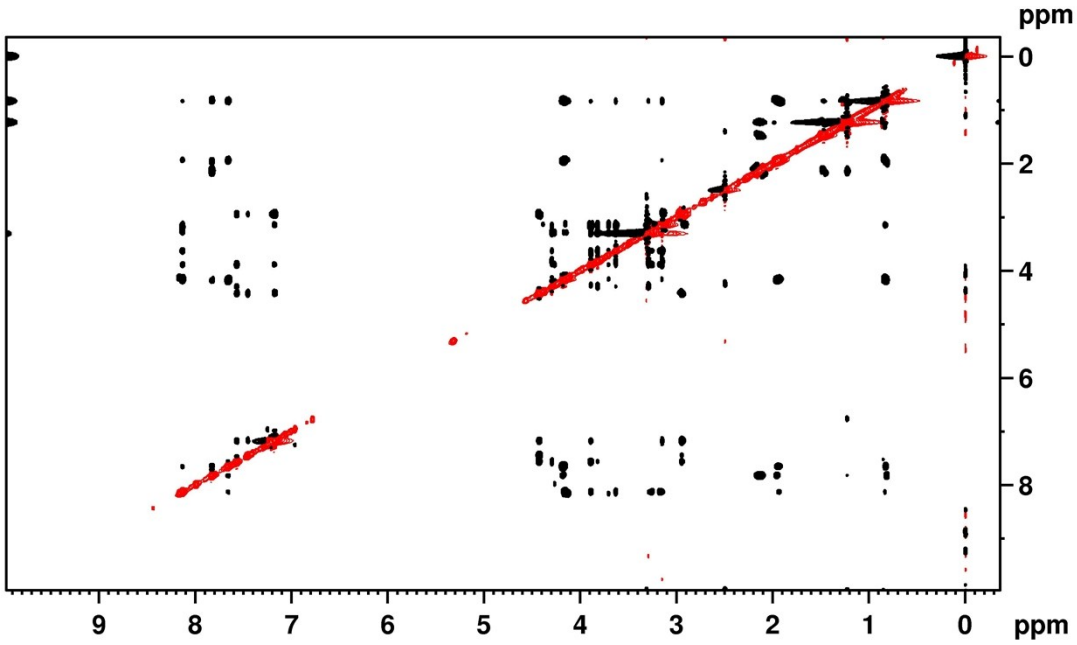


Figure S2: 2D-ROESY NMR spectrum (DMSO-d_6, 400 MHz) of compound 4P

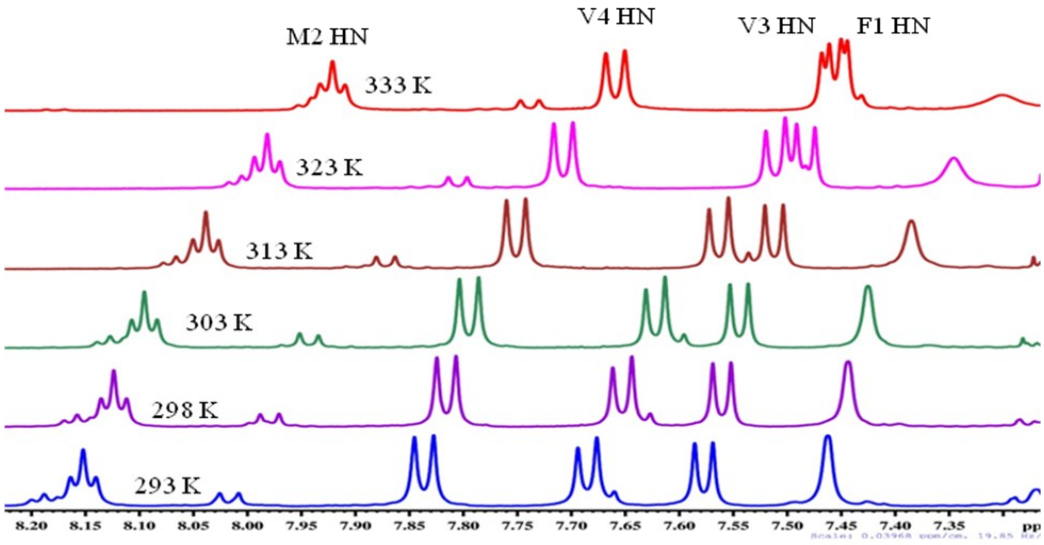


Figure S3: Stacked 1H-spectra of **4P** collected from 293 K-333 K

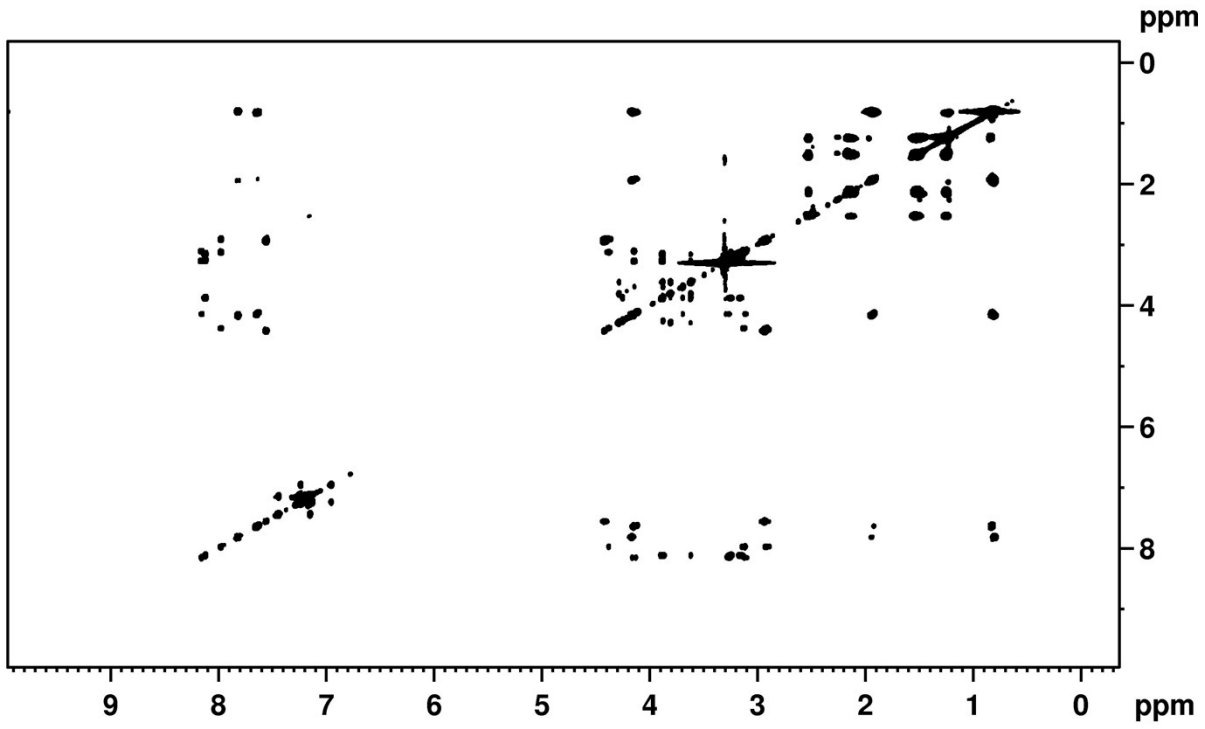


Figure S4: 2D-TOCSY NMR spectrum (DMSO-d_6, 400 MHz) of compound 4V

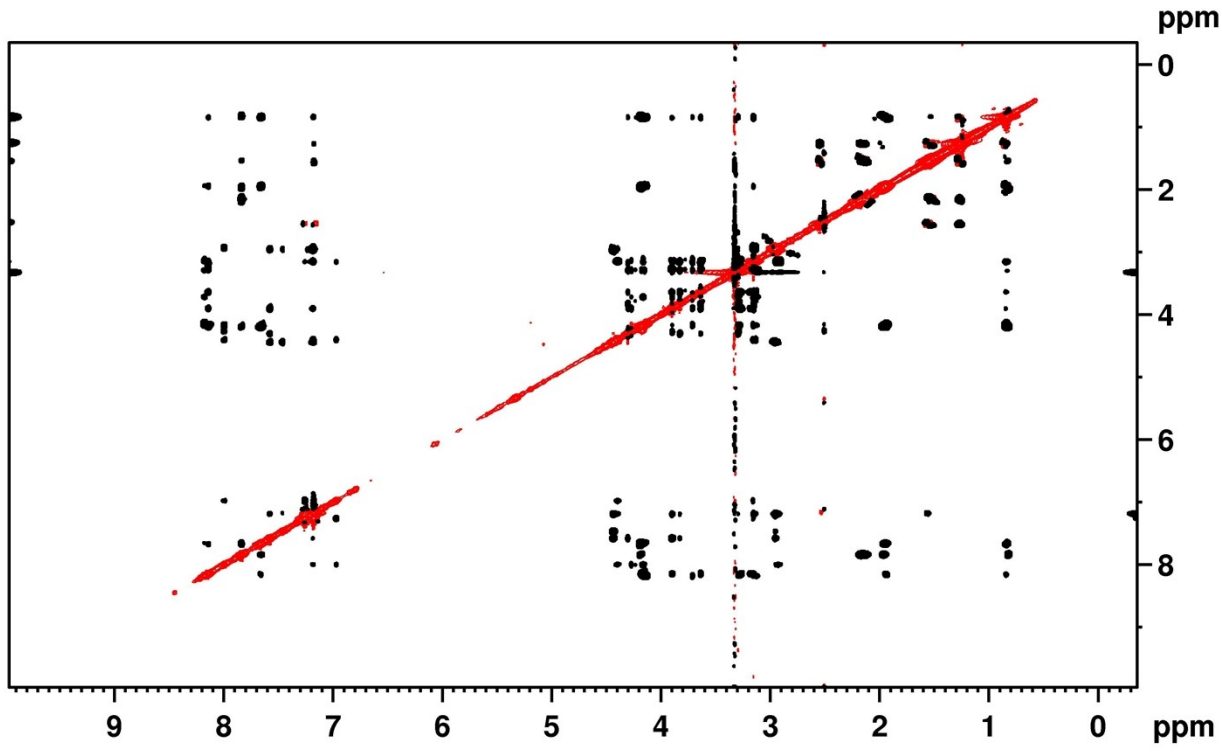


Figure S5: 2D-ROESY NMR spectrum (DMSO-d_6, 400 MHz) of compound 4V

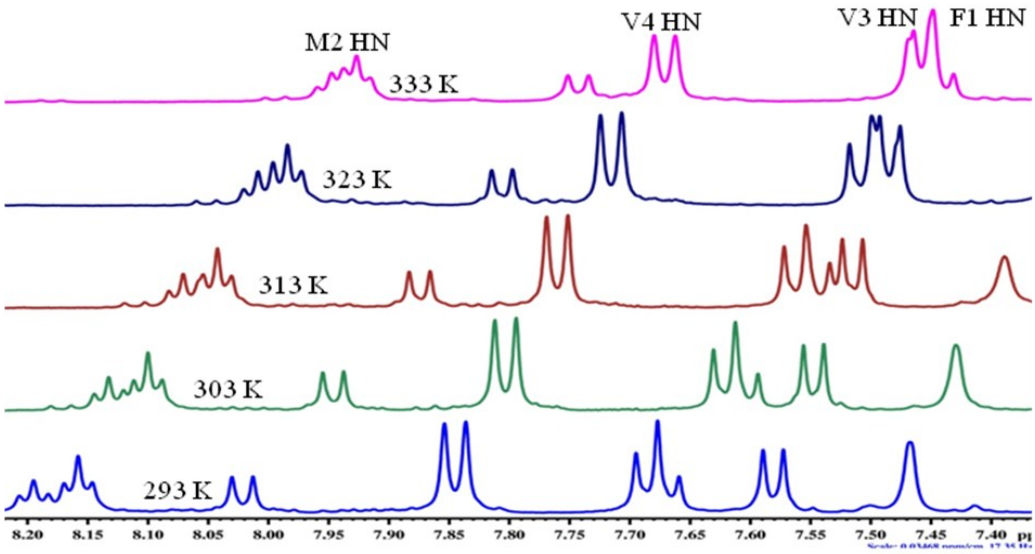


Figure S6: Stacked 1H-spectra of **4V** collected from 293 K-333 K

Table S3: Chemical shift (δ in ppm) and coupling constants (J in Hz) for **4V** in DMSO-d_6 (~8 mM, 500 MHz, 300K)

Residues	**NH**	**CαH**	**CβH**	**CγH**	**CδH**	**CεH**	**Δδ/ΔT**
[1]PHE	7.56 (*d,* $^3J_{NH\text{-}c\alpha H}$ = 8.4	4.41 (*ddd,* 1H, $^3J_{C\alpha H\text{-}c\beta H}$ = 5.4 Hz, $^3J_{C\alpha H\text{-}c\beta' H}$=7.8 Hz)	2.93 (m, 2H)	-----		----	3.6
[2]MAA	8.11 (*t,* $^3J_{NH\text{-}c\varepsilon H,\ C\varepsilon H'}$=5.7 Hz)	4.26 (d, $^3J_{C\alpha H\text{-}c\beta H}$ = 1.9 Hz)	3.81 (1H, $^3J_{c\beta H\text{-}C\gamma H}$ = 1.9Hz)	3.62 (dd, 1H, $^3J_{c\gamma H\text{-}C\delta H}$ = 2.7 Hz)	3.87 (dt, 1H, $^3J_{C\delta H\text{-}C\varepsilon H,\ H'}$ = 6.8 Hz)	3.14(m, 1H), 3.25 (m, 1H)	6.3
[3]VAL	7.62 (*d,* $^3J_{NH\text{-}c\alpha H}$ = 8.9	4.14 (*d,* $^3J_{C\alpha H\text{-}c\beta H}$ = 7.3	1.92 (*m, 1H)*	0.82 (d, 6H)			6.0
[4]VAL	7.81 (*d,* $^3J_{NH\text{-}c\alpha H}$ = 8.9 Hz)	4.16 (dd, $^3J_{C\alpha H\text{-}c\beta H}$=7.3 Hz)	1.94 (*m,* 1H)	0.80 (*d,* 6H)	___	___	4.8

Acetyl	----	2.134	1.462	1.212	__	__	4.5 for 7.44

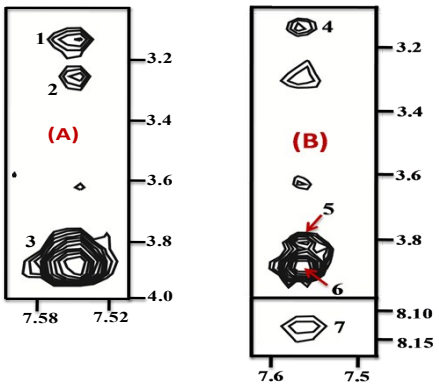


Figure S7: Expanded ROESY spectra of **4P** and **4V** in DMSO-d_6 (~8 mM, 300 K). The nOes MaaCεH(pro-S)↔PheNH, MaaCεH(pro-R)↔PheNH, MaaCδH↔PheNH, MaaCεH(pro-R)↔PheNH, MaaCβH↔PheNH, MaaCδH↔PheNH, MaaNH↔PheNH are marked as **1-7**.

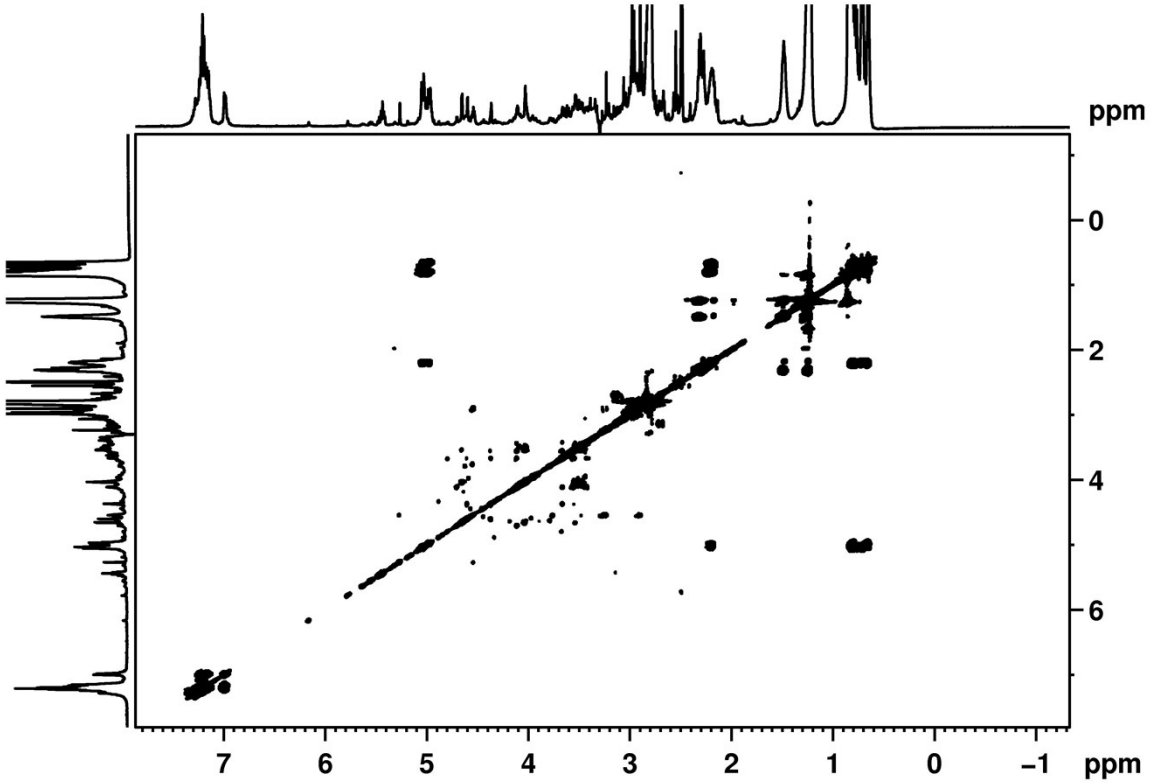


Figure S8: 2D-TOCSY NMR spectrum (DMSO-d_6, 400 MHz) of compound 4Q

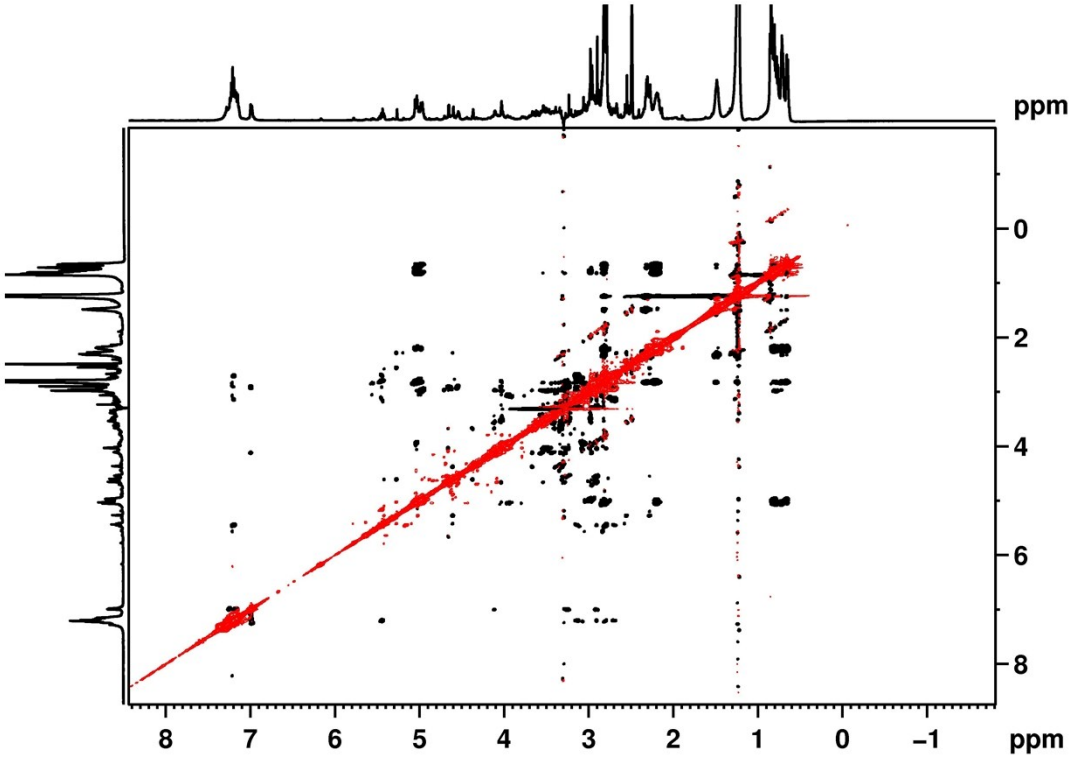


Figure S9: 2D-ROESY NMR spectrum (DMSO-d_6, 400 MHz) of compound 4Q

Table S4: Chemical shift (δ in ppm) and coupling constants (J in Hz) for **4Q** in DMSO-d_6 (~8 mM, 500 MHz, 300K)

AA	NH	CαH	CβH	CγH	CδH	CεH	Others	Δδ/ΔT
[1]PHE	-----	5.43	2.70, 3.13	-----	-----	-----	2.78	-----
[2]MAA	-----	4.65	-----	-----	4.02	-----	-----	-----
[3]VAL	-----	4.98	2.19	0.65, 0.81	-----	-----	2.97	-----
[4]VAL	-----	5.04	2.19	0.71, 0.77	-----	-----	2.81	-----
ACetyl	-----	2.134	1.462	1.212	-----	-----	-----	-----

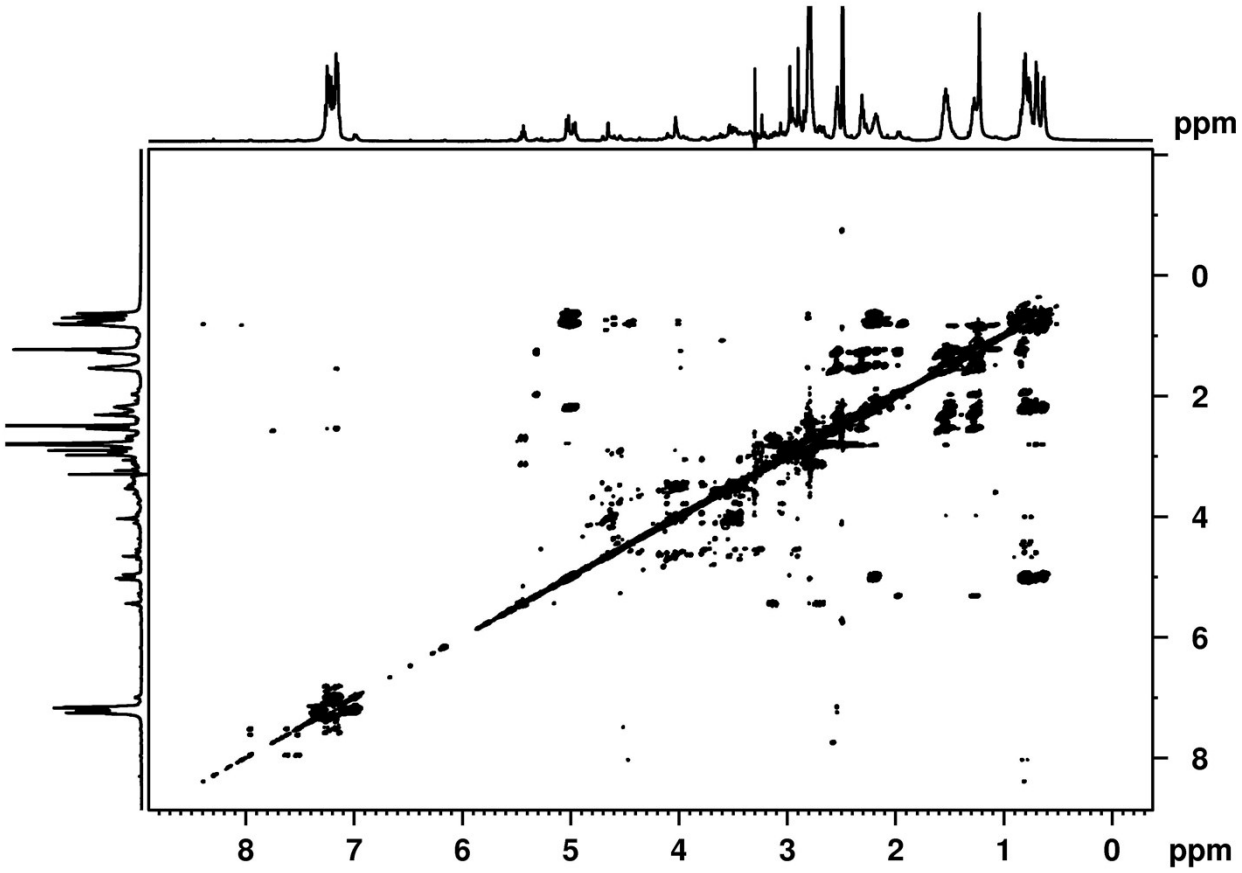


Figure S10: 2D-TOCSY NMR spectrum (DMSO-d_6, 400 MHz) of compound 4W

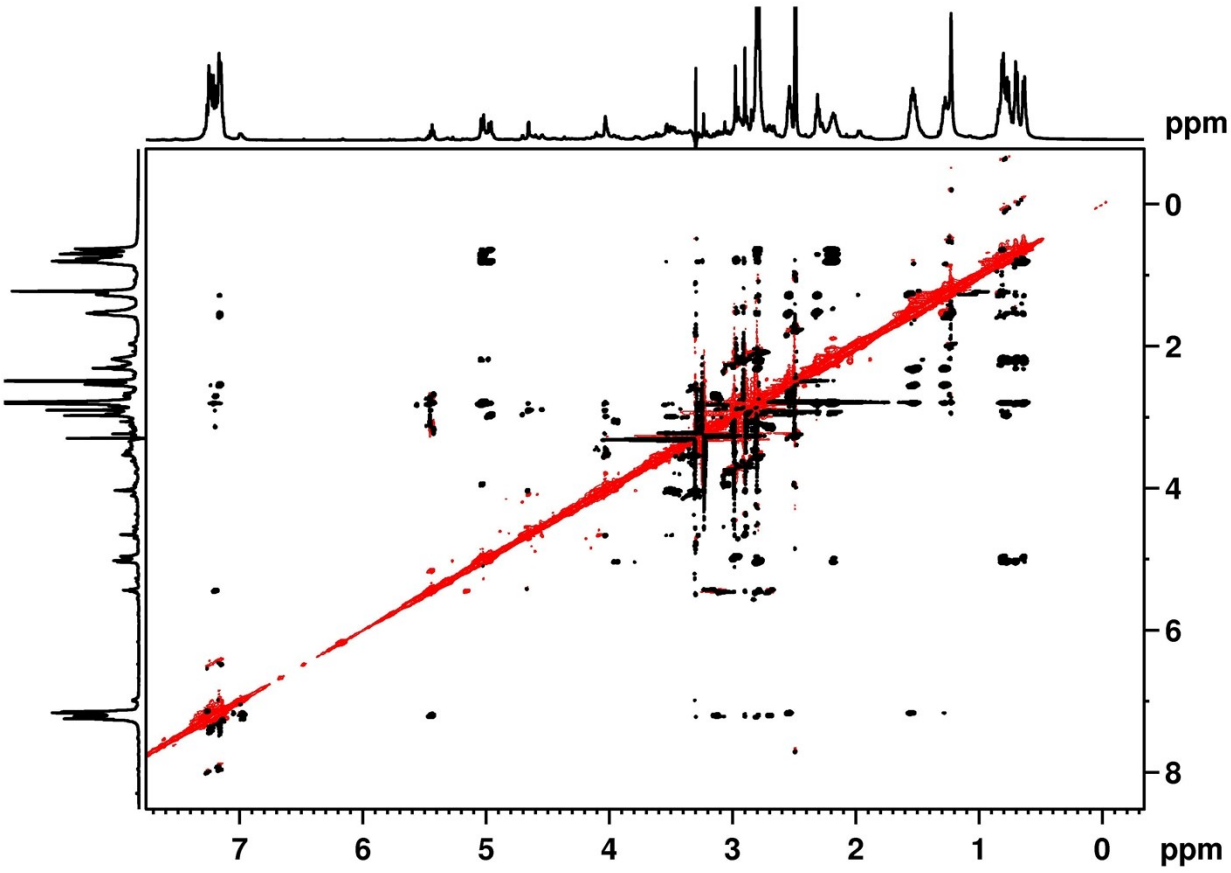


Figure S11: 2D-ROESY NMR spectrum (DMSO-d_6, 400 MHz) of compound 4W

Molecular dynamics: The Discovery studio 3.0 client Program was used for the restrained molecular dynamics and energy minimization calculation using CHARMm force field with default parameters throughout the simulation with the aid of distance dependent dielectric constant = 38. A force constant of 10 K cal/Å and 5 K cal/Å was used for distance and torsional restraints respectively. Minimizations were done initially with steepest descent algorithm followed by conjugate gradient methods for maximum 1000 iterations or RMS Deviation of 0.001 Kcal /mol, whichever was earlier. The molecules were initially equilibrated for 5ps and then after subjected to 1nS production run. Starting from 50 K, they were heated to 300 K in five steps increasing the temperature 50 K at each step. 20 structures were stored from the production run and are again energy minimized with the above mentioned protocol. Out of

these 20 structures 15 least energy structures were superimposed and are presented as Stereo view figures for each foldamer.

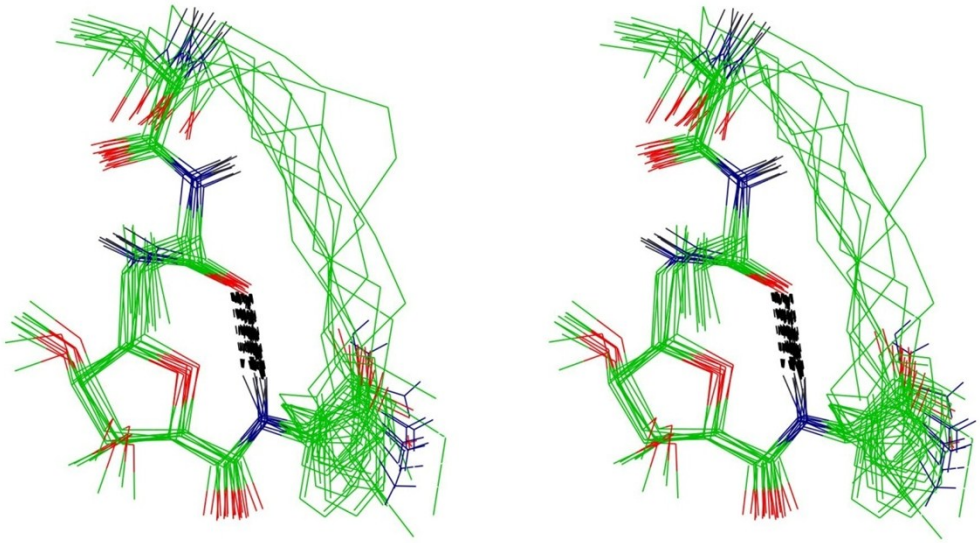


Figure S12. Stereo view of 15 minimum energy superimposed structures with H-bond for **4P.**

Table S5. Distance constraints used in MD calculation for **4P** derived from ROESY experiment in DMSO-d_6 (~8 mM, 500 MHz, 300 K).

Residue-Residue	Volume	Distance (Max.)	Distance (Min.)
^{1}PheCαH-HN	6.07E+06	4.5	3.5
^{1}PHECβH-^{3}ValHN	5.45E+06	4.5	3.5
^{2}MAACαH-^{1}PHEHN	3.40E+06	4.5	3.5
^{2}MAACαH-HN	4.42E+05	5.5	4.5
^{2}MAACδH-^{1}PHEHN	6.70E+06	4.5	3.5
^{2}MAA CδH-HN	3.87E+06	4.5	3.5
^{2}MAACεH(pro-R)-HN	5.82E+06	4.5	3.5
^{2}MAACεH(pro-S)-^{1}PHEHN	4.04E+05	5.5	4.5
^{2}MAAHE(pro-S)-HN	6.83E+06	4.5	3.5
^{2}MAAHG-HN	4.79E+06	4.5	3.5
^{3}VALCαH-^{2}MAAHN	2.39E+07	5.5	4.5
^{3}VALCβH-^{2}MAAHN	3.86E+06	4.5	3.5
^{3}VALHG-^{2}MAAHN	2.28E+06	4.5	5.5
^{4}VALHG-^{1}PHEHN	9.50E+05	5.5	4.5

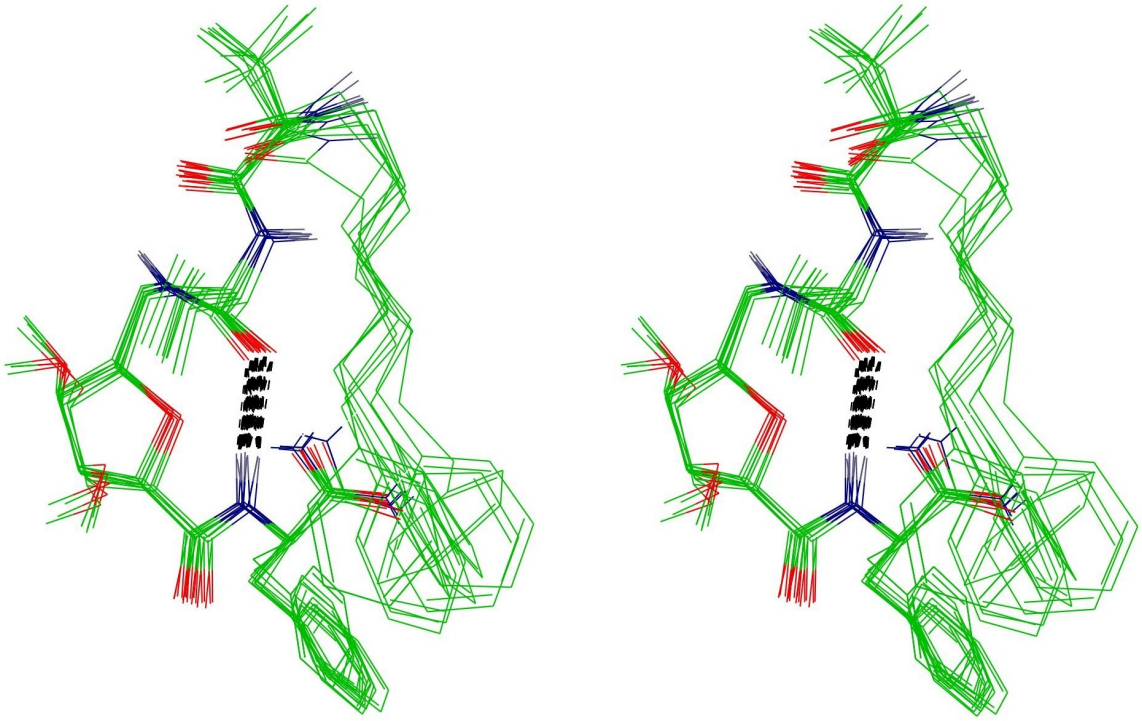


Figure S13. Stereo view of 15 minimum energy superimposed structures with H-bond for **4V.**

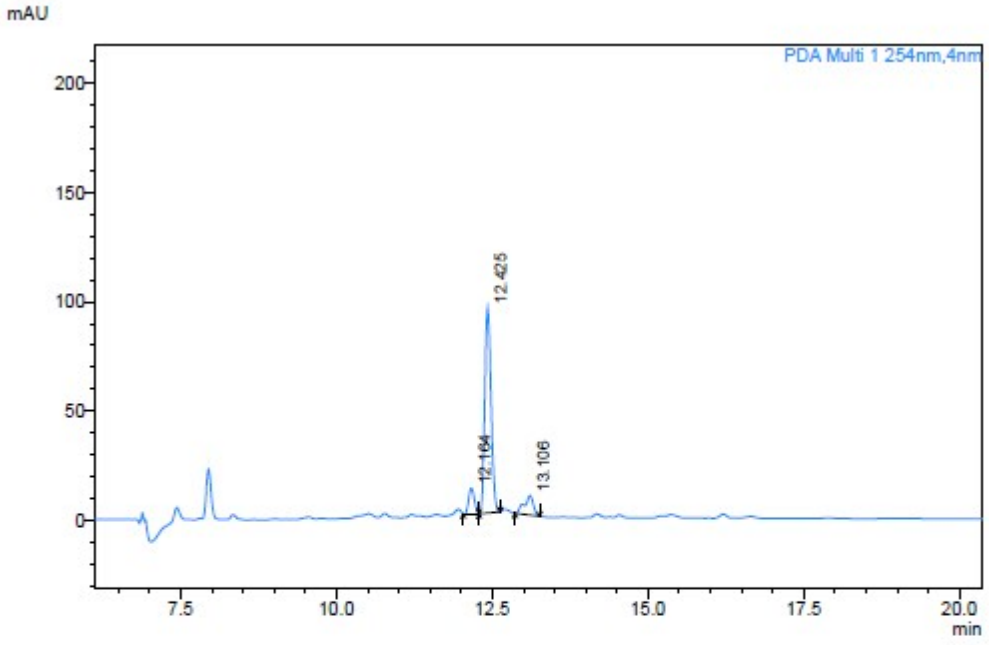
Table S6. Distance constraints used in MD calculation for **4V** derived from ROESY experiment in DMSO-d_6 (~8 mM, 500 MHz, 300 K).

Residue-Residue	Volume	Distance (Max)	Distance (Min)
^{2}CαH-TNH2-A	3.60E+05	5.5	4.5
^{1}PHE CβH-^{2}MAACαH	6.09E+05	5.5	4.5
^{3}VALCβH-^{2}MAACαH	6.42E+05	5.5	4.5
^{2}MAAHE(pro-R)-TNH2-A	6.71E+05	5.5	4.5
^{2}MAACαH-HN	8.27E+05	5.5	4.5
^{2}MAAHN-^{1}PHEHN	8.65E+05	5.5	4.5
^{2}MAACεH$_{(pro-R)}$-^{1}PHEHN	1.04E+06	4.5	3.5
^{1}PHEHN-TNH2-A	1.40E+06	4.5	3.5
^{3}VALCγ,γ'H-^{1}PHEHN	1.64E+06	4.5	3.5
Ace-CγH-^{4}VALHN	2.39E+06	4.5	3.5
^{2}MAACβH-^{1}PHEHN	2.44E+06	4.5	3.5
^{3}VALCγH,CγH'-2MAACαH	2.65E+06	4.5	3.5
^{2}MAAHG-CαH	3.35E+06	4.5	3.5
TNH2-CβH-^{1}PHEHN	3.60E+06	4.5	3.5
ACHE-ACFH-Ar	3.79E+06	4.5	3.5

^{3}VALCγH,Cγ'H-^{2}MAAHD	3.79E+06	4.5	3.5
^{1}PHECβ,β'H-TNH2-A	4.47E+06	4.5	3.5
^{2}MAACεH(*pro-R*)-CαH	4.73E+06	4.5	3.5
Ace-CβH-^{4}VALHN	5.72E+06	4.5	3.5
^{2}MAACαH-^{1}PHEHN	6.82E+06	4.5	3.5
2MAACδH-HN	7.26E+06	4.5	3.5
2MAACγH-HD	8.27E+06	4.5	3.5
2MAACγH-HN	9.87E+06	4.5	3.5
1PHECβ,β'H-HN	1.02E+07	3.5	2.5
3VALHN-4VALHN	1.13E+07	3.5	2.5
4VALHN-3VALHN	1.17E+07	3.5	2.5
3VALCβH-2MAAHN	1.18E+07	3.5	2.5
2MAACδH-1PHEHN	1.23E+07	3.5	2.5
3VALCγ.γ'H-^{2}MAAHN	1.24E+07	3.5	2.5
^{2}MAAHN-3VALHN	1.26E+07	3.5	2.5
1PHECαH-HN	1.28E+07	3.5	2.5
^{2}MAACγH-HD	1.32E+07	3.5	2.5
4VALCαH-HN	1.38E+07	3.5	2.5
1PHECαH-TNH2-A	1.39E+07	3.5	2.5
3VALCγH,Cγ'H-ACHE	1.44E+07	3.5	2.5
^{2}MAACεH(*pro-S*)- CαH	1.46E+07	3.5	2.5
^{2}MAACεH(*pro-R*)-CβH	1.58E+07	3.5	2.5
^{2}MAACβH-CαH	1.61E+07	3.5	2.5
4VALCβH-HN	1.62E+07	3.5	2.5
^{2}MAACεH(*pro-S*)-HN	2.08E+07	3.5	2.5
^{2}MAACγH-CβH	2.09E+07	3.5	2.5
4VALCγH,Cγ'H-HN	2.12E+07	3.5	2.5
3VALCβH-HN	2.18E+07	3.5	2.5
3VALCγH,Cγ'H-HN	2.27E+07	3.5	2.5
^{2}MAA CεH(*pro-S*)- CβH	2.27E+07	3.5	2.5
^{2}MAA CεH(*pro-R*)-CδH	2.70E+07	3.5	2.5
AceCδH -ACFH-Ar	4.21E+07	3.5	2.5
^{2}MAACεH(*pro-R*)-HN	4.67E+07	3.5	2.5
Ace-CαH-4VALHN	5.09E+07	3.5	2.5
^{3}VALHN-^{2}MAAHN	6.81E+07	3.5	2.5
^{4}VALCαH-^{3}VALHN	7.18E+07	3.5	2.5
^{3}VALCαH-^{2}MAAHN	7.49E+07	3.5	2.5
^{2}MAACδH -CαH	1.21E+08	3.5	2.5

RPHPLC Chromatograms:

- **HPLC chromatogram of compound 20.**

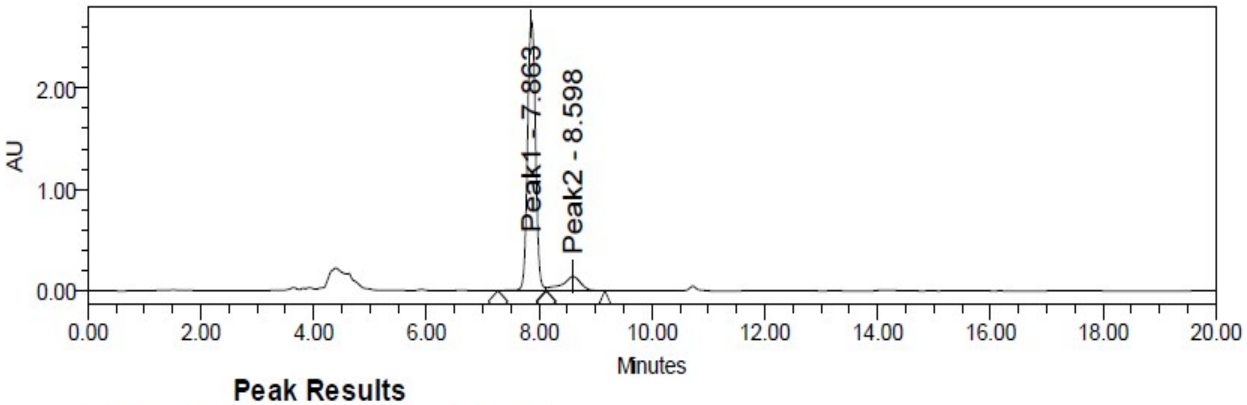


Summary
Injection Volume : 20

PDA Ch1 254nm

Ret. Time	Area	Area%
12.164	73218	8.899
12.425	660164	80.236
13.106	89400	10.866
	822782	100.000

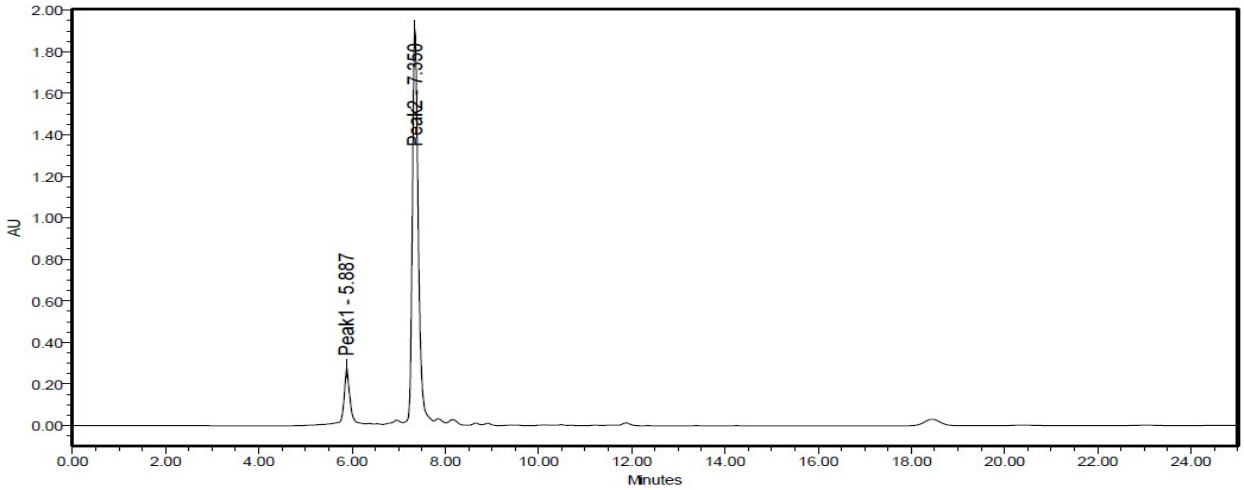
- **HPLC chromatogram of compound 4A.**



Peak Results

	Name	RT	Area	% Area	Height
1	Peak1	7.863	26356871	89.04	2661136
2	Peak2	8.598	3245626	10.96	141080

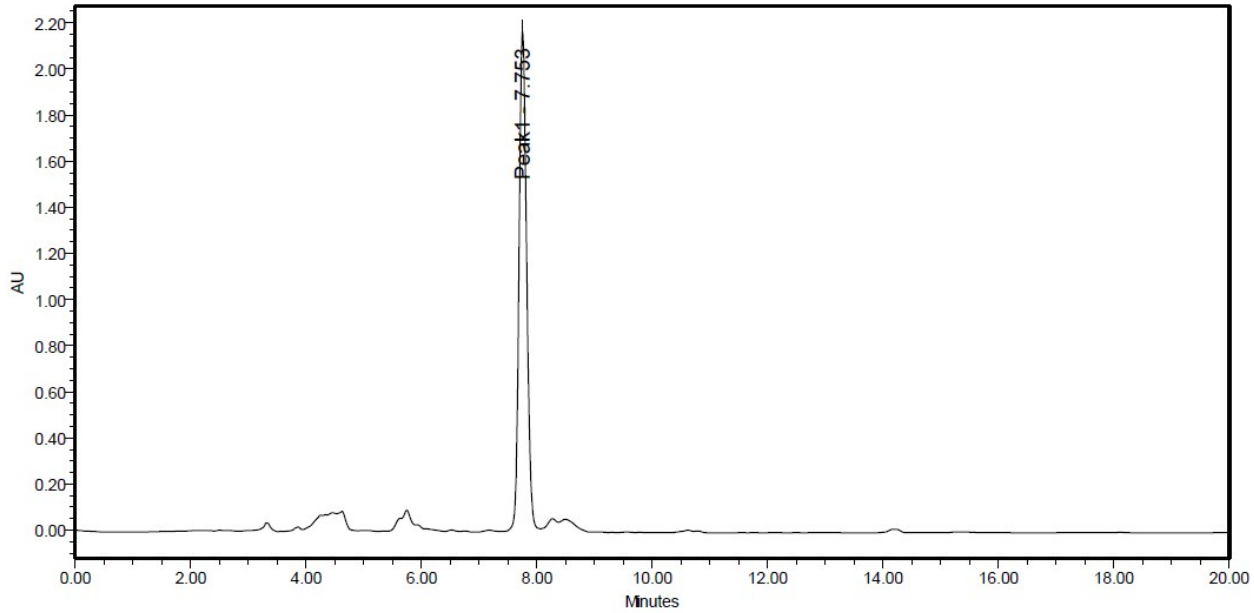
- **HPLC chromatogram of compound 4B.**



Peak Results

	Name	RT	Area	% Area	Height
1	Peak1	5.887	2693124	13.54	276755
2	Peak2	7.350	17201969	86.46	1908732

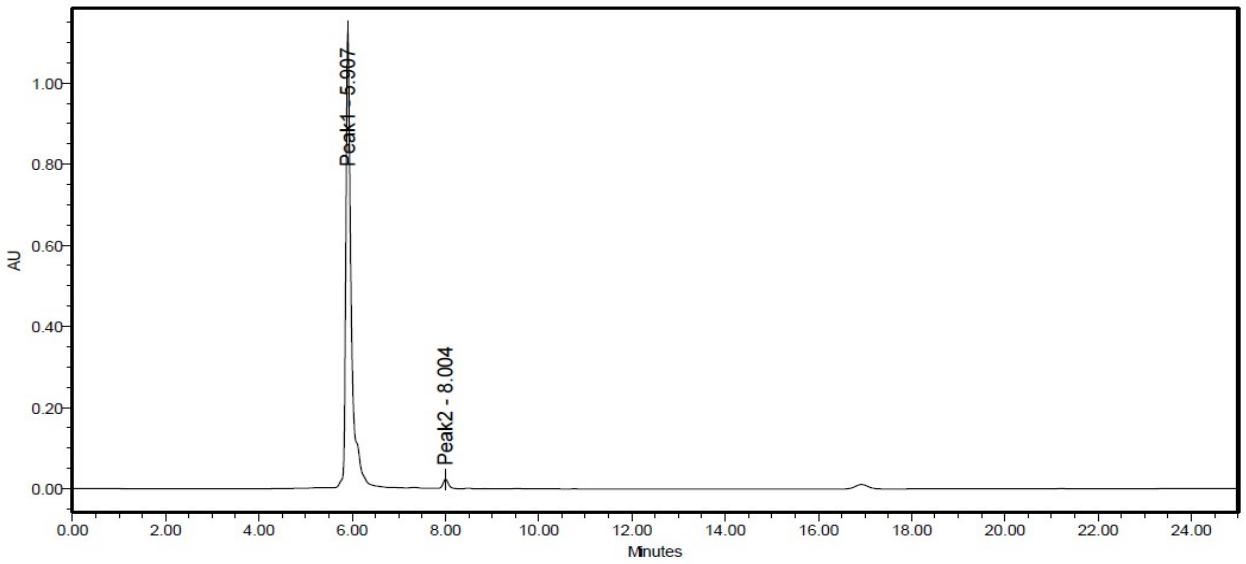
- **HPLC chromatogram of compound 4C.**



Peak Results

	Name	RT	Area	% Area	Height
1	Peak1	7.753	20073184	100.00	2171260

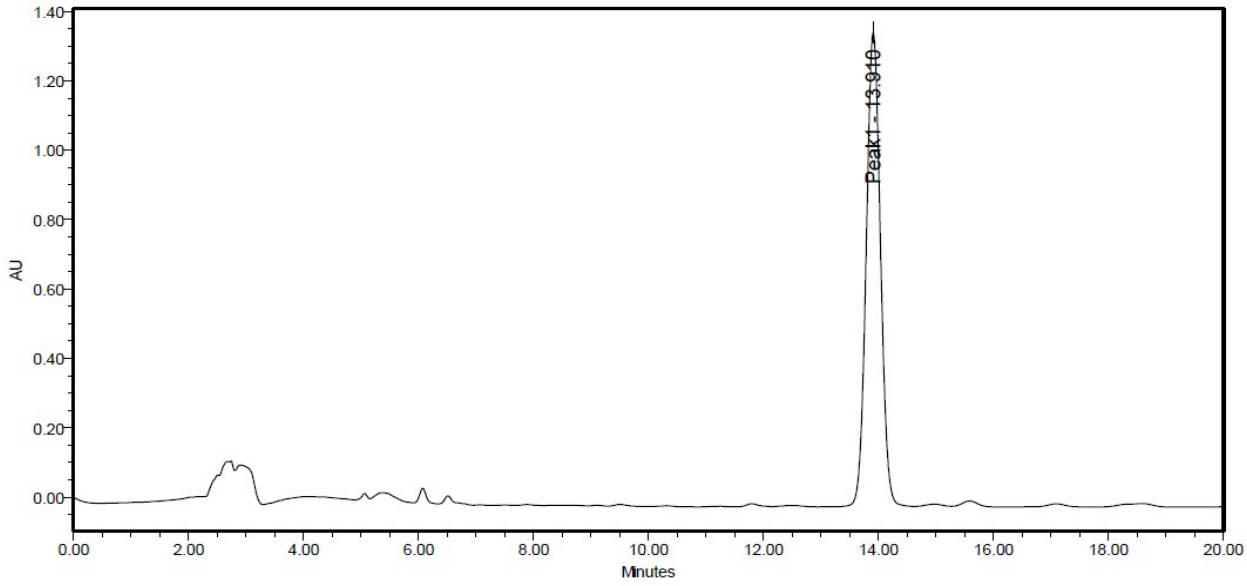
- **HPLC chromatogram of compound 4D.**



Peak Results

	Name	RT	Area	% Area	Height
1	Peak1	5.907	9047991	98.04	1125542
2	Peak2	8.004	180432	1.96	22606

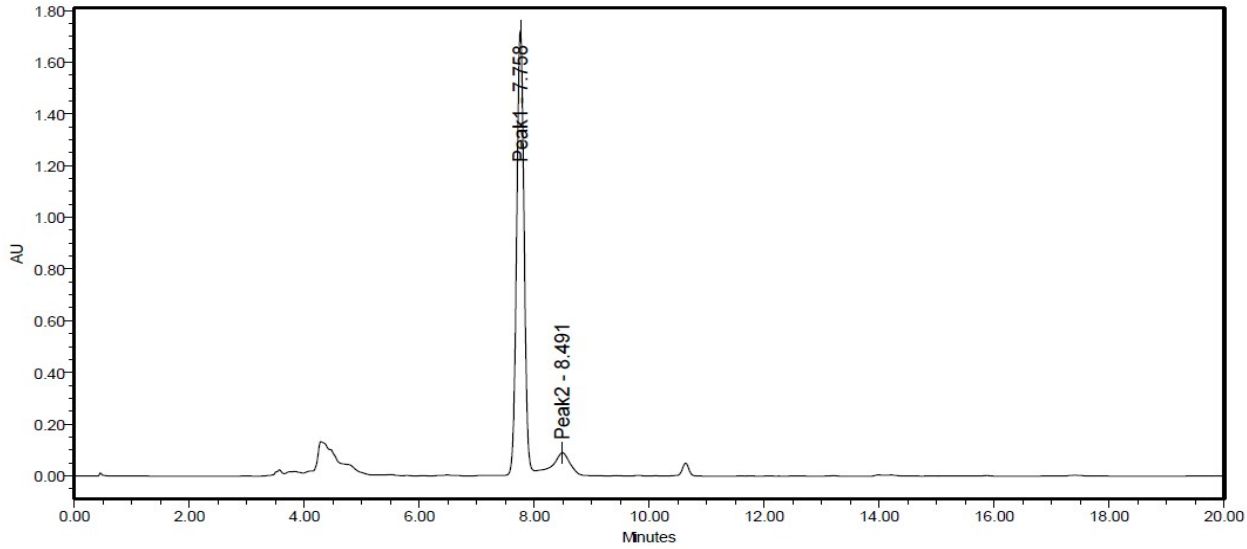
- **HPLC chromatogram of compound 4E.**



Peak Results

	Name	RT	Area	% Area	Height
1	Peak1	13.910	23516236	100.00	1367071

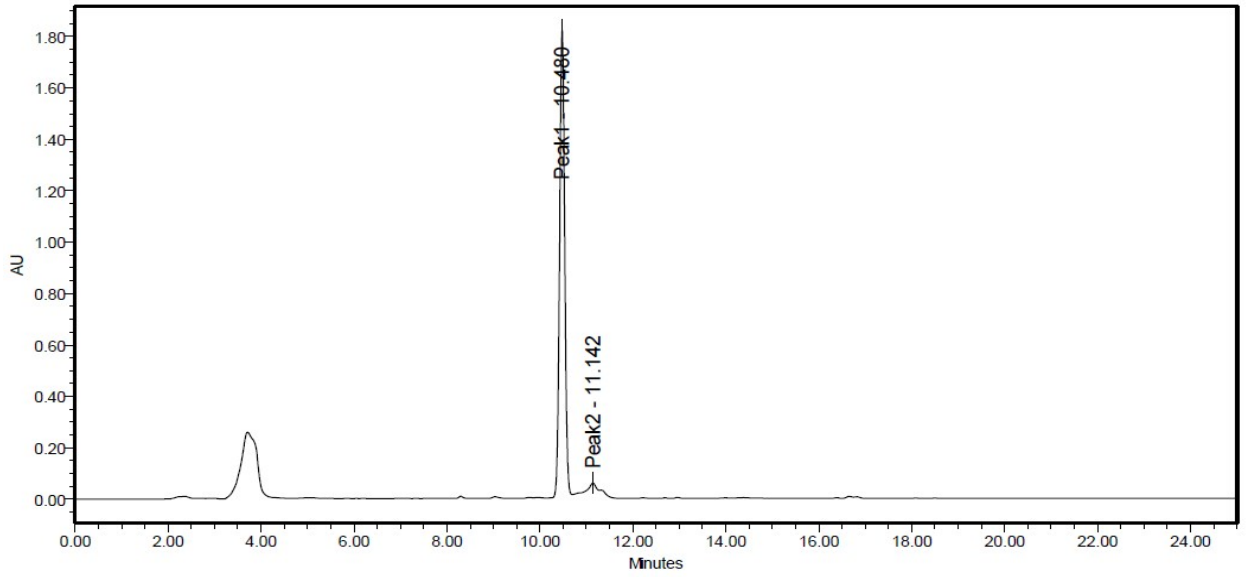
- **HPLC chromatogram of compound 4F.**



Peak Results

	Name	RT	Area	% Area	Height
1	Peak1	7.758	15537780	88.42	1722583
2	Peak2	8.491	2033933	11.58	89966

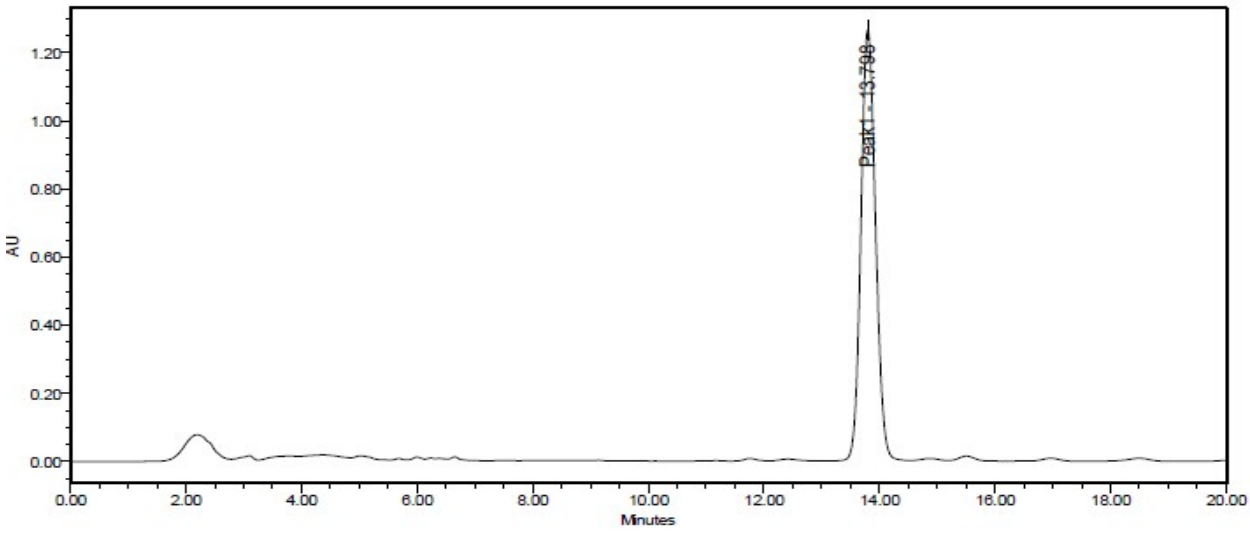
- **HPLC chromatogram of compound 4G.**



Peak Results

	Name	RT	Area	% Area	Height
1	Peak1	10.480	13921983	91.70	1820587
2	Peak2	11.142	1260056	8.30	59480

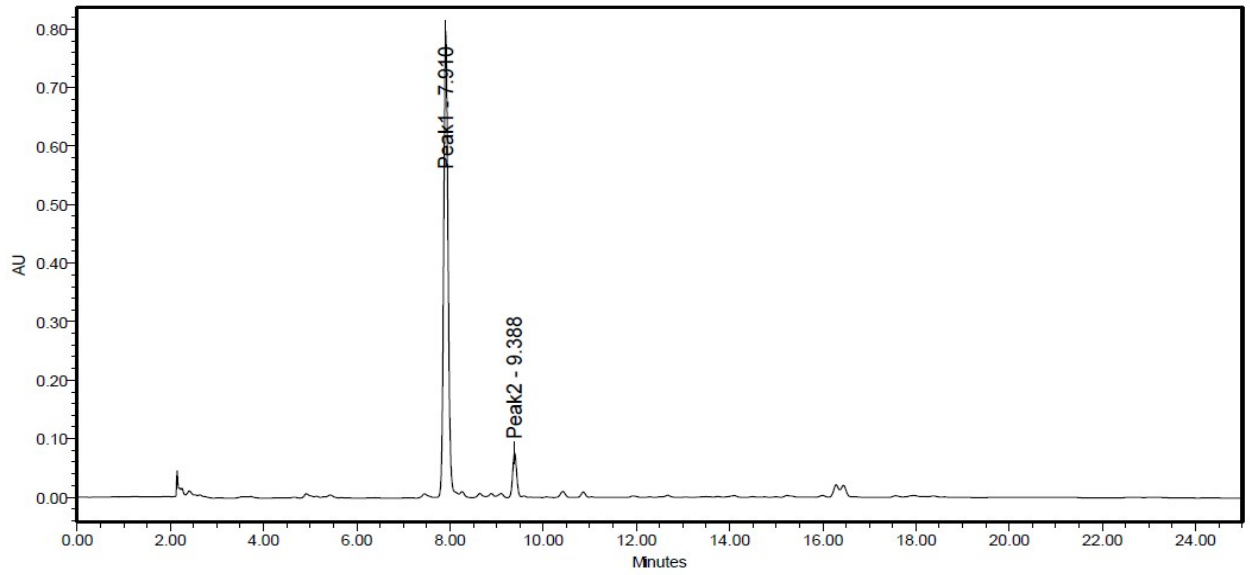
- **HPLC chromatogram of compound 4H.**



Peak Results

	Name	RT	Area	% Area	Height
1	Peak1	13.798	22222537	100.00	1265532

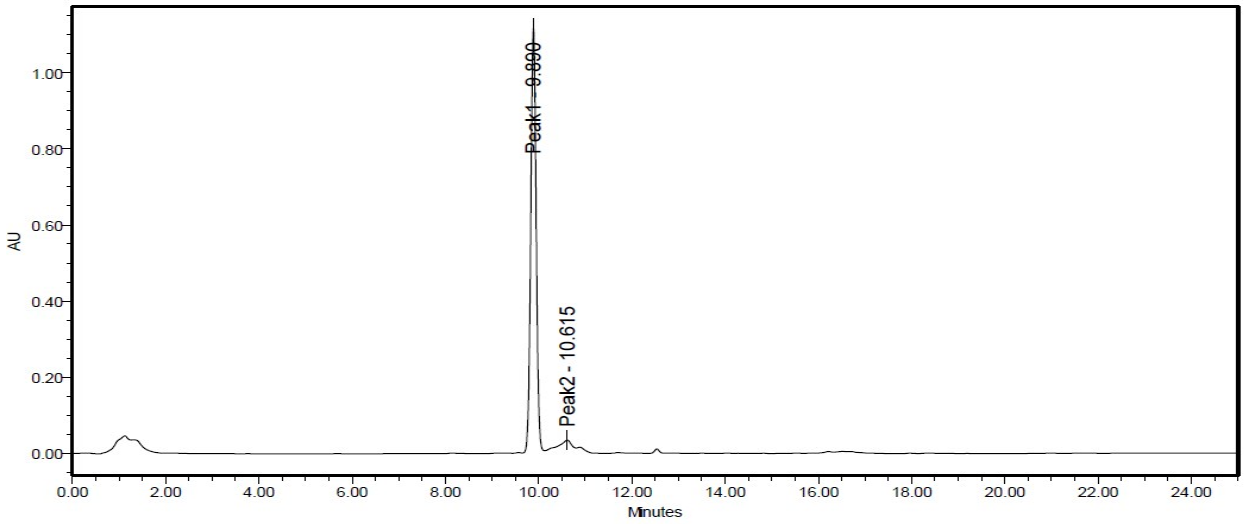
- **HPLC chromatogram of compound 4I.**



Peak Results

	Name	RT	Area	% Area	Height
1	Peak1	7.910	5232683	91.91	798043
2	Peak2	9.388	460532	8.09	76658

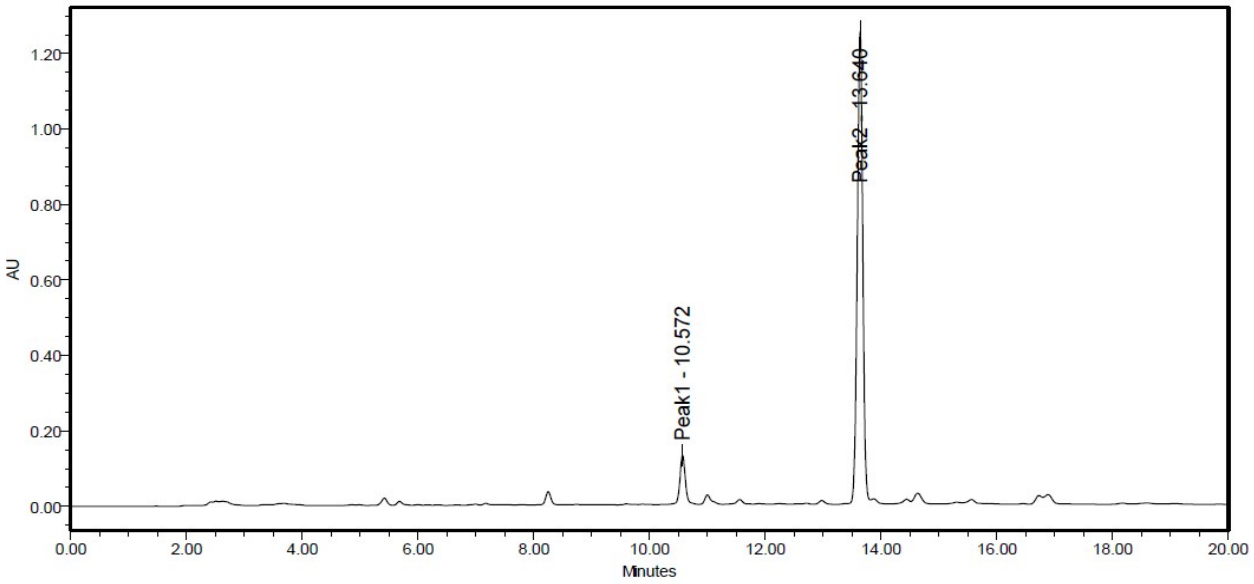
- **HPLC chromatogram of compound 4J.**



Peak Results

	Name	RT	Area	% Area	Height
1	Peak1	9.890	9061598	91.78	1117011
2	Peak2	10.615	811374	8.22	35026

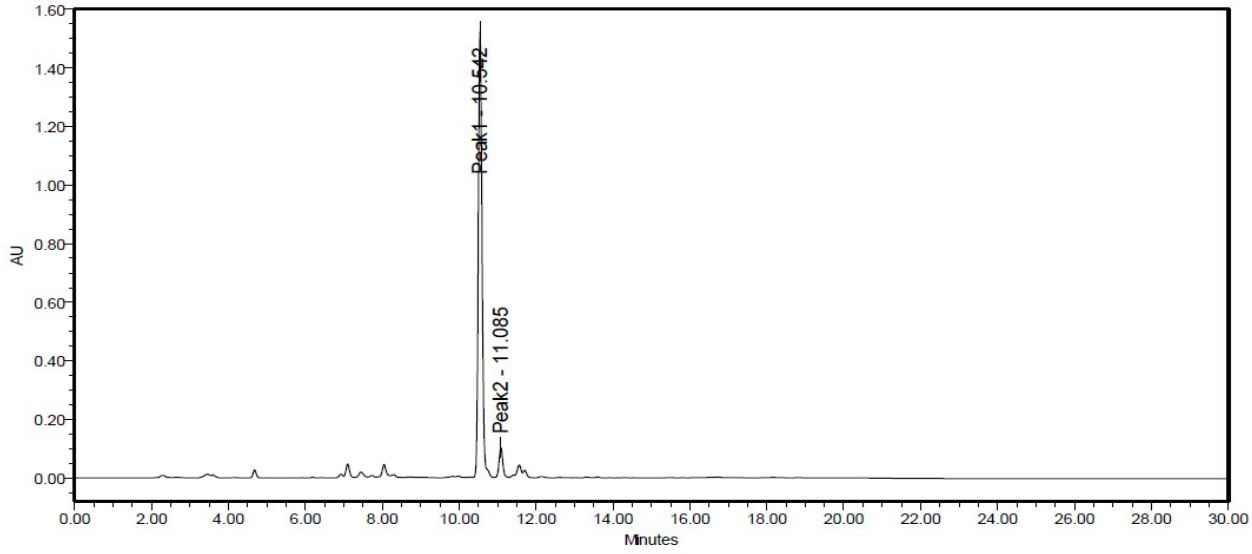
- **HPLC chromatogram of compound 4K.**



Peak Results

	Name	RT	Area	% Area	Height
1	Peak1	10.572	850881	9.26	130315
2	Peak2	13.640	8338843	90.74	1252836

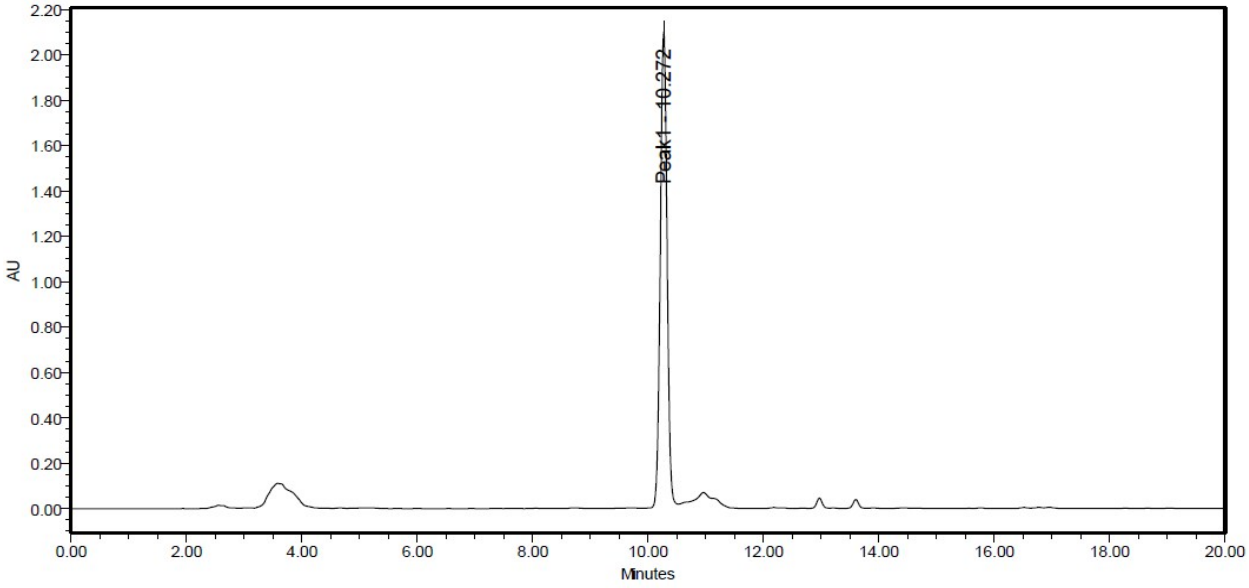
- **HPLC chromatogram of compound 4L.**



Peak Results

	Name	RT	Area	% Area	Height
1	Peak1	10.542	10232675	93.72	1522078
2	Peak2	11.085	686054	6.28	102474

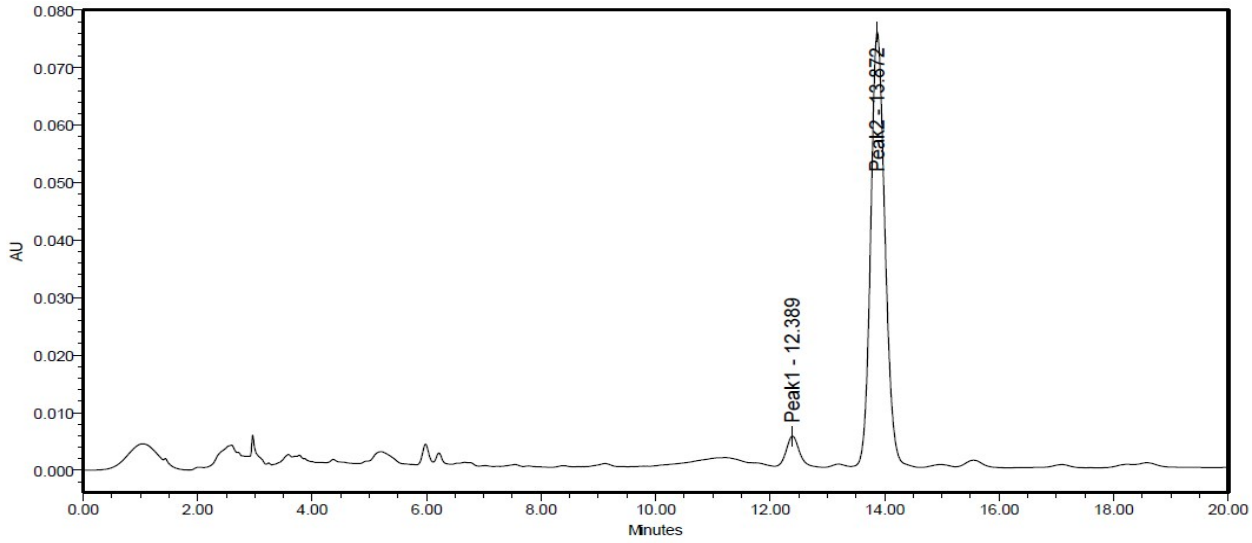
- **HPLC chromatogram of compound 4M.**



Peak Results

	Name	RT	Area	% Area	Height
1	Peak1	10.272	17280535	100.00	2099870

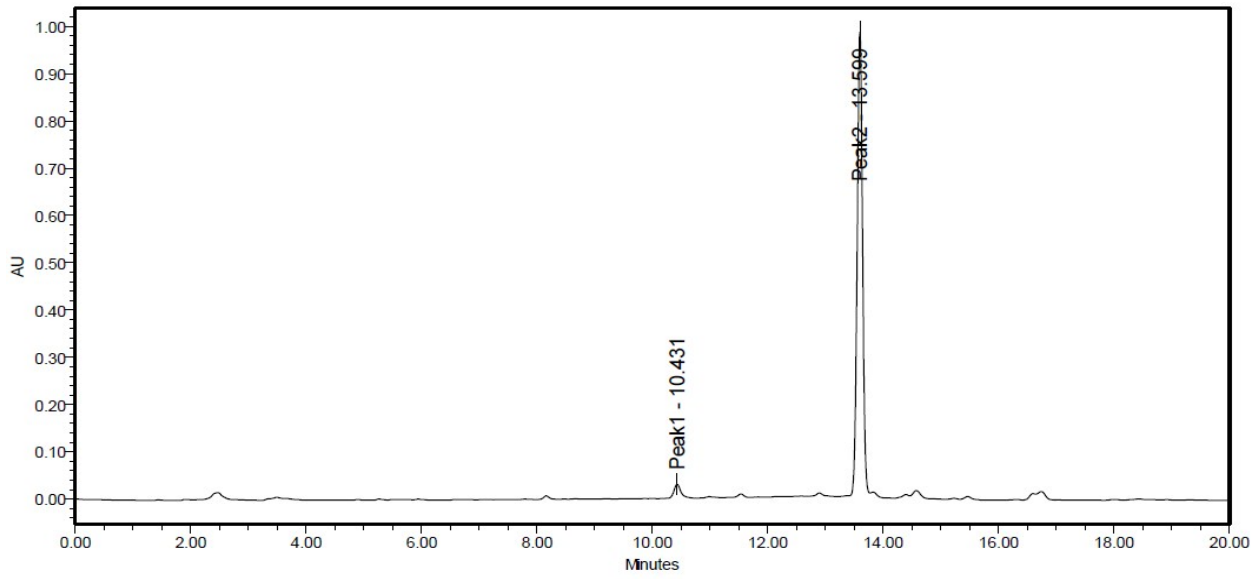
- **HPLC chromatogram of compound 4N.**



Peak Results

	Name	RT	Area	% Area	Height
1	Peak1	12.389	82519	5.93	5306
2	Peak2	13.872	1310125	94.07	75644

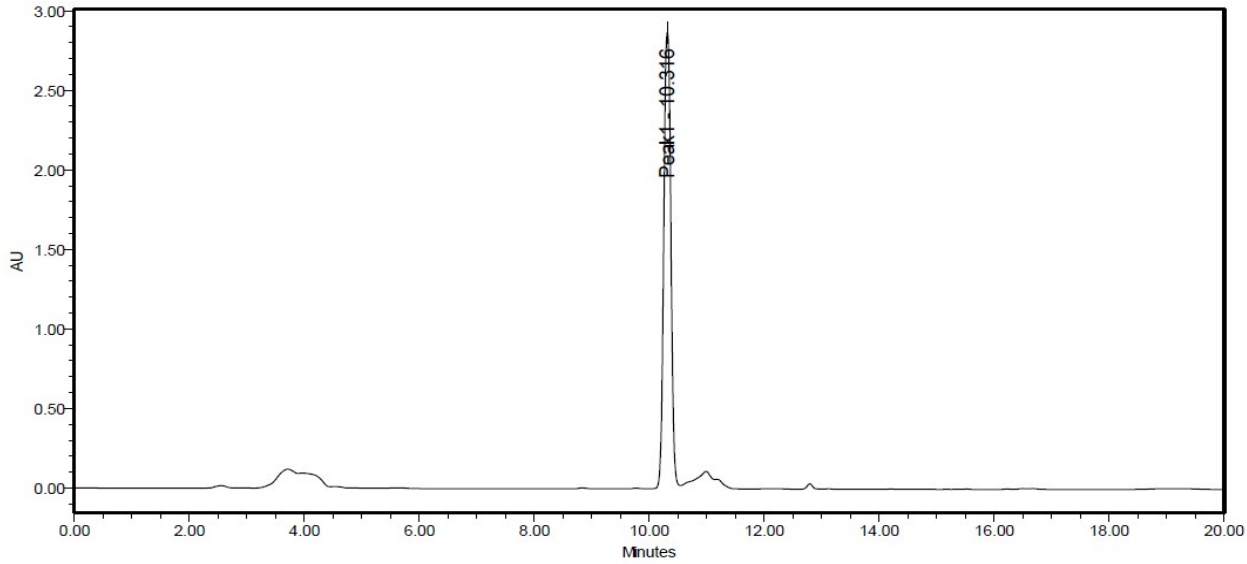
- **HPLC chromatogram of compound 4O.**



Peak Results

	Name	RT	Area	% Area	Height
1	Peak1	10.431	265735	3.89	30199
2	Peak2	13.599	6573111	96.11	986338

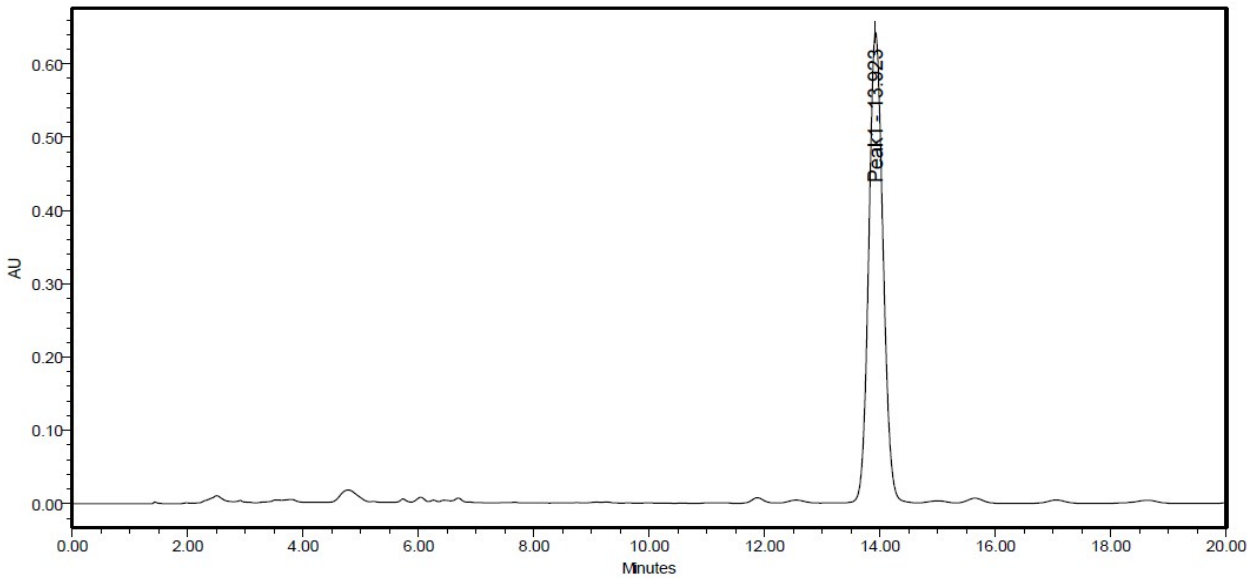
- **HPLC chromatogram of compound 4P.**



Peak Results

	Name	RT	Area	% Area	Height
1	Peak1	10.316	24654312	100.00	2868261

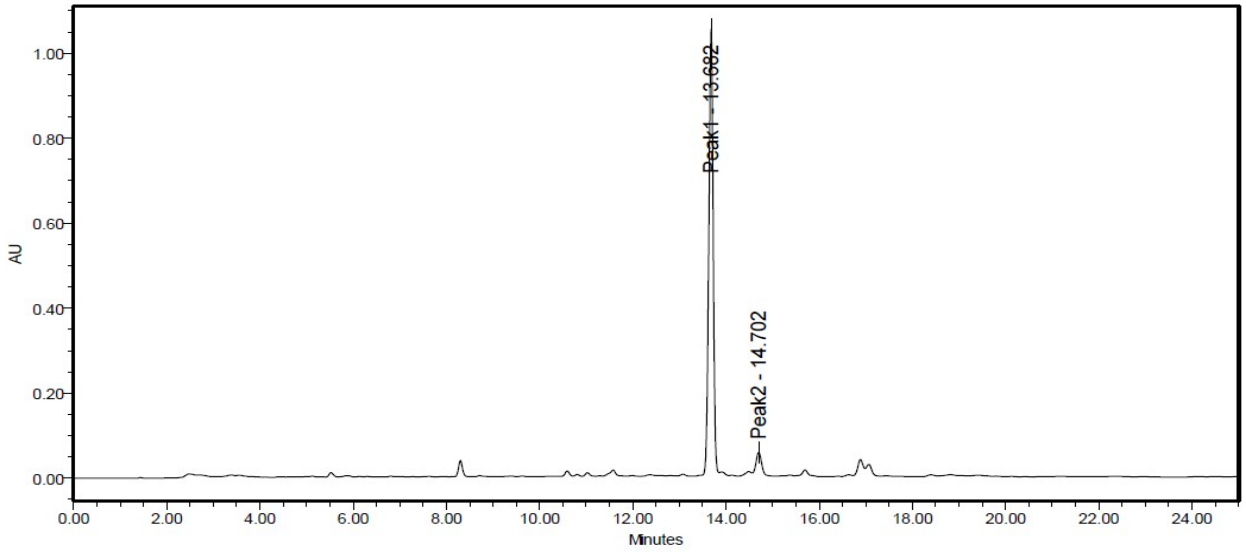
- **HPLC chromatogram of compound 4Q.**



Peak Results

	Name	RT	Area	% Area	Height
1	Peak1	13.923	11000711	100.00	642052

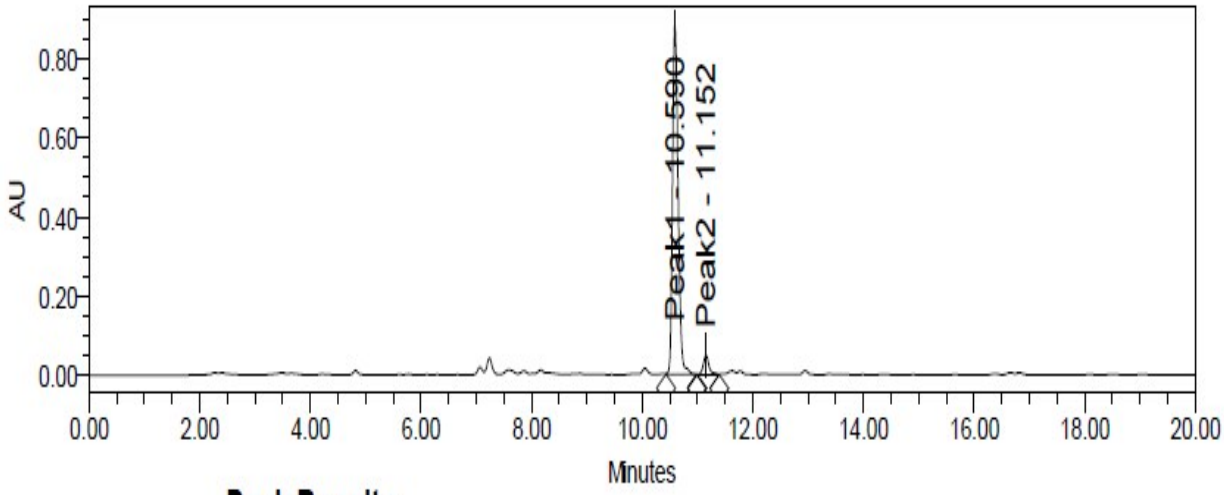
- **HPLC chromatogram of compound 4R.**



Peak Results

	Name	RT	Area	% Area	Height
1	Peak1	13.682	6906085	93.04	1053216
2	Peak2	14.702	516476	6.96	56945

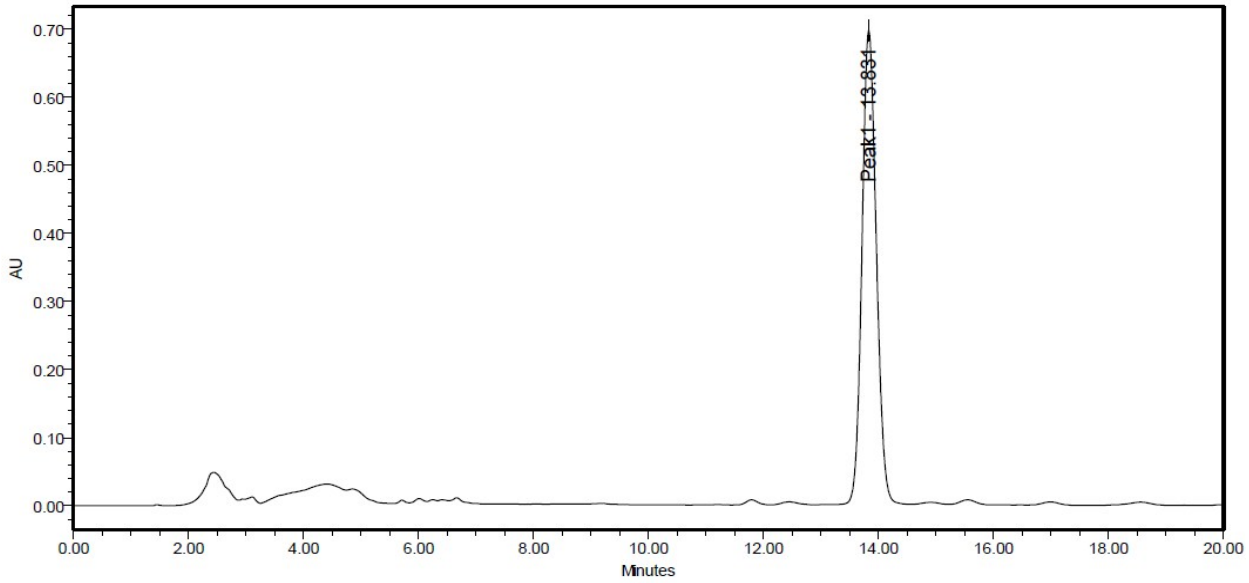
- **HPLC chromatogram of compound 4S.**



Peak Results

	Name	RT	Area	% Area	Height
1	Peak1	10.590	6220236	94.76	883480
2	Peak2	11.152	343730	5.24	48174

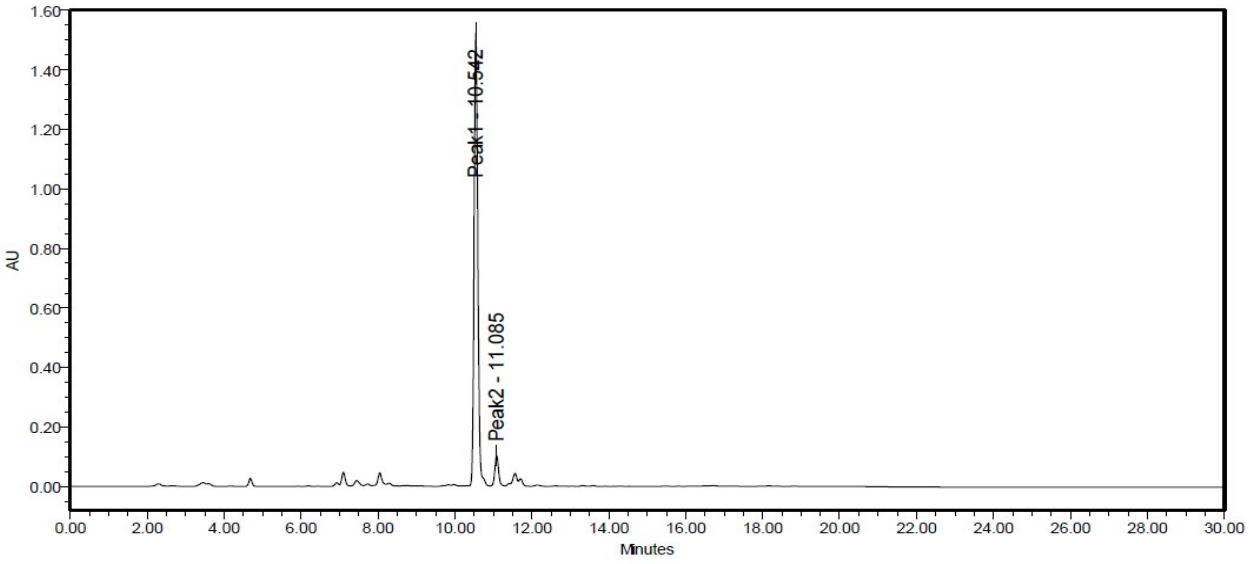
- **HPLC chromatogram of compound 4T.**



Peak Results

	Name	RT	Area	% Area	Height
1	Peak1	13.831	12043197	100.00	696290

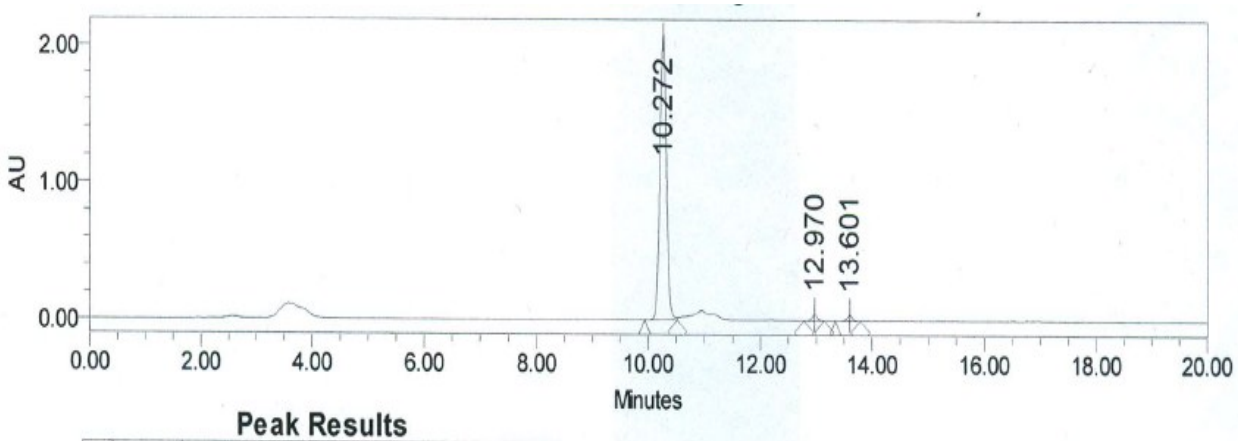
- **HPLC chromatogram of compound 4U.**



Peak Results

	Name	RT	Area	% Area	Height
1	Peak1	10.542	10232675	93.72	1522078
2	Peak2	11.085	686054	6.28	102474

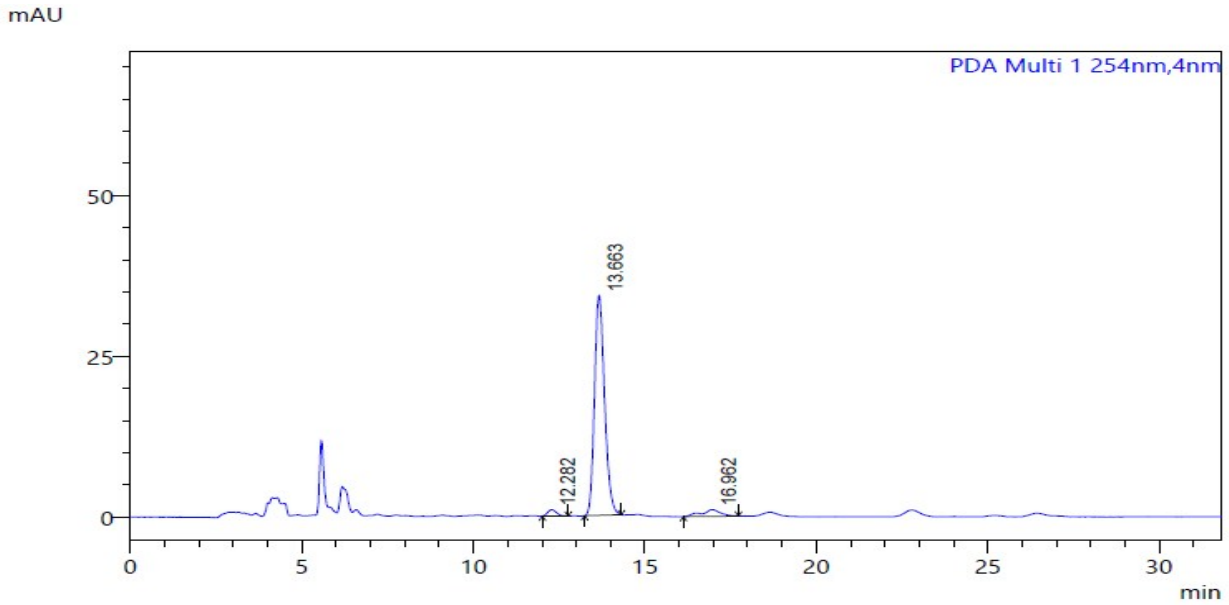
- **HPLC chromatogram of compound 4V.**



Peak Results

	Name	RT	Area	% Area	Height
1		10.272	17157580	96.87	2089490
2		12.970	299022	1.69	45422
3		13.601	255394	1.44	38710

- **HPLC chromatogram of compound 4W.**



Summary(Data)
PDA Ch1 254nm

Ret. Time	Area	Area%
12.282	18001	2.392
13.663	694831	92.341
16.962	39630	5.267
	752462	100.000