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

SUPPORTING INFORMATION

Table of Content:

Chemical reactivity parameters:

The global chemical reactivity parameters contain total energy, electrophilicity (ω), chemical hardness (η) and electronic chemical potential (μ). The stability and reactivity of the molecules are assessed by these parameters.[1] The HOMO-LUMO energy gap is responsible for the chemical hardness of the molecular structure and can be determined by equation (1) as follows:

$$\eta = (E_{HOMO} - E_{LUMO})/2 \qquad (1)$$

This HOMO-LUMO energy gap also used to determine the molecular stability. It is known that higher the HOMO-LUMO energy gap more stable and chemically harder the molecules as compare to the softer and less stable molecules. Another parameter electrophilicity index (ω) is defined as lowering in energy of molecules due to the flow of electrons from HOMO to LUMO. Hence, it measures the energy changes that take place when a molecule is saturated by the addition of electrons and governs chemical reactivity behaviour of molecules. The equation (2) represents the electrophilicity index (ω) of molecules.[2]

$$\omega = \mu^2/2\eta \qquad (2)$$

Where, η represents chemical hardness and μ represents the electronic chemical potential. Electronic chemical potential (μ) is described as the negative of electronegetivity[3] and given by the equation (3):

$$\mu = (E_{HOMO} + E_{LUMO})/2 \qquad (3)$$

It depicts the transfer of charge that takes place within the molecule in ground state which describes the tendency of electrons to escape from the equilibrium state. Hence, chemically reactive molecules show greater chemical potential. **Table SI-3** lists and described chemical reactivity parameter of synthesized triazole **5a-f** and **9a-f**. On comparing the reactivity parameters of compound **3** and **8** with these synthesized triazoles, we conclude that introduction of 1,2,3-triazole moiety in the structure lowers the HOMO-LUMO energy gap along with lowering the chemical hardness and increasing chemical potential of a molecule except for **5b**, **5f**, **9b** and **9f** as shown in table by red background highlighter. However, this effect was more pronounced observed with **5e** and **9e** as shown in table by green background highlighter. Hence, ultimately this results into increasing the chemical reactivity and bioactivity of molecules by 1,2,3-triazole moiety.

Table SI-1 Molinspiration Property Engine

Compound	%ABS	MiLogP	TPSA	natoms	MW	nON	nOHNH	nviolations	Nrotb	volume
3	82.53	1.51	76.72	16	217.23	5	3	0	4	198.02
5a	71.93	2.37	107.44	25	336.36	8	3	0	6	295.64
5b	71.93	2.54	107.44	26	354.35	8	3	0	6	300.57
5c	71.93	3.05	107.44	26	370.80	8	3	0	6	309.17
5d	71.93	3.18	107.44	26	415.25	8	3	0	6	313.52
5e	56.13	2.33	153.26	28	381.35	11	3	1	7	318.97
5f	68.75	2.43	116.67	27	366.38	9	3	0	7	321.18
8	82.53	1.56	76.72	16	217.23	5	3	0	4	198.02
9a	71.93	2.42	107.44	25	336.36	8	3	0	6	295.64
9b	71.93	2.59	107.44	26	354.35	8	3	0	6	300.57
9c	71.93	3.10	107.44	26	370.80	8	3	0	6	309.17
9d	71.93	3.23	107.44	26	415.25	8	3	0	6	313.52
9e	56.13	2.38	153.26	28	381.35	11	3	1	7	318.97
9f	68.75	2.48	116.67	27	366.38	9	3	0	7	321.18

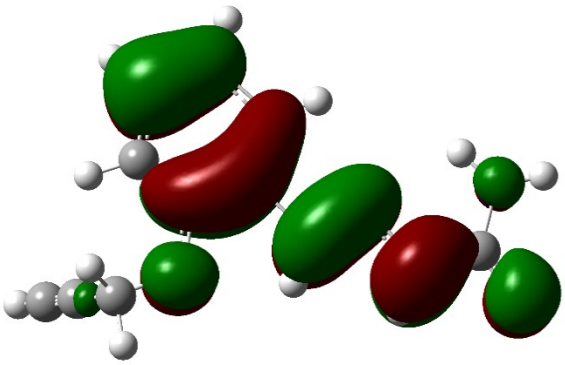
Table SI-2 Molinspiration Bioactivity Score

Compound	GPCR ligand	Ion Channel modulator	Kinnase Inhibitor	Nuclear receptor ligand	Protease Inhibitor	Enzyme Inhibitor
3	-0.65	-0.95	-0.88	-1.07	-0.79	-0.38
5a	-0.11	-0.41	-0.27	-0.65	-0.30	-0.06
5b	-0.10	-0.41	-0.23	-0.60	-0.31	-0.07
5c	-0.11	-0.40	-0.28	-0.65	-0.33	-0.09
5d	-0.20	-0.46	-0.30	-0.73	-0.40	-0.13
5e	-0.24	-0.42	-0.37	-0.67	-0.41	-0.16
5f	-0.14	-0.43	-0.28	-0.63	-0.31	-0.09
8	-0.68	-0.84	-0.86	-1.06	-0.84	-0.35
9a	-0.13	-0.34	-0.26	-0.64	-0.32	-0.04
9b	-0.12	-0.34	-0.22	-0.59	-0.34	-0.06
9c	-0.13	-0.33	-0.27	-0.64	-0.36	-0.07
9d	-0.22	-0.40	-0.29	-0.72	-0.43	-0.11
9e	-0.26	-0.35	-0.36	-0.67	-0.43	-0.14
9f	-0.68	-0.84	-0.86	-1.06	-0.84	-0.35

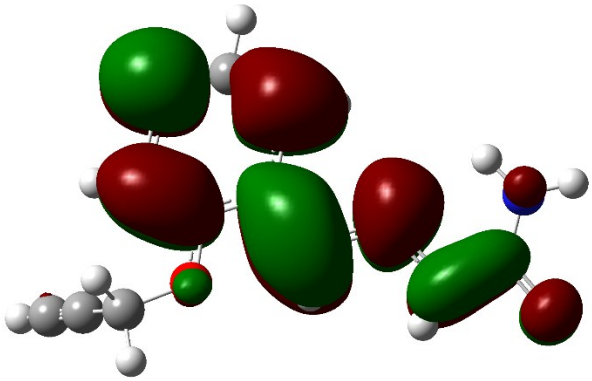
Table SI-3 Reactivity indices of semicarbazone-triazole hybrid molecules (**3**, **5a-f**, **8** & **9a-f**)

Compd.	E_{HOMO} (eV)	E_{LUMO} (eV)	$E_{LUMO-HOMO}$ (eV)	μ (eV)	η (eV)	ω (eV)
3	-5.91	-1.54	4.37	-3.73	2.19	3.18
5a	-5.82	-1.56	4.26	-3.69	2.13	3.20
5b	-6.13	-1.66	4.47	-3.90	2.24	3.39
5c	-5.99	-1.69	4.3	-3.84	2.15	3.43
5d	-5.99	-1.68	4.31	-3.84	2.16	3.41
5e	-6.53	-2.71	3.82	-4.62	1.91	5.59
5f	-5.78	-1.31	4.47	-3.55	2.24	2.81
8	-5.69	-1.06	4.63	-3.38	2.32	2.46
9a	-5.82	-1.31	4.51	-3.57	2.26	2.82
9b	-6.2	-1.48	4.72	-3.84	2.36	3.12
9c	-6.22	-1.7	4.52	-3.96	2.26	3.47
9d	-5.87	-1.57	4.3	-3.72	2.15	3.22
9e	-6.31	-3.04	3.27	-4.68	1.64	6.68
9f	-6.13	-1.25	4.88	-3.69	2.44	2.79

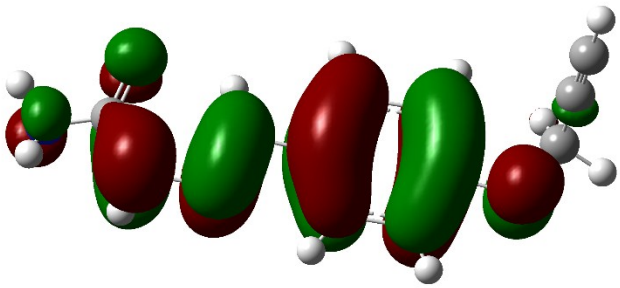
Table SI-4 FMOs distribution pattern figures of **3** & **8.**



HOMO (**3**)



LUMO (**3**)



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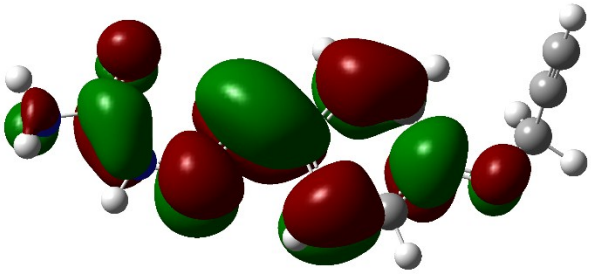
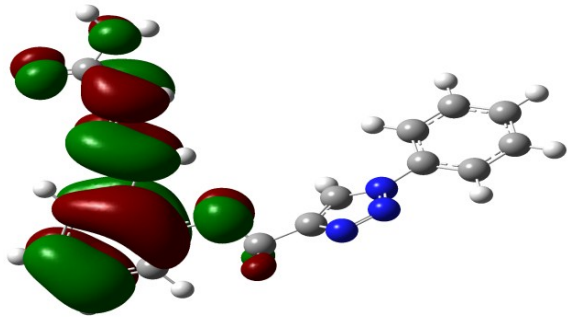
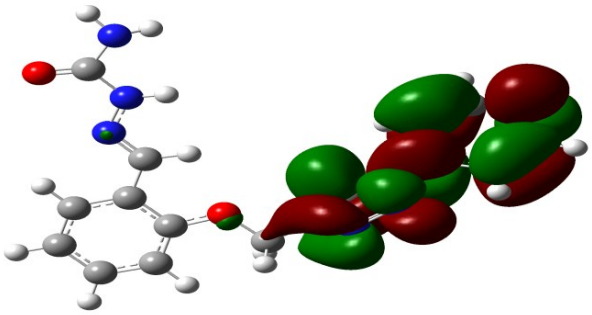


LUMO (**8**)

Table SI-5 FMOs distribution pattern figures of **5a-f** & **9a-f.**



HOMO (**5a**)



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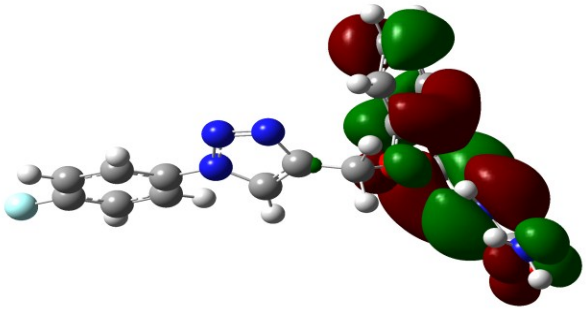

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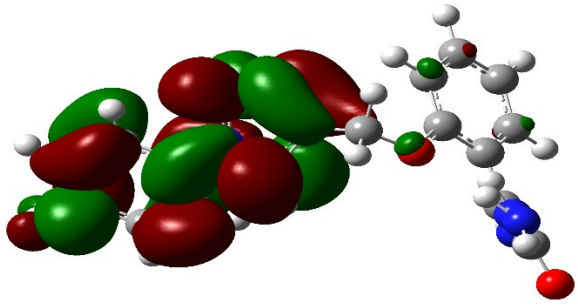
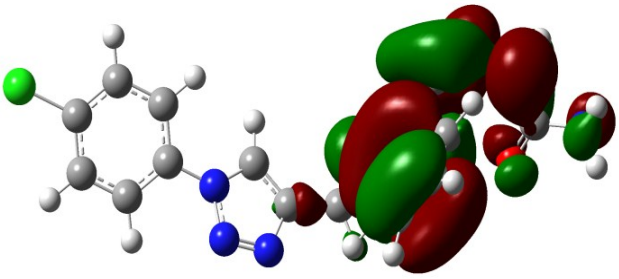


LUMO (**5b**)



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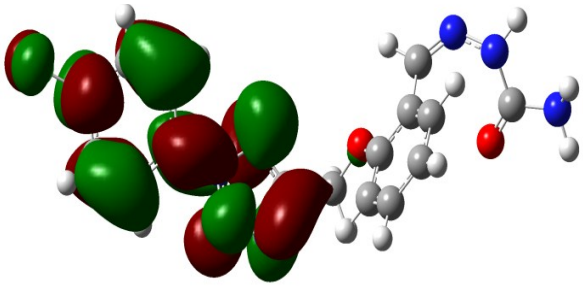

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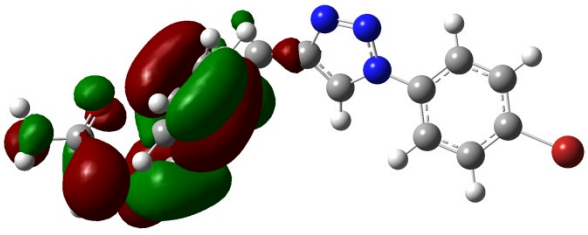

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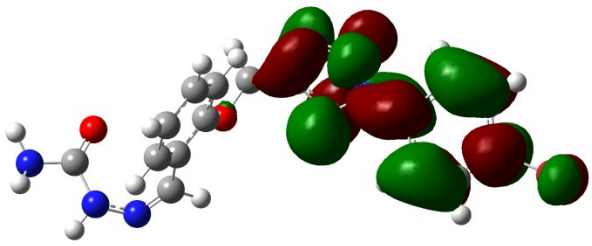

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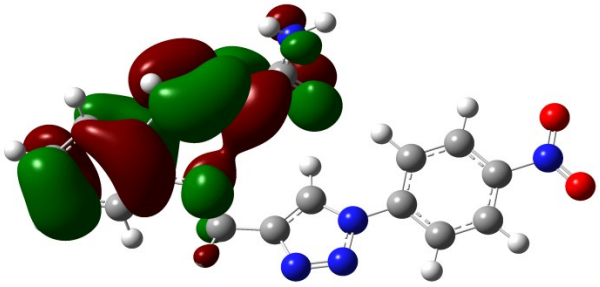

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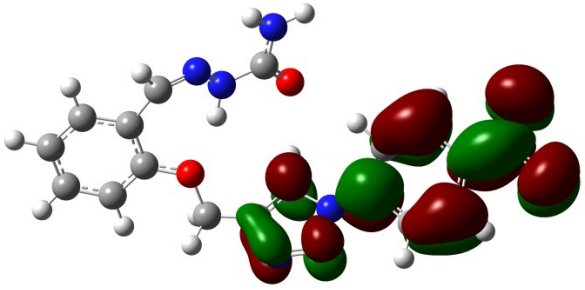

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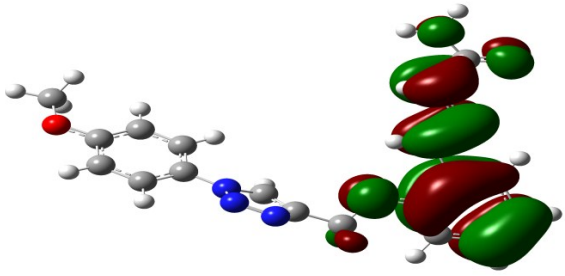

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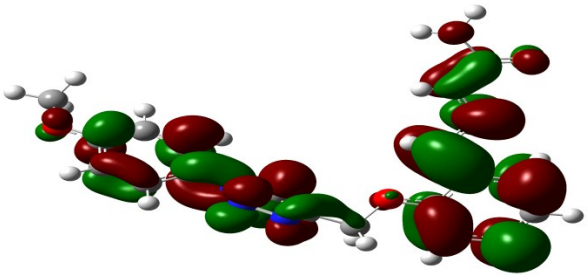
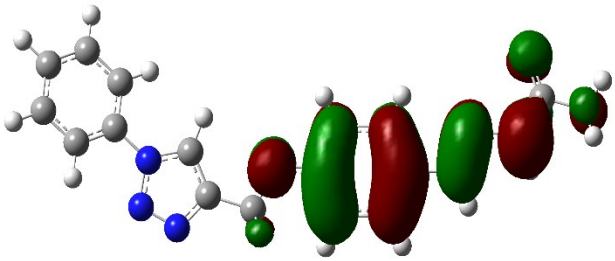


LUMO (**5f**)



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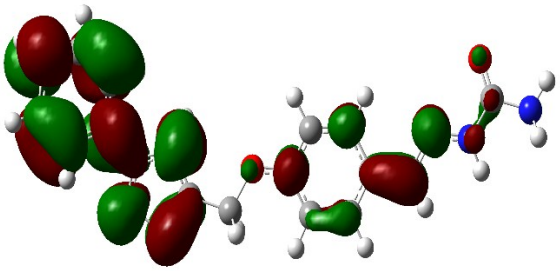
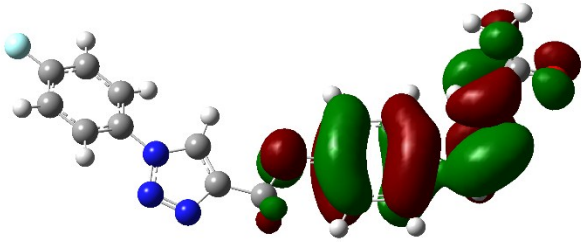
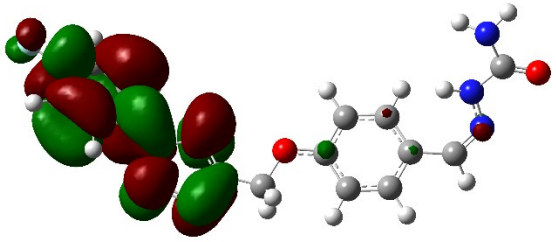


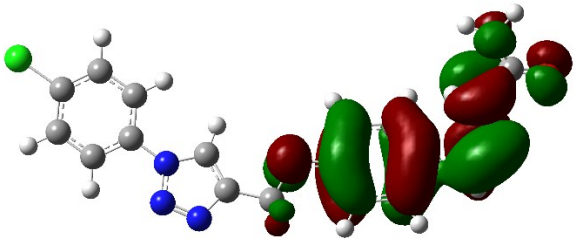
LUMO (**9a**)



HOMO (**9b**)



LUMO (**9b**)



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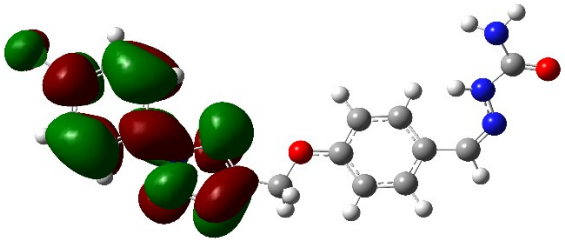
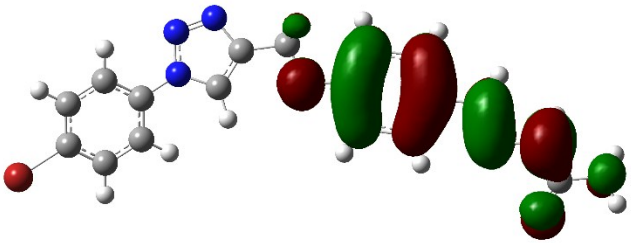
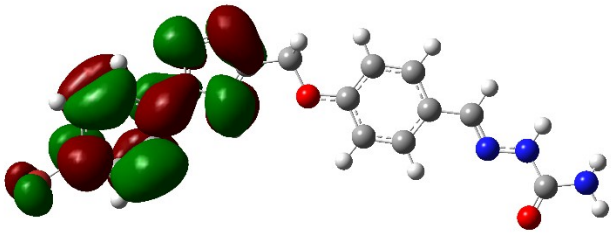


LUMO (**9c**)



HOMO (**9d**)



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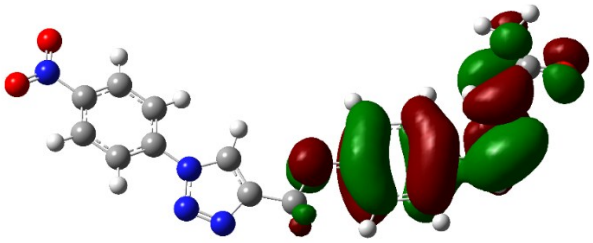

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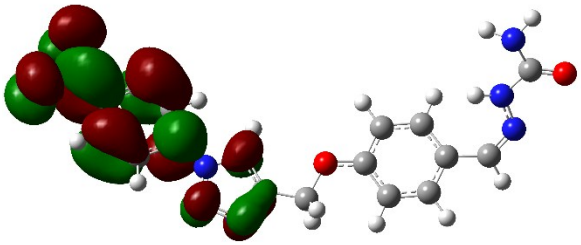

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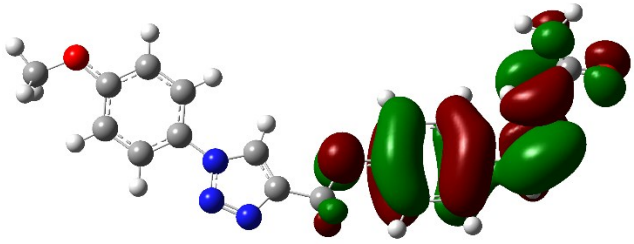
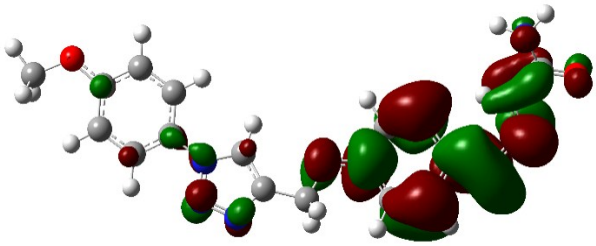


HOMO (**9f**)



LUMO (**9f**)

Experimental Section (General)

The starting chemicals were purchased from commercial suppliers and were used without further purification. The melting point of all compounds was recorded in open capillaries and is incorrect. All the newly synthesised triazole derivatives were satisfactorily characterized by various analytical and spectral techniques i.e. IR, ^{1}H-NMR, ^{13}C-NMR and HRMS spectrometry. The IR spectra were recorded on Shimazdu IR Affinity FTIR spectrophotometer using potassium bromide (KBr). The ^{1}H-NMR and ^{13}C-NMR spectra were recorded on Bruker Avance II 400 nano bay spectrophotometer operating at 400 and 100 MHz in deuterated (DMSO-d6) using tetramethyl silane (TMS) as internal standard. Chemical shift (δ) values are given in ppm and coupling constant (*J*) values are given in Hertz (Hz). Splitting pattern is indicated as follows: s for singlet peak; d for doublet peak; t for triplet peak; m for multiplet peak and dd for double of doublet peak. The appearance of characteristic singlet ^{1}H-NMR in region of 7.6 is due to triazolyl protons. Mass spectra were recorded with instrument Bruker Compass Data Analysis

4.0 at IIT New Delhi. The progress of reaction and the purity of the compounds were monitored by thin layer chromatography (TLC) using readymade silica gel plates (SIL G /UV 254, ALUGRAM) and the chromatogram were visualised under ultraviolet lamp.

Procedure for the synthesis of a terminal alkyne (**2**):

To a solution of ortho/para substituted hydroxy benzaldehyde (1.0 mmol) in 20 mL acetone, anhydrous potassium carbonate (1.5 mmol) was added and the resulting suspension was refluxed for 30 min. Propargyl bromide (80% in toluene, 1.5 mmol) was added to it slowly and the reaction mixture was refluxed for 7-8 hrs by following reported procedure but little modifications were used as and when required.[4] After completion of the reaction as monitored by TLC, the solvent was evaporated and the resulting solid residue was washed with ice cold water and recrystallized from chloroform:hexane (7:3 v/v ratio).

General procedure for the synthesis of semicarbazone linked alkyne (**3**):

As per the reported procedure with slight modifications a solution of semicarbazide (1mmol) and 4-(prop-2-yn-1-yloxy)benzaldehyde (1mmol) in ethanol (70 ml) was refluxed for 4 h. The crystalline solid product separated out on cooling the reaction mixture. Filtered the product and washed with cold ethanol and recrystallized with EtOH-$CHCl_3$ to yield the pure semicarbazone alkyne (**3**) in 93 % yield.[5]

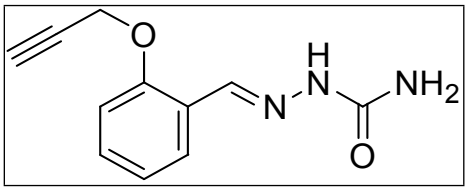
Semicarbazide hydrochloride (1 mmol dissolved in 10 mL water) was added to a stirred solution of O-proparagylated benzaldehyde (1 mmol) in ethanol at 70 C. The reaction mixture was stirred for another 2-3 hours at the same temperature. The reaction was monitored by TLC. After completion of the reaction, cool the reaction mixture. White coloured precipitate started to appear in the reaction mixture. Then add 20 mL of ice cold water to the reaction mixture. When amount of precipitates increased, then filter and dry the precipitates. Then wash the precipitate with warm ethyl acetate to remove unreacted started materials to produce the compounds in pure form.

General procedure for the synthesis of semicarbazone linked triazoles (5a-5f):

A mixture of substituted phenyl azide **4a-4f** (1.0 mmol), alkyne **2** (1.0 mmol) in DMF/water (1:1), $CuSO_4.5H_2O$ (10 mol %) and sodium ascorbate (20 mol %) was stirred for 2-3 h at room temperature. The progress of the reaction was monitored by TLC and after completion of the reaction, the reaction mixture was diluted with ice cold water (30 mL). The solid residues were filtered, washed with aqueous ammonium chloride:ammonia solution (9:1) followed by water and recrystallized with ethyl acetate:hexane (4:1 v/v) to get the desired 1,2,3-triazole derivatives (**5a-5f**) in 90-95 % yield.[5]

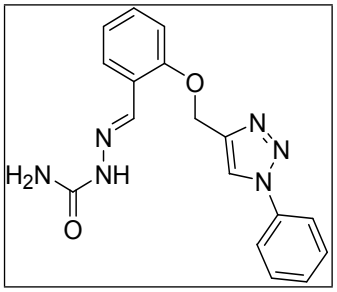
Spectroscopic data of (3, 5a-f):

(E)-2-(2-(prop-2-yn-1-yloxy)benzylidene)hydrazine-1-carboxamide (**3**)



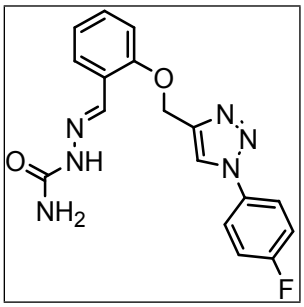
Appearance: white, solid; Yield: 93 %; m. p. 210-212 ºC, reaction time 4 h. ^{1}H-NMR (400 MHz, DMSO): δ 10.27 (s, 1H), 8.18 (s, 1H), 8.02 (d, *J* = 7.7 Hz, 1H), 7.34 (t, *J* = 7.8 Hz, 1H), 7.12 (d, *J* = 8.4 Hz, 1H), 7.00 (t, *J* = 7.5 Hz, 1H), 6.46 (s, 2H), 4.88 (d, *J* = 1.9 Hz, 2H), 3.61 (s, 1H). ^{13}C-NMR (101 MHz, DMSO): δ 157.18 (C), 155.49 (C), 134.95 (CH), 130.55 (CH), 126.22 (CH), 123.96 (CH), 121.80 (CH), 113.64 (CH), 79.56 (C), 79.00 (C), 56.48 (CH_2) ppm. FTIR (KBr): ν_{max} 3263(s), 1691(s), 1577(m), 1433(m), 1606(m) cm^{-1}

(E)-2-(2-((1-phenyl-1*H*-1,2,3-triazol-4-yl)methoxy)benzylidene)hydrazine-1-Carboxamide (**5a**)



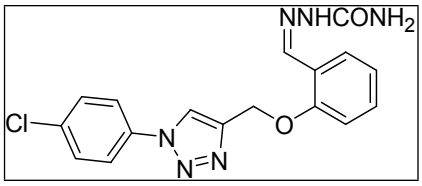
Appearance: white colour solid; Yield: 92 %; m. p.: 240-242 ºC, reaction time 3 h. ^{1}H-NMR (400 MHz, DMSO): δ 10.19 (s, 1H), 8.94 (s, 1H), 8.22 (s, 1H), 8.02 (dd, *J* = 7.7, 1.6 Hz, 1H), 7.93 (d, *J* = 7.5 Hz, 2H), 7.63 (t, *J* = 7.8 Hz, 2H), 7.53 (t, *J* = 7.4 Hz, 1H), 7.40 – 7.33 (m, 1H), 7.29 (d, *J* = 7.8 Hz, 1H), 7.00 (t, *J* = 7.4 Hz, 1H), 6.45 (s, 2H), 5.32 (s, 2H). ^{13}C-NMR (101 MHz, DMSO): δ 157.13 (C), 156.35 (C), 144.43 (C), 137.02 (C), 135.26 (CH), 130.77 (CH), 130.42 (CH), 129.31 (CH), 126.12 (CH), 123.71 (C), 123.16 (s), 121.58 (CH), 120.70 (CH), 113.52 (CH), 62.32 (CH_2) ppm; FT-IR (KBr): ν_{max} 3134(m), 3060(w), 1693(s), 1575(m), 1450(m), 1606(m), 3473(s) cm^{-1}; HRMS $[M+Na]^+$: m/z cal. for $C_{17}H_{16}N_6O_2Na$ 359.1227, found 359.1231.

(E)-2-(2-((1-(4-fluorophenyl)-1*H*-1,2,3-triazol-4-yl)methoxy)benzylidene)hydrazine-1-carboxamide (**5b**)



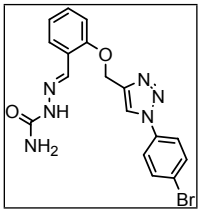
Appearance: white colour solid; Yield: 90 %; m. p.: 250-252 ºC, reaction time 2.5 h. ^{1}H-NMR (400 MHz, DMSO): δ 10.17 (s, 1H), 8.92 (s, 1H), 8.21 (s, 1H), 8.02 (dd, *J* = 7.8, 1.5 Hz, 1H), 7.98 (dd, *J* = 9.1, 4.7 Hz, 2H), 7.49 (t, *J* = 8.8 Hz, 2H), 7.36 (t, *J* = 7.8 Hz, 1H), 7.29 (d, *J* = 7.8 Hz, 1H), 7.00 (t, *J* = 7.4 Hz, 1H), 6.44 (s, 2H), 5.32 (s, 2H). ^{13}C-NMR (101 MHz, DMSO) δ 157.12 (C), 156.34 (C), 144.47 (C), 135.28 (C), 133.60 (C), 130.77 (CH), 126.13 (CH), 123.71 (CH), 123.41 (CH), 123.09 (CH) (d, *J* = 8.8 Hz), 121.59 (CH), 117.39 (CH), 117.16 (CH), 113.53 (CH), 62.31 (CH_2) ppm; FT-IR (KBr): v_{max} 3143(m), 3062(w), 1693(s), 1577(m), 1456(m), 1604(m), 3458(s) cm^{-1}. HRMS $[M+Na]^+$: m/z cal. for $C_{17}H_{15}N_6O_2FNa$ 377.1133, found 377.1142.

(E)-2-(2-((1-(4-chlorophenyl)-1*H*-1,2,3-triazol-4-yl)methoxy)benzylidene)hydrazine-1-Carboxamide (**5c**)



Appearance: white colour solid; Yield: 91 %; m. p.: 260-262 ºC, reaction time 2.5 h. ^{1}H-NMR (400 MHz, DMSO): δ 10.18 (s, 1H), 8.97 (s, 1H), 8.21 (s, 1H), 8.02 (d, *J* = 7.7 Hz, 1H), 7.92 (d, *J* = 9.0 Hz, 2H), 7.84 (d, *J* = 9.0 Hz, 2H), 7.41–7.34 (m, 1H), 7.29 (d, *J* = 8.3 Hz, 1H), 7.00 (t, *J* = 7.4 Hz, 1H), 6.45 (s, 2H), 5.32 (s, 2H). ^{13}C-NMR (101 MHz, DMSO): δ 157.12 (C), 156.31 (C), 144.62 (C), 136.21 (C), 135.25 (CH), 133.32 (CH), 130.77 (CH), 126.14 (CH), 123.71 (C), 123.20 (CH), 122.59 (CH), 121.97 (CH), 121.60 (CH), 113.51 (CH), 62.25 (CH_2) ppm; FT-IR (KBr): v_{max} 3147(s), 3064(w), 1697(s), 1583(m), 1454(m), 1600(m), 3464(s) cm^{-1}; HRMS $[M+Na]^+$: m/z cal. for $C_{17}H_{15}N_6O_2FNa$ 393.0837, found 393.0855.

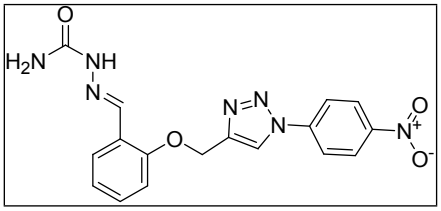
(E)-2-(2-((1-(4-bromophenyl)-1*H*-1,2,3-triazol-4-yl)methoxy)benzylidene)hydrazine-1-carboxamide (**5d**)



Appearance: white colour solid; Yield: 94 %; m. p.: 280-282 ºC, reaction time 2.5 h. ^{1}H-NMR (400 MHz, DMSO): δ 10.18 (s, 1H), 8.97 (s, 1H), 8.21 (s, 1H), 8.02 (d, *J* = 7.7 Hz, 1H), 7.92 (d, *J* = 9.0 Hz, 2H), 7.84 (d, *J* = 9.0 Hz, 2H), 7.41-7.34 (m, 1H), 7.29 (d, *J* = 8.3 Hz, 1H), 7.00 (t, *J* = 7.4 Hz,

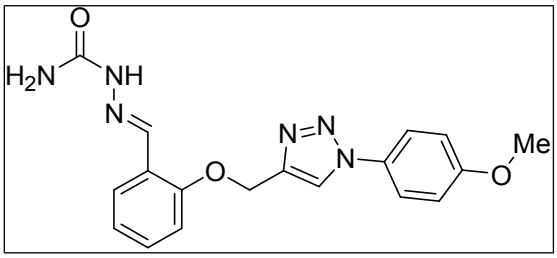
1H), 6.45 (s, 2H), 5.32 (s, 2H). ^{13}C-NMR (101 MHz, DMSO): δ 157.12 (C), 156.31 (C), 144.62 (C), 136.21 (C), 135.25 (CH), 133.32 (C), 130.77 (CH), 126.14 (CH), 123.71 (C), 123.20 (CH), 122.59 (CH), 121.97 (CH), 121.60 (CH), 113.51 (CH), 62.25 (CH_2) ppm; FT-IR (KBr): ν_{max} 3147(s), 3064(w), 1697(s), 1583(m), 1454(m), 1600(m), 3464(s) cm^{-1}; HRMS $[M+Na]^+$: m/z cal. for $C_{17}H_{15}N_6O_2FNa$ 437.0332, found 437.0343.

(E)-2-(2-((1-(4-nitrophenyl)-1*H*-1,2,3-triazol-4-yl)methoxy)benzylidene)hydrazine-1-carboxamide (**5e**)



Appearance: Yellow colour solid; Yield: 95 %; m. p.: 230-232 ºC, reaction time 2 h. ^{1}H-NMR (400 MHz, DMSO) δ 10.17 (s, 1H), 9.15 (s, 1H), 8.49 (d, *J* = 9.1 Hz, 2H), 8.26 (d, *J* = 9.2 Hz, 2H), 8.22 (s, 1H), 8.02 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.41 – 7.34 (m, 1H), 7.29 (d, *J* = 7.8 Hz, 1H), 7.01 (t, *J* = 7.4 Hz, 1H), 6.44 (s, 2H), 5.35 (s, 2H). ^{13}C-NMR (101 MHz, DMSO): δ 157.12 (C), 156.27 (C), 147.32 (C), 145.08 (C), 141.22 (C), 135.25 (CH), 130.78 (CH), 126.17 (CH), 126.10 (CH), 123.74 (C), 123.64 (CH), 121.66 (CH), 121.25 (CH), 113.55 (CH), 62.16 (CH_2) ppm; FT-IR (KBr): ν_{max} 3142 (m), 3062(w), 1695(s), 1595(m), 1452(m), 1608(w), 3444(m) cm^{-1}; HRMS $[M+Na]^+$: m/z cal. for $C_{17}H_{15}N_7O_4Na$ 404.1078, found 404.1094.

(E)-2-(2-((1-(4-methoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methoxy)benzylidene)hydrazine-1-carboxamide (**5f**)



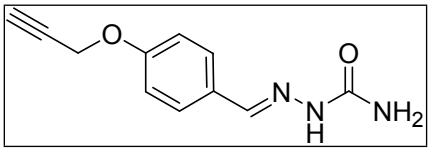
Appearance: white colour solid; Yield: 92 %; m. p.: 310-312 ºC, reaction time 3 h. ^{1}H-NMR (400 MHz, DMSO) δ 10.17 (s, 1H), 8.83 (s, 1H), 8.21 (s, 1H), 8.01 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.40–7.32 (m, 1H), 7.29 (d, *J* = 7.8 Hz, 1H), 7.20 – 7.11 (m, 2H), 7.00 (t, *J* = 7.4 Hz, 1H), 6.43 (s, 2H), 5.30 (s, 2H), 3.85 (s, 3H). ^{13}C-NMR (101 MHz, DMSO): δ 159.57 (C), 157.12 (C), 156.37 (C), 144.17 (C), 135.29 (CH), 130.77 (CH), 130.44 (CH), 126.12 (CH), 123.70 (C), 123.13 (CH), 122.37 (C), 121.56 (CH), 115.41 (CH), 113.52 (CH), 62.36 (CH_2), 56.07 (CH_3); FT-IR (KBr): ν_{max} 3138(m), 3062(w), 1693(s), 1581(m), 1456(m), 1608(s), 3456(s) cm^{-1}; HRMS $[M+Na]^+$: m/z cal. for $C_{18}H_{18}N_6O_3Na$ 389.1333, found 389.1352.

General procedure for the synthesis of semicarbazone linked triazoles (9a-9f):

A mixture of substituted phenyl azide **4a-f** (1.0 mmol), alkyne **8** (1.0 mmol) in DMF/water (1:1 v/v), $CuSO_4.5H_2O$ (10 mol %) and sodium ascorbate (20 mol %) was stirred for 2-3 h at room temperature. After completion of the reaction, as confirmed by the TLC; the reaction mixture was diluted with ice cold water (30 mL). The solid residues were filtered, washed with aqueous ammonium chloride:ammonia solution (9:1 v/v) followed by water and recrystallized with ethyl acetate:hexane (4:1 v/v) to get the desired 1,2,3-triazole derivatives (**9a-9f**) in 88-94 % yield.

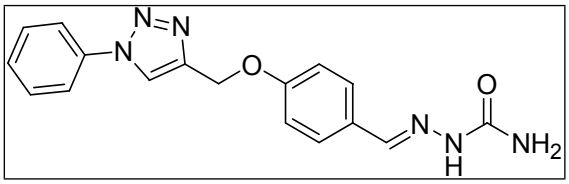
Spectroscopic data (8 & 9a-f):

(E)-2-(4-(prop-2-yn-1-yloxy)benzylidene)hydrazine-1-carboxamide **(8)**



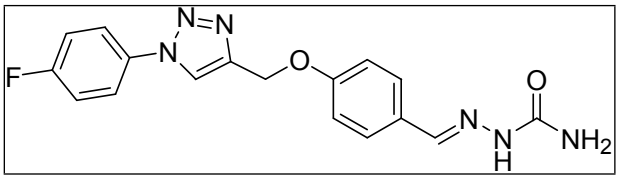
Appearance: white colour solid; Yield: 94 %; m. p.: 210-212 ºC, reaction time 4 h. ^{1}H-NMR (400 MHz, DMSO) δ 10.13 (s, 1H), 7.79 (s, 1H), 7.67 (d, *J* = 8.8 Hz, 2H), 7.00 (d, *J* = 8.8 Hz, 2H), 6.44 (s, 2H), 4.84 (d, *J* = 2.3 Hz, 2H), 3.58 (t, *J* = 2.3 Hz, 1H). ^{13}C-NMR (101 MHz, DMSO): δ 158.36 (C), 157.30 (C), 139.45 (CH), 128.64 (CH), 128.40 (CH), 115.42 (CH), 79.56 (C), 78.83 (C), 55.96 (CH_2). FT-IR (KBr): ν_{max} 3263(s), 1691(w), 1577(s), 1433(s), 1606(s) ppm.

(E)-2-(4-((1-phenyl-1H-1,2,3-triazol-4-yl)methoxy)benzylidene)hydrazine-1-carboxamide (**9a**)



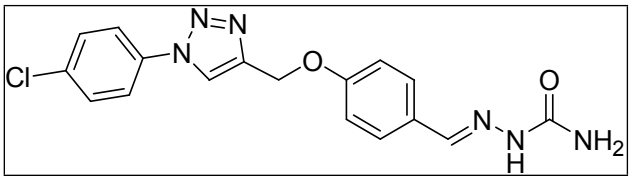
Appearance: white colour solid; Yield: 94 %; m p.: 220-222 ºC, reaction time 3 h. ^{1}H-NMR (400 MHz, DMSO) δ 10.12 (s, 1H), 8.97 (s, 1H), 7.92 (d, *J* = 7.6 Hz, 2H), 7.80 (s, 1H), 7.68 (d, *J* = 8.8 Hz, 2H), 7.62 (t, *J* = 7.8 Hz, 2H), 7.51 (t, *J* = 7.4 Hz, 1H), 7.10 (d, *J* = 8.8 Hz, 2H), 6.43 (s, 2H), 5.28 (s, 2H). ^{13}C-NMR (101 MHz, DMSO): δ 159.20 (C), 157.30 (C), 144.21 (C), 139.50 (CH), 137.03 (C), 130.40 (CH), 129.27 (CH), 128.53 (CH), 128.38 (C), 123.41 (CH), 120.65 (CH), 115.35 (CH), 61.58 (CH_2) ppm; FTIR (KBr): ν_{max} 3140 (m), 3060(w), 1691(s), 1597(s), 1433(s), 1606(w), 3462(s) cm^{-1}; HRMS [M+Na]+: m/z cal. for $C_{17}H_{16}N_6O_2Na$ 359.1227, found 359.1231.

(E)-2-(4-((1-(4-fluorophenyl)-1H-1,2,3-triazol-4-yl)methoxy)benzylidene)hydrazine-1-carboxamide (**9b**)



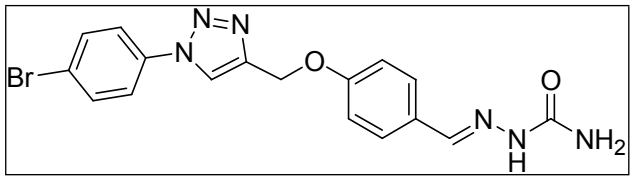
Appearance: white colour solid; Yield: 92 %; m. p.: 235-237 ºC, reaction time 2.5 h. ^{1}H-NMR (400 MHz, DMSO) δ 10.12 (s, 1H), 8.95 (s, 1H), 7.97 (dd, *J* = 9.1, 4.7 Hz, 2H), 7.80 (s, 1H), 7.68 (d, *J* = 8.8 Hz, 2H), 7.47 (t, *J* = 8.8 Hz, 2H), 7.10 (d, *J* = 8.8 Hz, 2H), 6.43 (s, 2H), 5.28 (s, 2H). ^{13}C-NMR (101 MHz, DMSO): δ 163.39 (C), 160.94 (C), 159.17 (C), 157.29 (C), 144.22 (C), 139.50 (CH), 133.58 (CH) (d, *J* = 2.8 Hz), 128.52 (CH), 128.38 (C), 123.64 (CH), 123.07 (CH), 122.98 (CH), 61.56 (CH_2) ppm; FTIR (KBr): v_{max}3143(m), 3064(w), 1693(s), 1577(s), 1444(s), 1608(s), 3481(s) cm^{-1}; HRMS $[M+Na]^+$: m/z cal. for $C_{17}H_{15}N_6O_2FNa$ 377.1133, found 377.1142.

(E)-2-(4-((1-(4-chlorophenyl)-1H-1,2,3-triazol-4-yl)methoxy)benzylidene)hydrazine-1-carboxamide (**9c**)



Appearance: white colour solid; Yield: 90 %; m. p.: 260-262 ºC, reaction time 2.5 h. ^{1}H-NMR (400 MHz, DMSO) δ 10.11 (s, 1H), 9.00 (s, 1H), 7.97 (d, *J* = 6.8 Hz, 2H), 7.80 (s, 1H), 7.70 (s, 2H), 7.68 (s, 2H), 7.09 (d, *J* = 8.8 Hz, 2H), 6.43 (s, 2H), 5.28 (s, 2H). ^{13}C-NMR (101 MHz, DMSO) δ 159.17 (C), 157.28 (C), 144.39 (C), 139.47 (s), 135.83 (C), 133.54 (C), 130.37 (CH), 128.53 (CH), 128.41 (C), 123.50 (CH), 122.34 (CH), 115.35 (CH), 61.55 (CH_2) ppm; FTIR (KBr): v_{max}3140(m), 3062(w), 1691(s), 1585(m), 1440(m), 1608(s), 3469(s) cm^{-1}; HRMS $[M+Na]^+$: m/z cal. for $C_{17}H_{15}N_6O_2FNa$ 393.0837, found 393.0855.

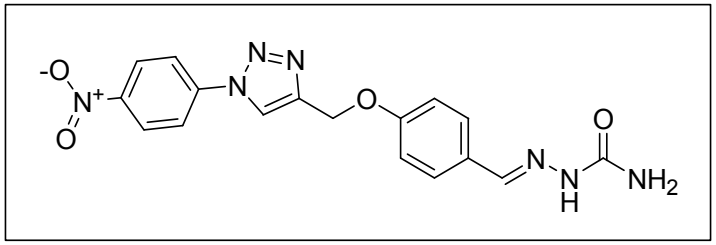
(E)-2-(4-((1-(4-bromophenyl)-1H-1,2,3-triazol-4-yl)methoxy)benzylidene)hydrazine-1-carboxamide (**9d**)



Appearance: white colour solid; Yield: 88 %; m. p.: 220-222 ºC, reaction time 2 h. ^{1}H NMR (400 MHz, DMSO) δ 10.11 (s, 1H), 9.00 (s, 1H), 7.90 (d, *J* = 8.9 Hz, 2H), 7.82 (d, *J* = 8.9 Hz, 2H), 7.80 (s, 1H), 7.68 (d, *J* = 8.8 Hz, 2H), 7.09 (d, *J* = 8.8 Hz, 2H), 6.43 (s, 2H), 5.28 (s, 2H). ^{13}C-NMR (101 MHz, DMSO): δ 159.15 (C), 157.27 (C), 144.40 (C), 139.48 (CH), 136.22

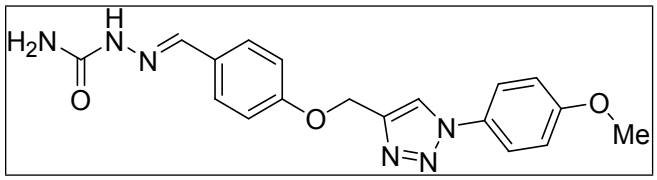
(C), 133.29 (C), 128.52 (CH), 128.39 (C), 123.44 (CH), 122.57 (CH), 121.91 (CH), 115.34 (CH), 61.54 (CH_2) ppm; FT-IR (KBr): v_{max}3142(m), 3062(w), 1693(s), 1581(m), 1433(m), 1604(m), 3471(s) cm^{-1}; HRMS $[M+Na]^+$: m/z cal. for $C_{17}H_{15}N_6O_2FNa$ 437.0332, found 437.0343.

(E)-2-(4-((1-(4-nitrophenyl)-1H-1,2,3-triazol-4-yl)methoxy)benzylidene)hydrazine-1-carboxamide (**9e**)



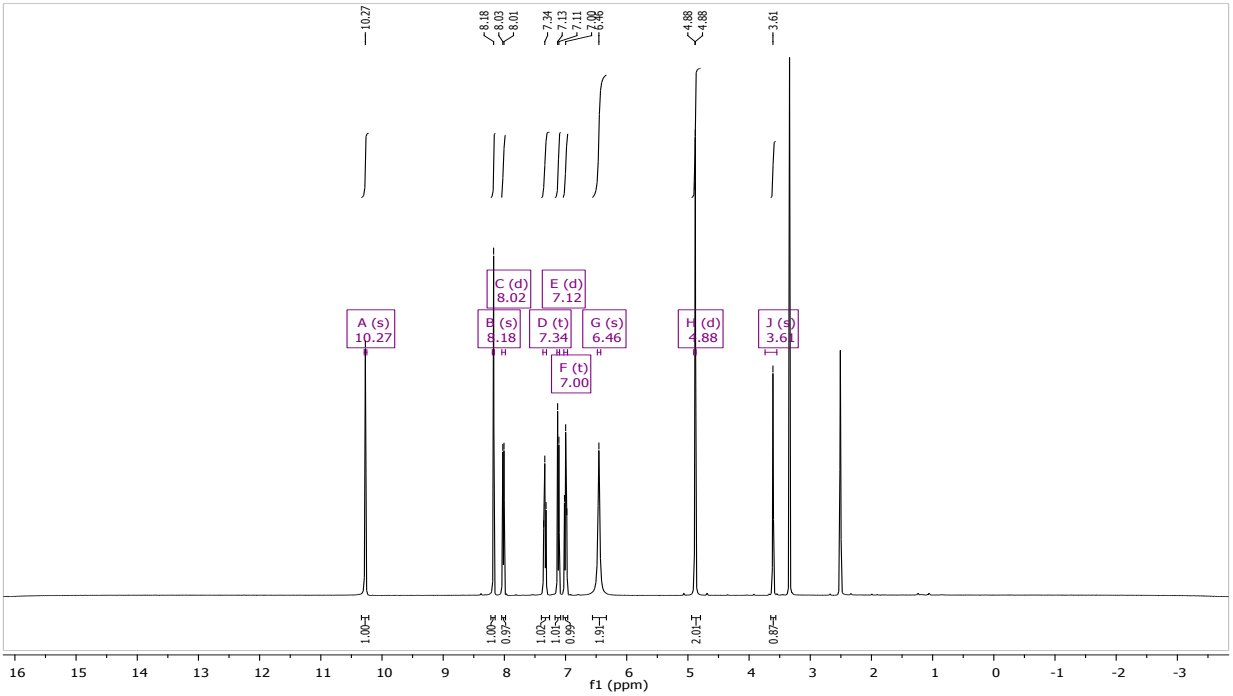
Appearance: Yellow colour solid; Yield: 93 %; m. p.: 230-232 ºC, reaction time 2 h. ^{1}H-NMR (400 MHz, DMSO) δ 10.11 (s, 1H), 9.18 (s, 1H), 8.47 (d, *J* = 9.2 Hz, 2H), 8.25 (d, *J* = 9.2 Hz, 2H), 7.80 (s, 1H), 7.69 (d, *J* = 8.8 Hz, 2H), 7.10 (d, *J* = 8.8 Hz, 2H), 6.43 (s, 2H), 5.32 (s, 2H). ^{13}C-NMR (101 MHz, DMSO): δ 159.12 (C), 157.28 (C), 147.29 (C), 144.90 (C), 141.25 (C), 139.47 (CH), 128.54 (CH), 128.47 (C), 126.06 (CH), 123.84 (CH), 121.21 (CH), 115.37 (CH), 61.50 (CH_2) ppm; FT-IR (KBr): v_{max}3142(m), 3060(w), 1689(s), 1597(s), 1463(s), 1604(s), 3475(s) cm^{-1}; HRMS $[M+Na]^+$: m/z cal. for $C_{17}H_{15}N_7O_4Na$ 404.1078, found 404.1094.

(E)-2-(4-((1-(4-methoxyphenyl)-1H-1,2,3-triazol-4-yl)methoxy)benzylidene)hydrazine-1-carboxamide (**9f**)

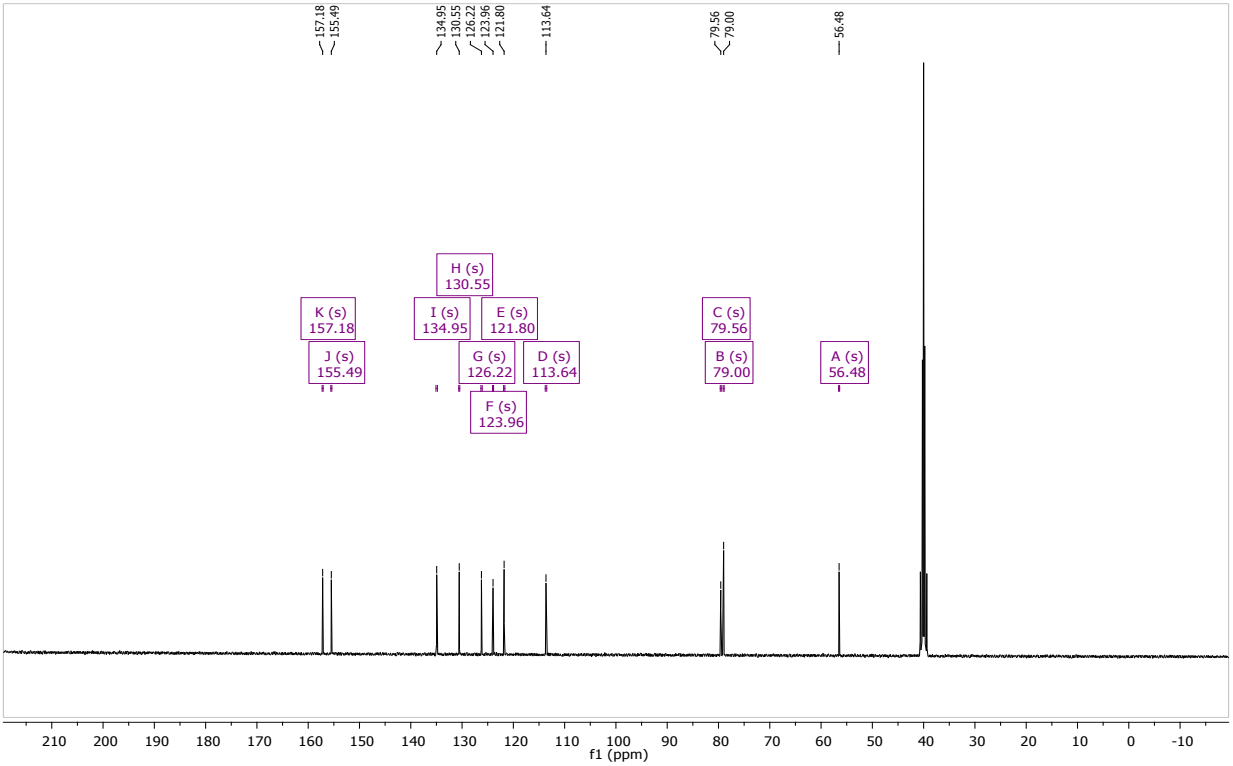


Appearance: white coloured solid; Yield: 92 %; m. p.: 245-247ºC, reaction time 3 hrs. ^{1}H-NMR (400 MHz, DMSO) δ 10.12 (s, 1H), 8.85 (s, 1H), 7.82 (d, *J* = 9.2 Hz, 3H), 7.68 (d, *J* = 8.7 Hz, 2H), 7.15 (d, *J* = 9.0 Hz, 2H), 7.10 (d, *J* = 8.7 Hz, 2H), 6.43 (s, 2H), 5.26 (s, 2H), 3.84 (s, 3H). ^{13}C-NMR (101 MHz, DMSO): δ 159.81 (C), 159.22 (C), 157.29 (C), 143.94 (C), 139.51 (CH), 130.44 (CH), 128.51 (CH), 128.35 (C), 123.35 (CH), 122.30 (CH), 115.37 (C), 115.34 (CH), 61.62 (CH_2), 56.04 (CH_3); FT-IR (KBr): v_{max}3155(m), 3062(w), 1693(s), 1589(m), 1450(m), 1600(s), 3458(s) cm^{-1}; HRMS $[M+Na]^+$: m/z cal. for $C_{18}H_{18}N_6O_3Na$ 389.1333, found 389.1352.

Physical Data (^{1}H-NMR, ^{13}C-NMR spectra of **3**)

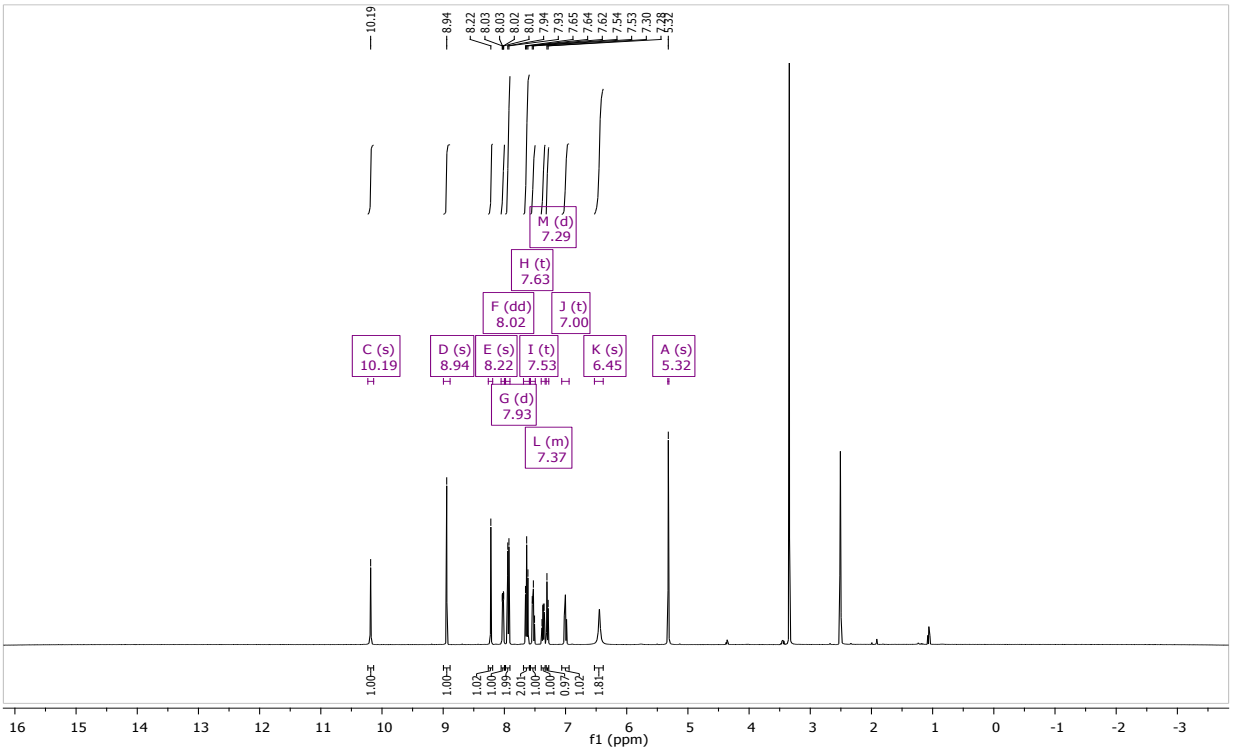


^{1}H-NMR (**3**)

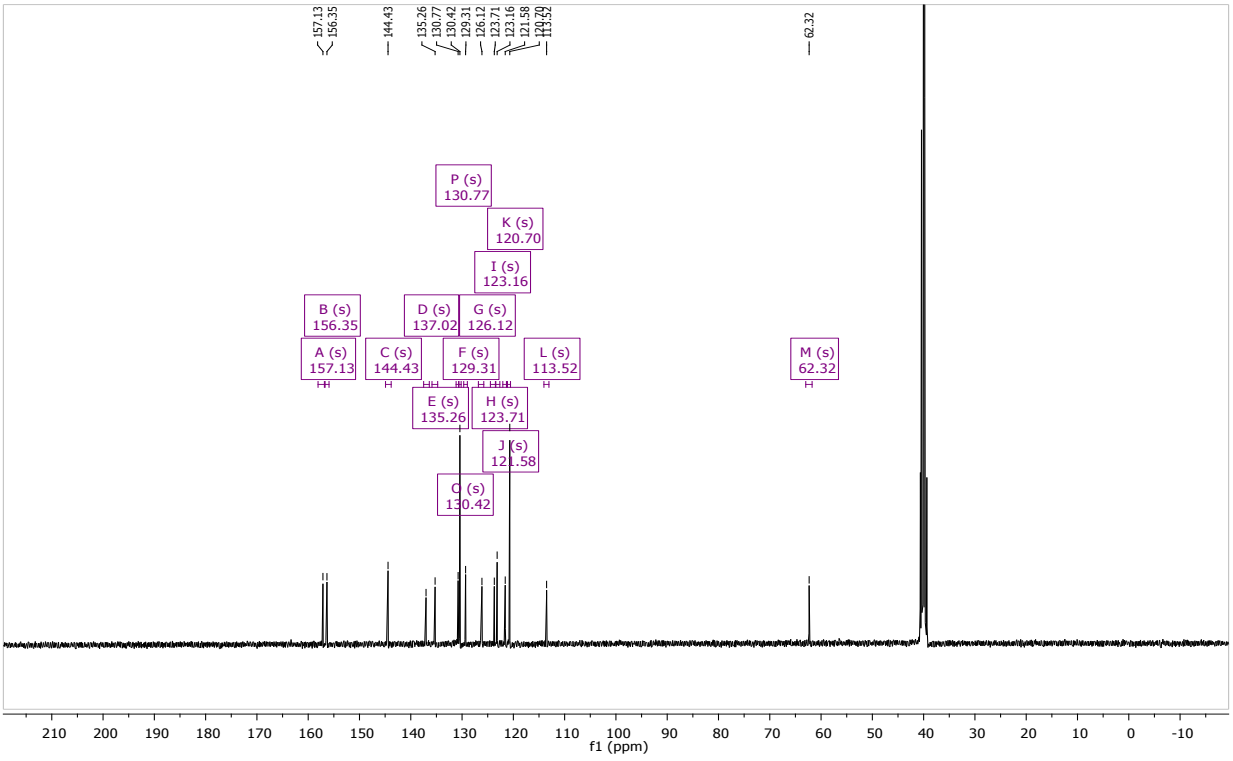


^{13}C-NMR (**3**)

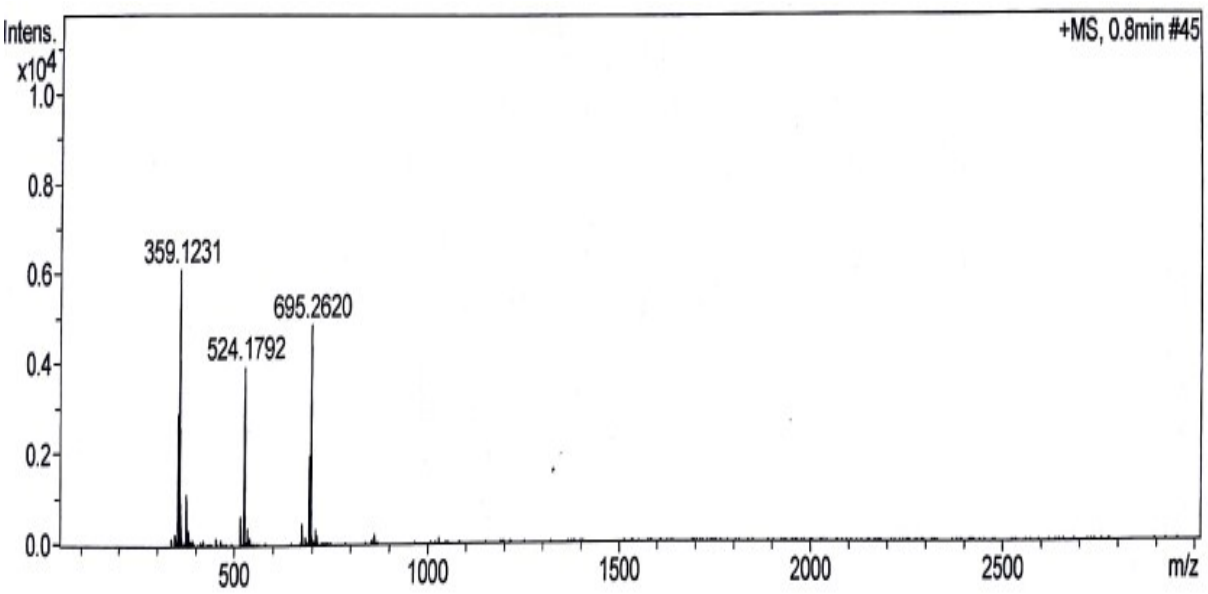
Physical Data (^{1}H-NMR, ^{13}C-NMR, HRMS of **5a-f**)



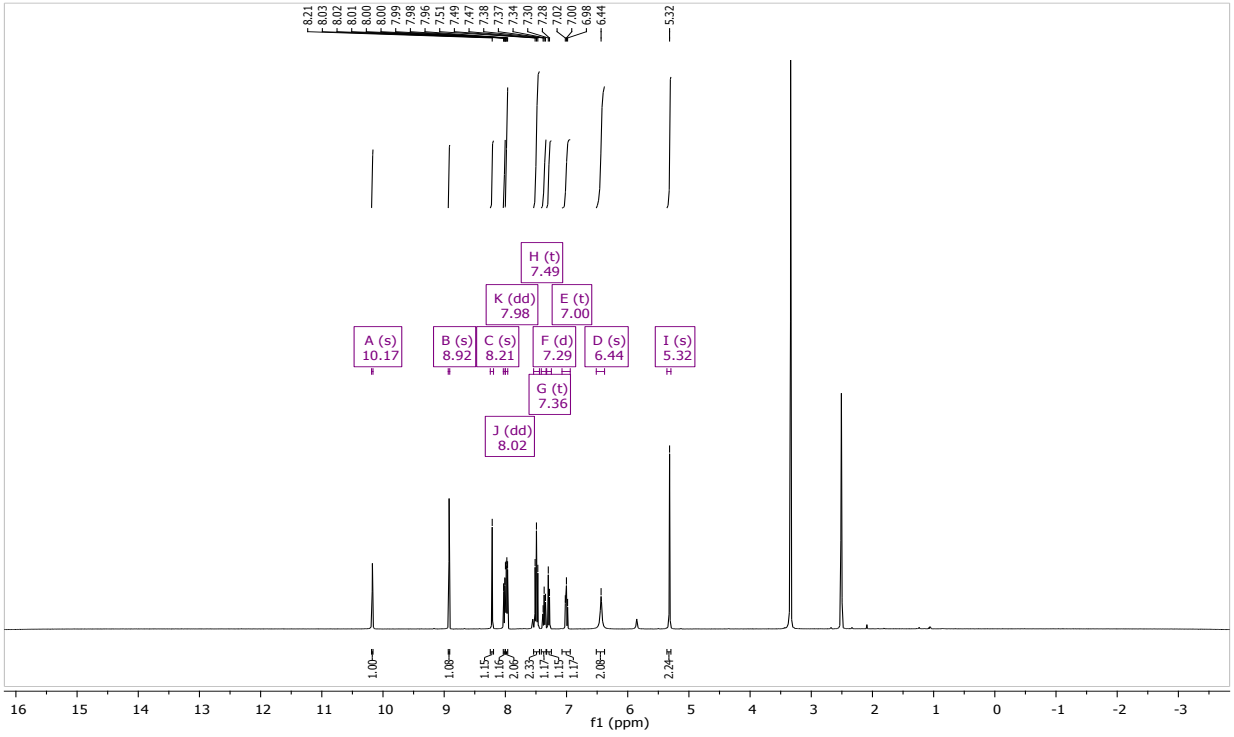
^{1}H-NMR (**5a**)



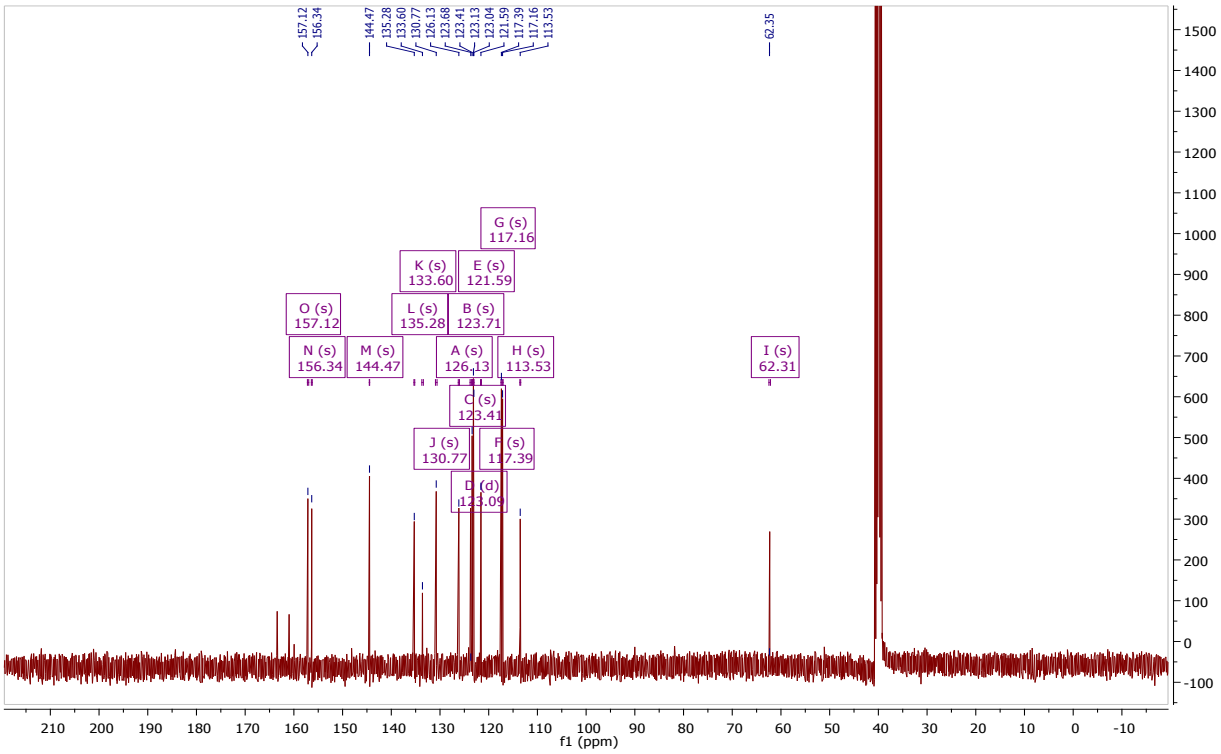
^{13}C-NMR (**5a**)



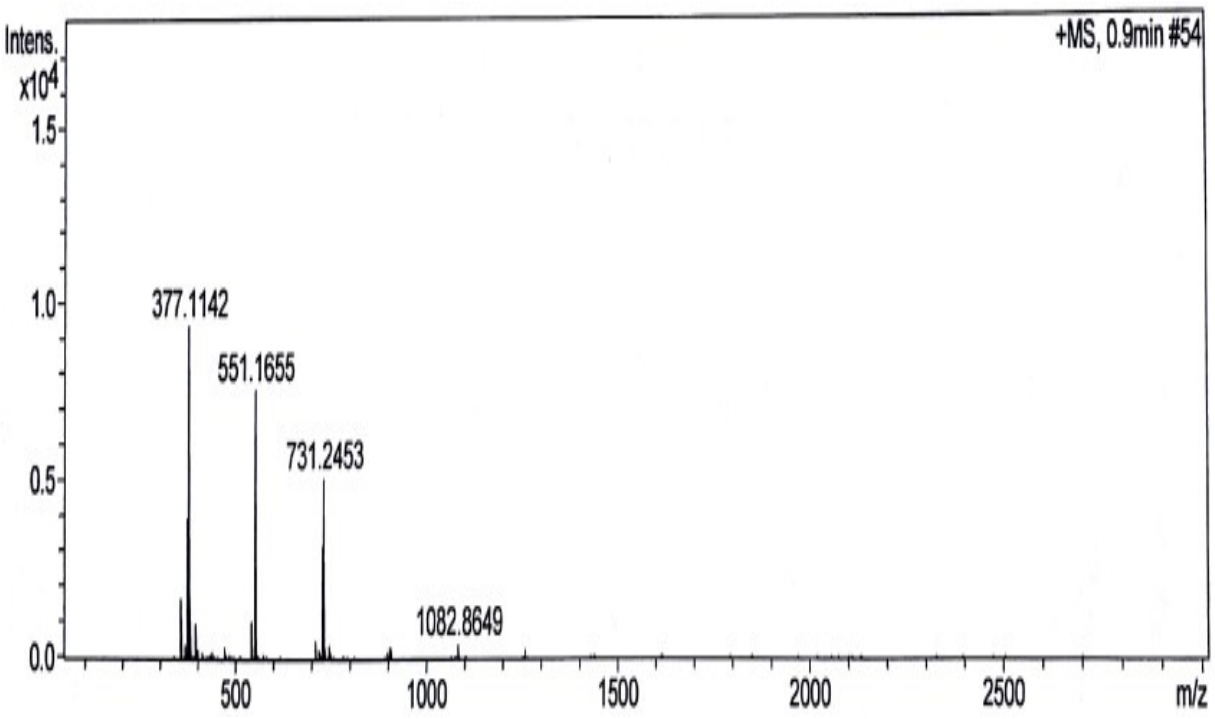
HRMS [M+Na]+: m/z cal. for $C_{17}H_{16}N_6O_2Na$ 359.1227, found 359.1231.



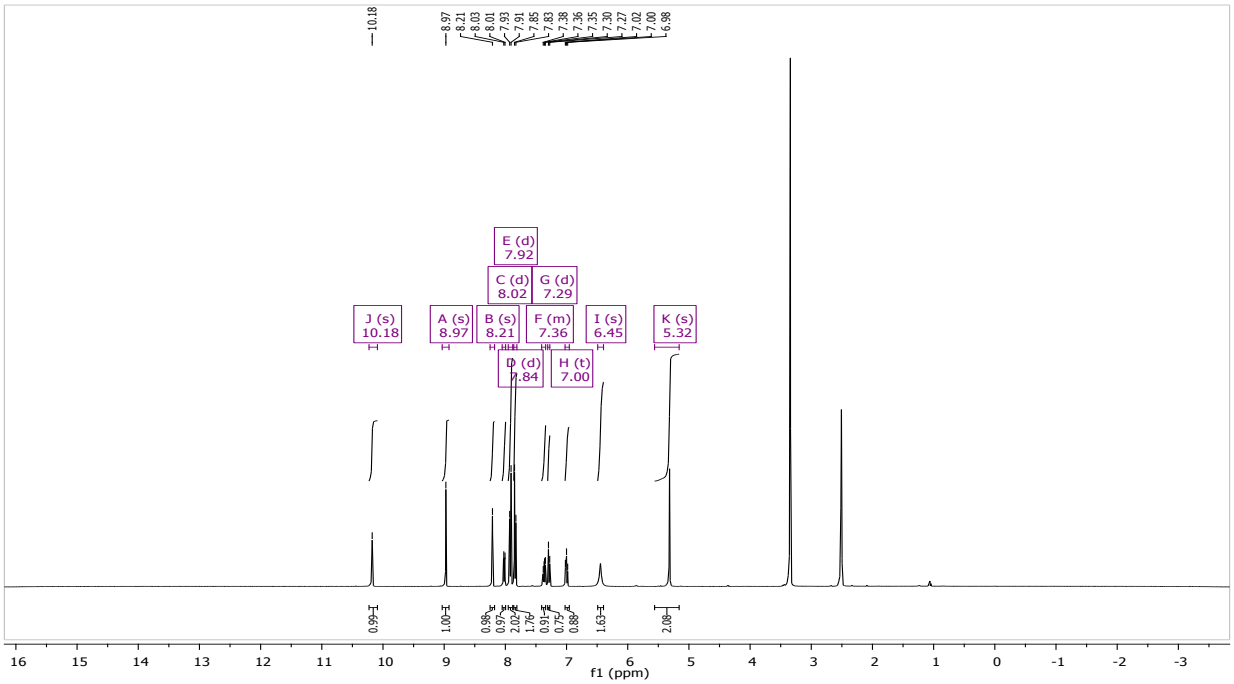
^{1}H-NMR (**5b**)



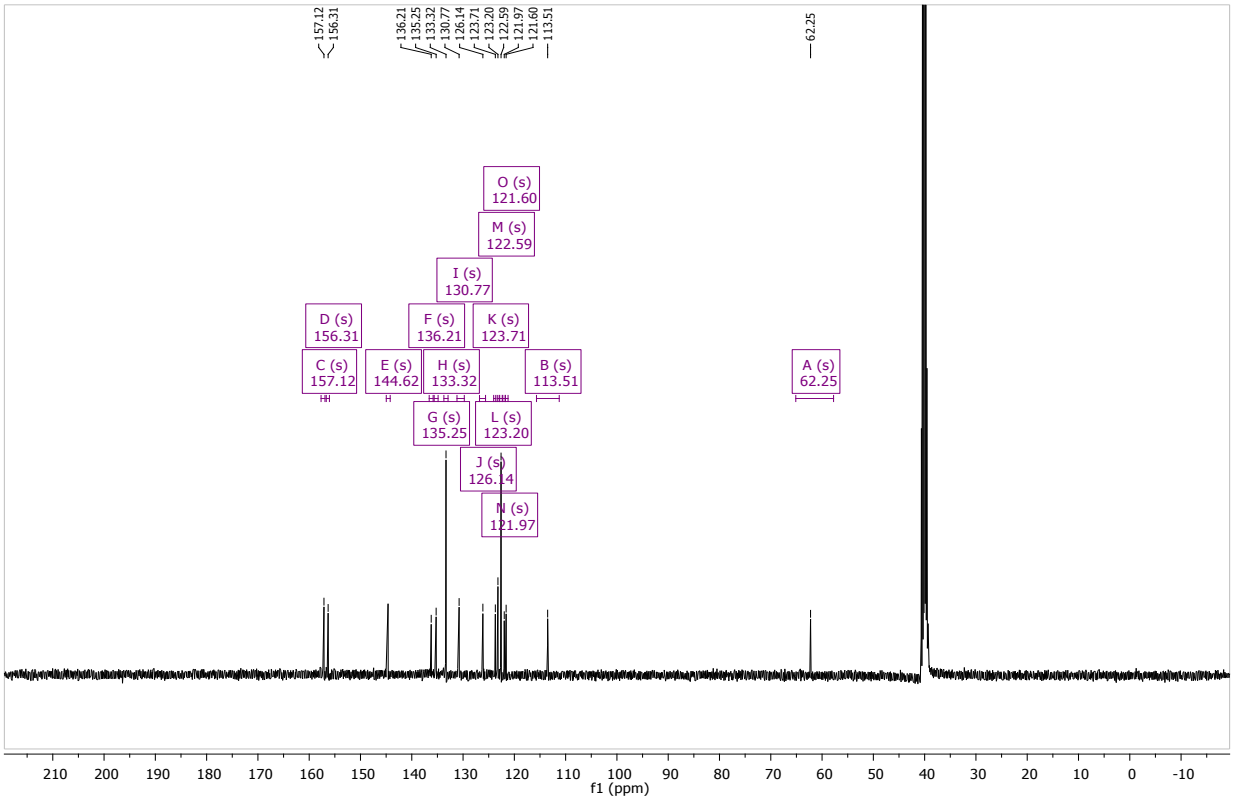
^{13}C-NMR (**5b**)



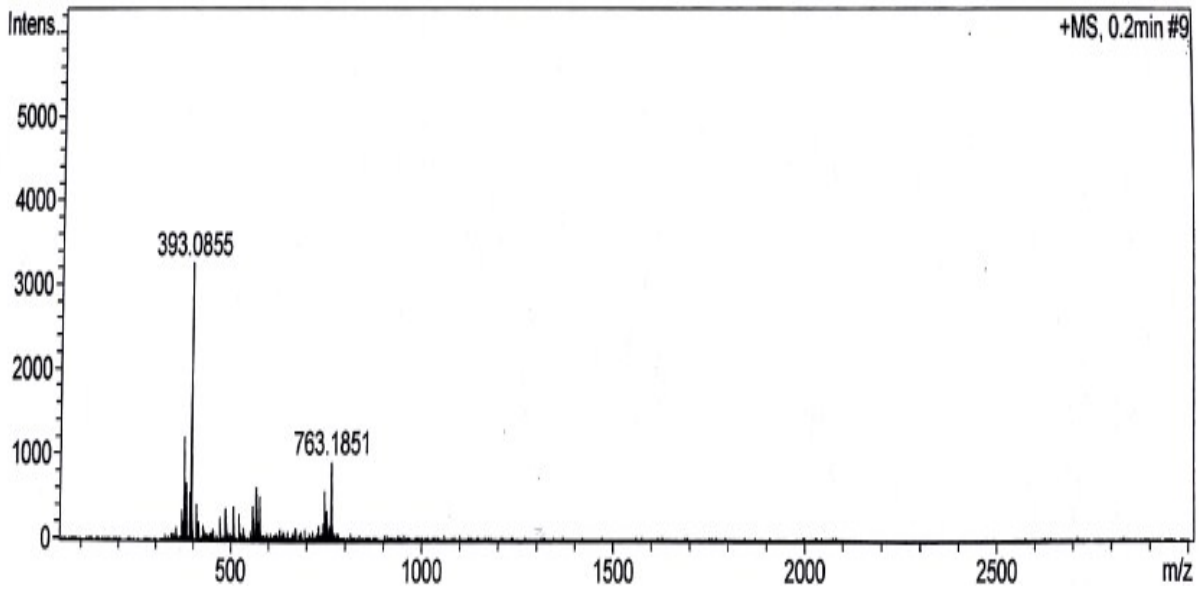
HRMS [M+Na]+: m/z cal. for $C_{17}H_{15}N_6O_2FNa$ 377.1133, found 377.1142.



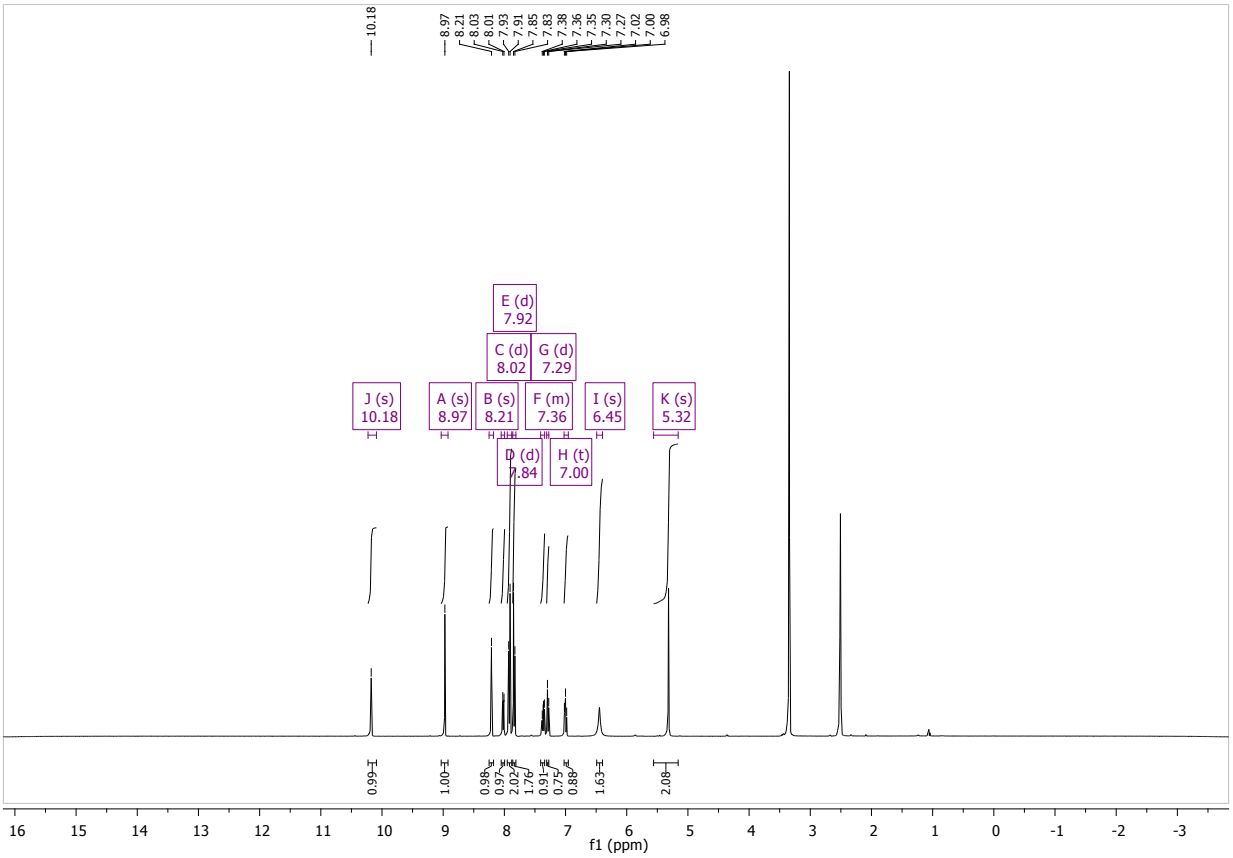
^{1}H-NMR (**5c**)



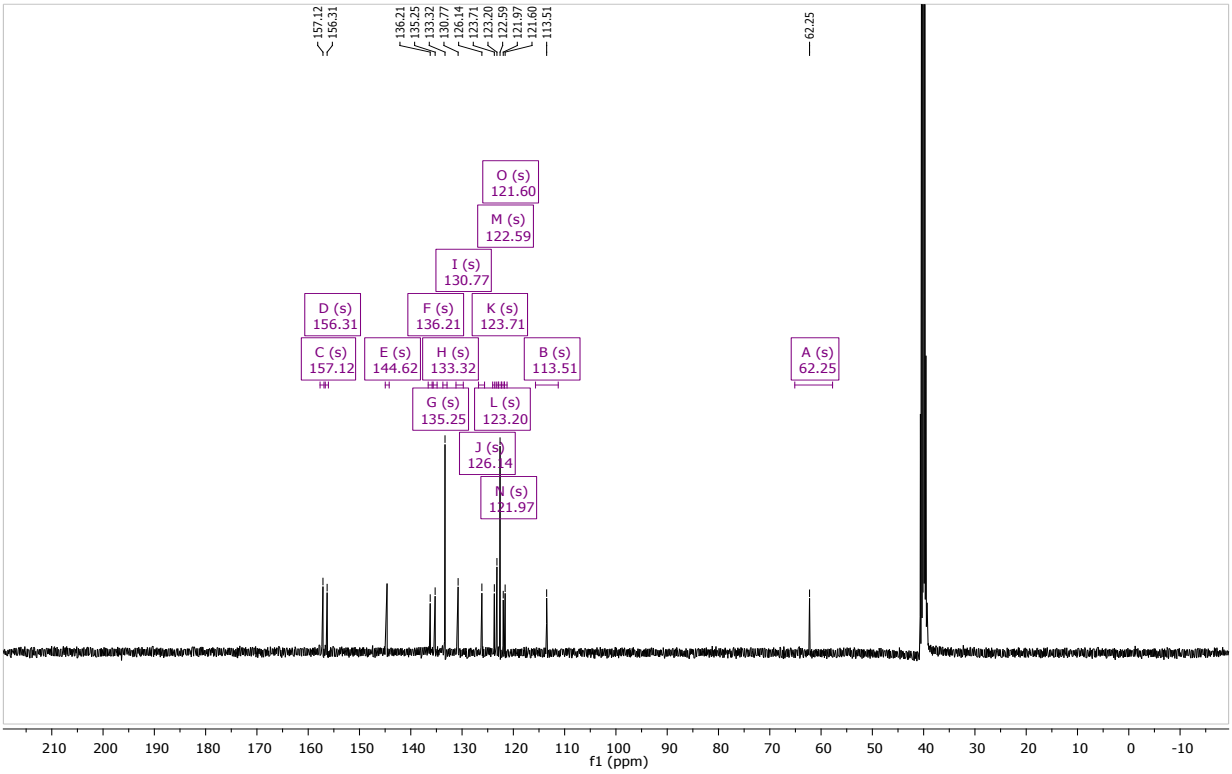
^{13}C-NMR (**5c**)



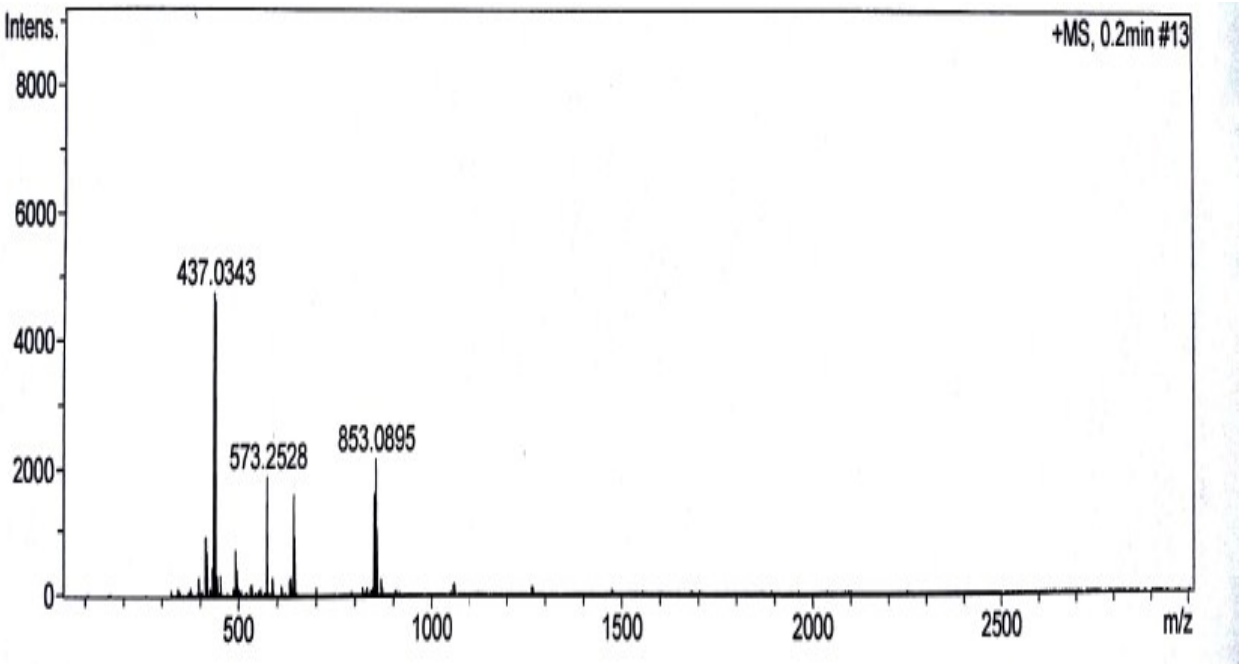
HRMS $[M+Na]^+$: m/z cal. for $C_{17}H_{15}N_6O_2FNa$ 393.0837, found 393.0855.



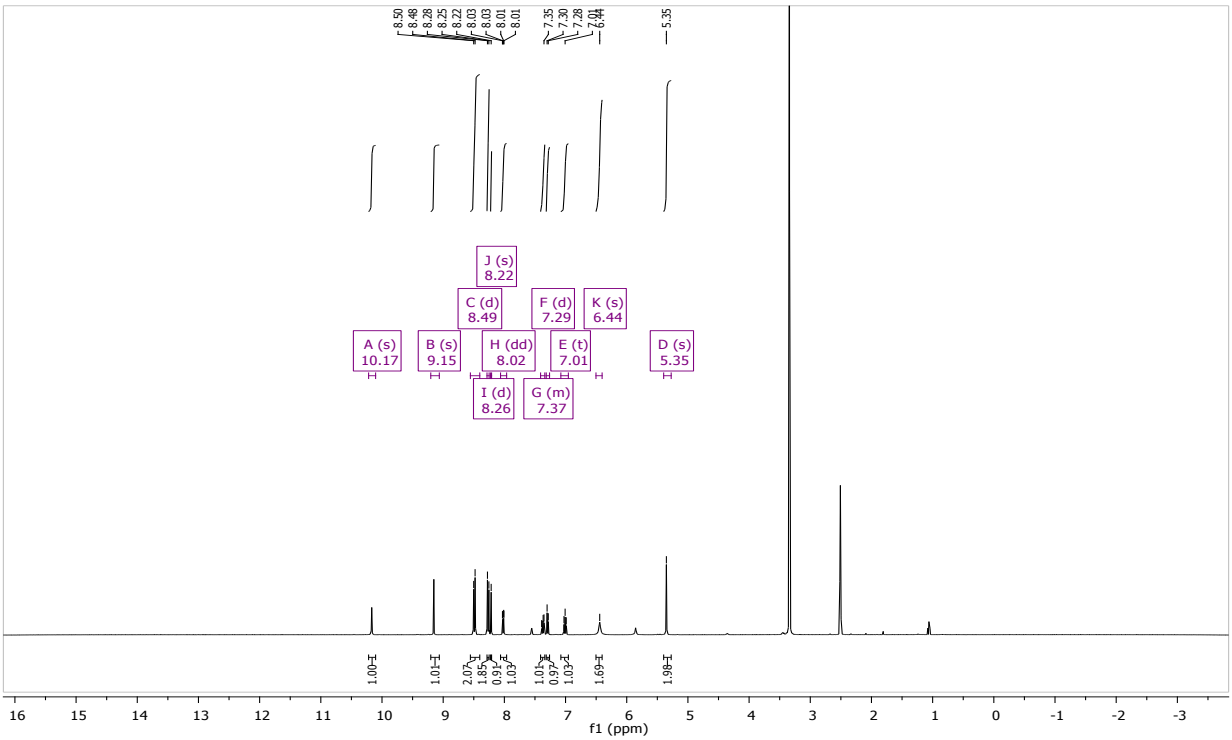
^{1}H-NMR (**5d**)



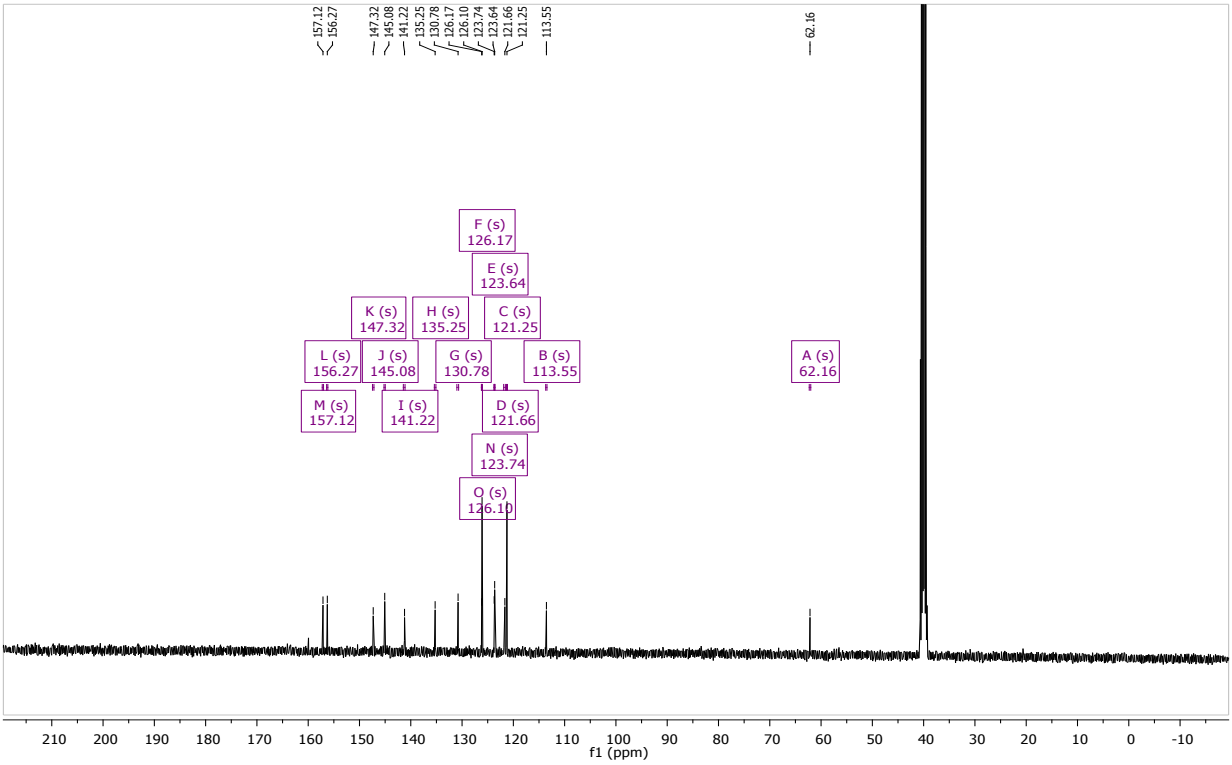
^{13}C-NMR (**5d**)



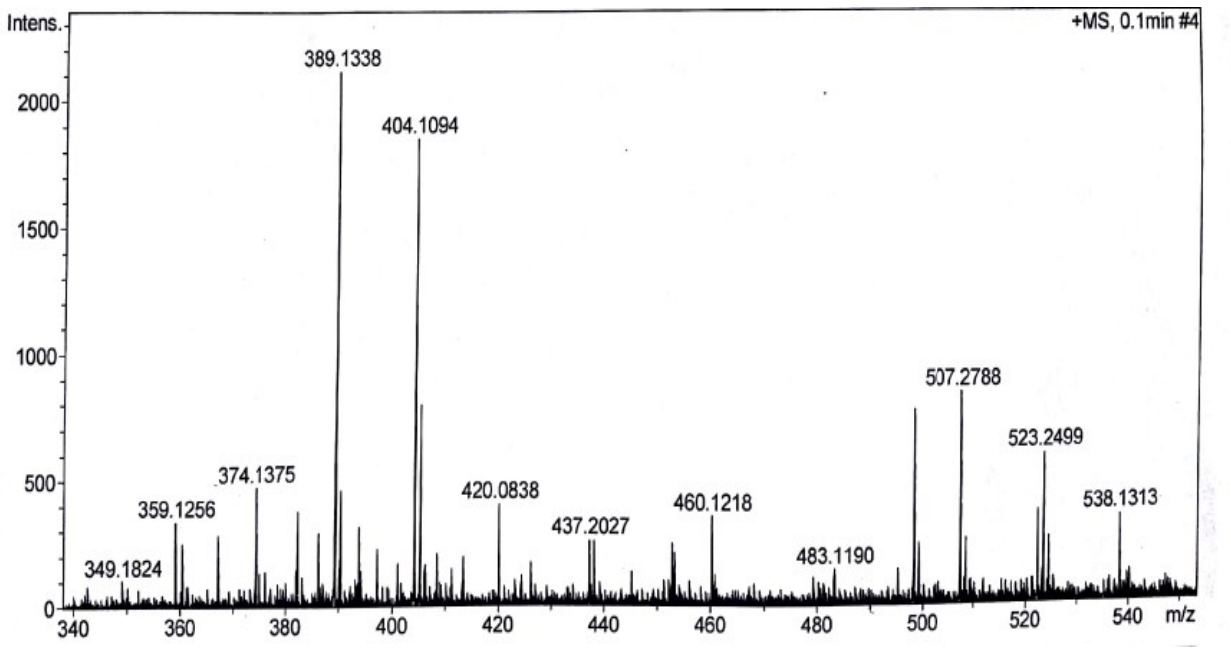
HRMS $[M+Na]^+$: m/z cal. for $C_{17}H_{15}N_6O_2FNa$ 437.0332, found 437.0343.



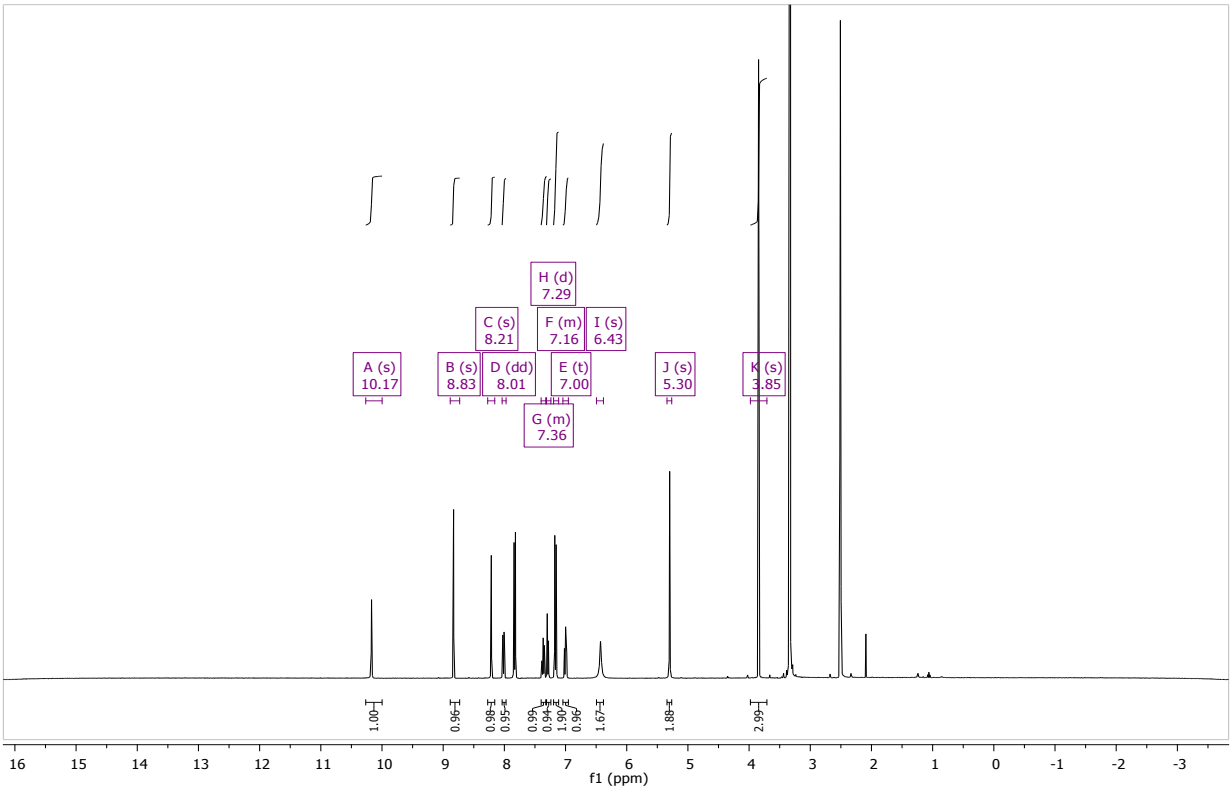
^{1}H-NMR (**5e**)



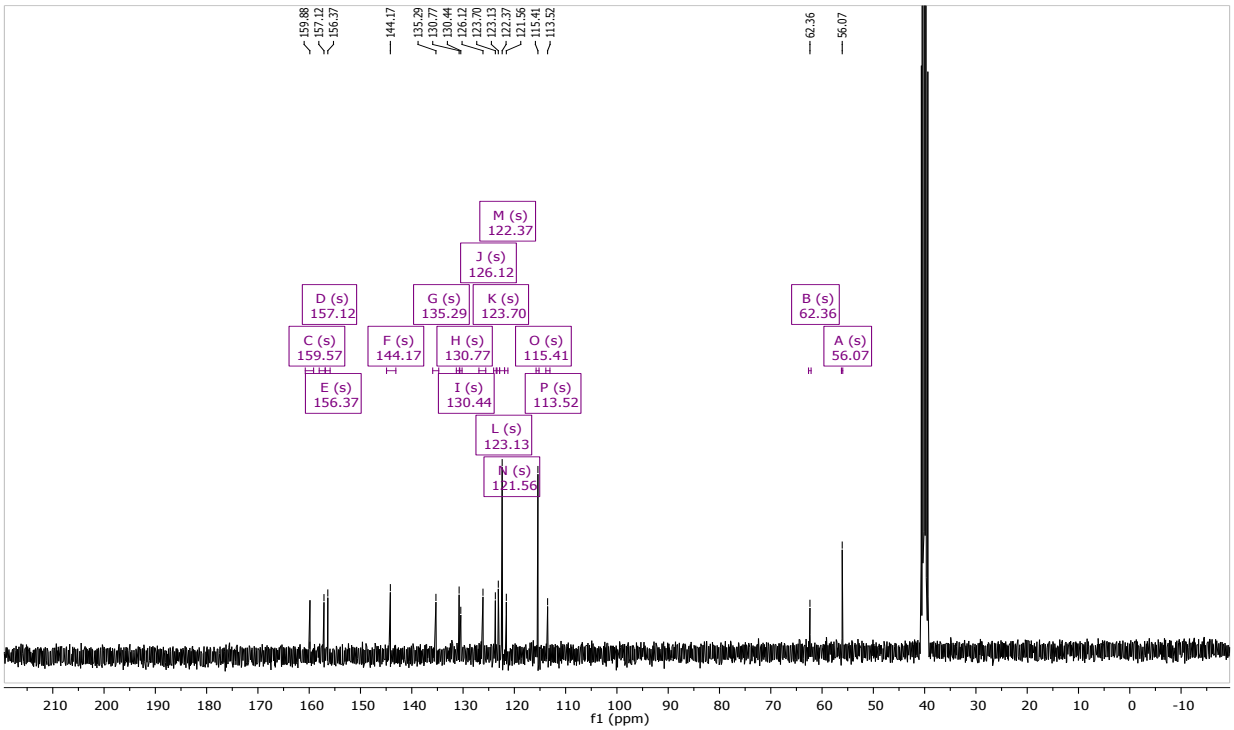
^{13}C-NMR (**5e**)



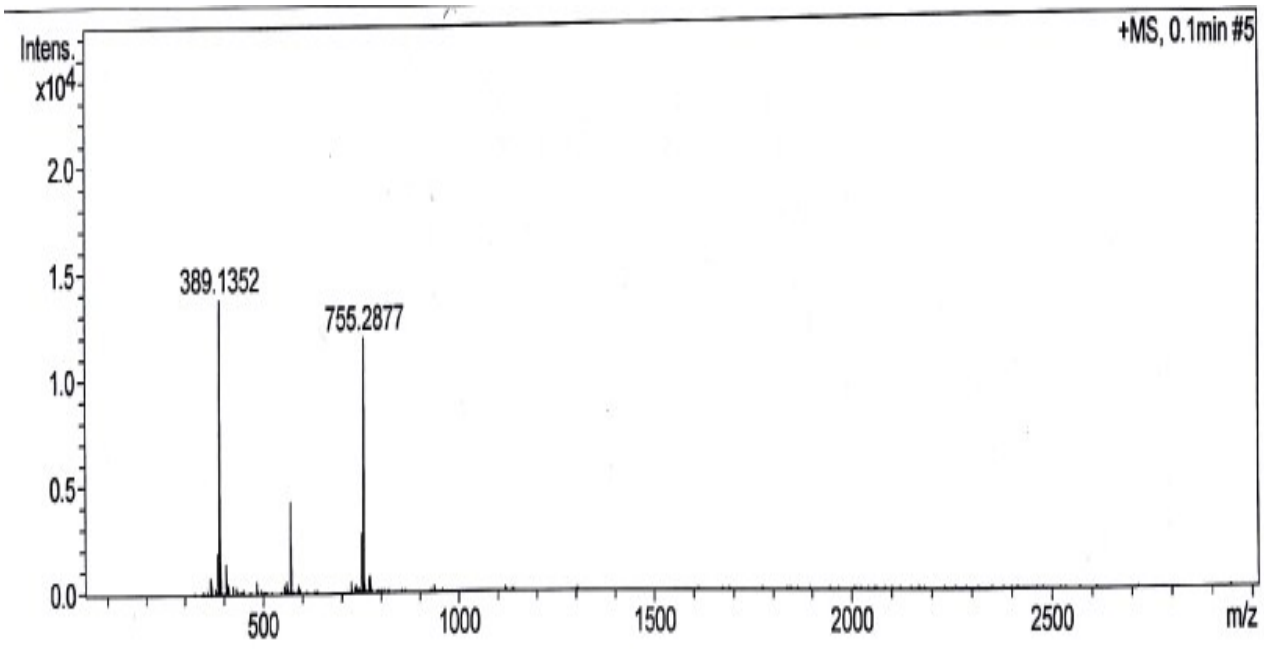
HRMS $[M+Na]^+$: m/z cal. for $C_{17}H_{15}N_7O_4Na$ 404.1078, found 404.1094.



^{1}H NMR (**5f**)

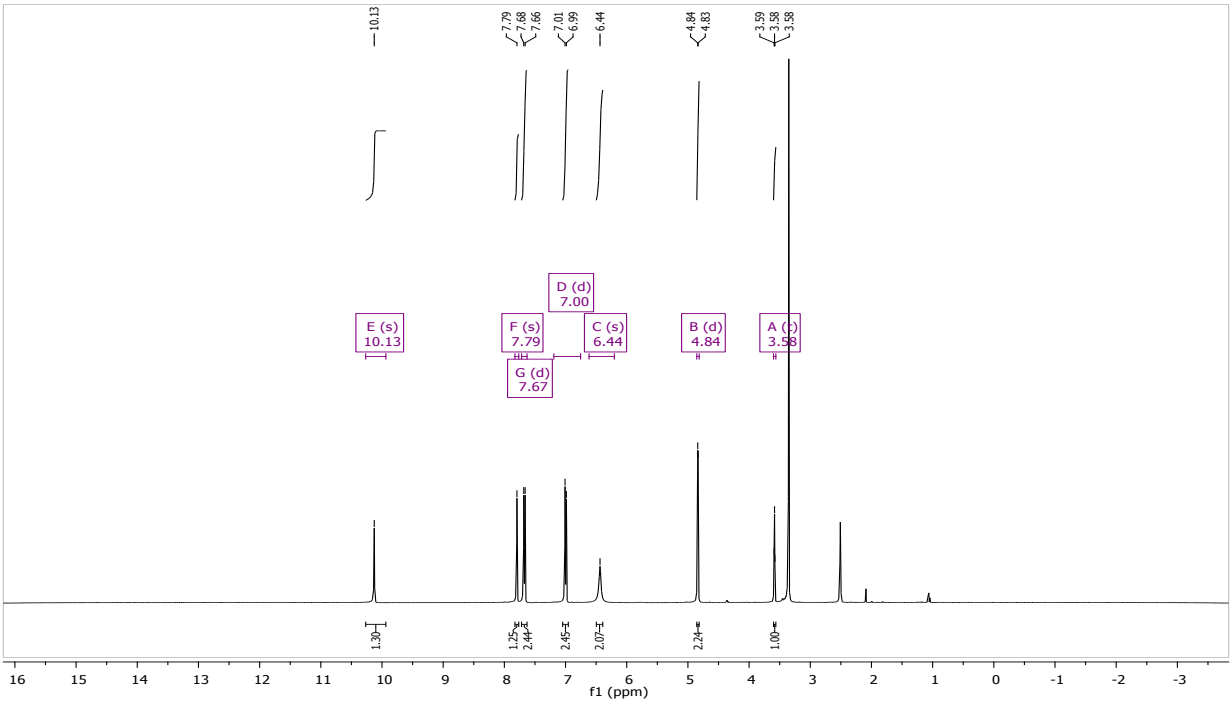


^{13}C-NMR (**5f**)

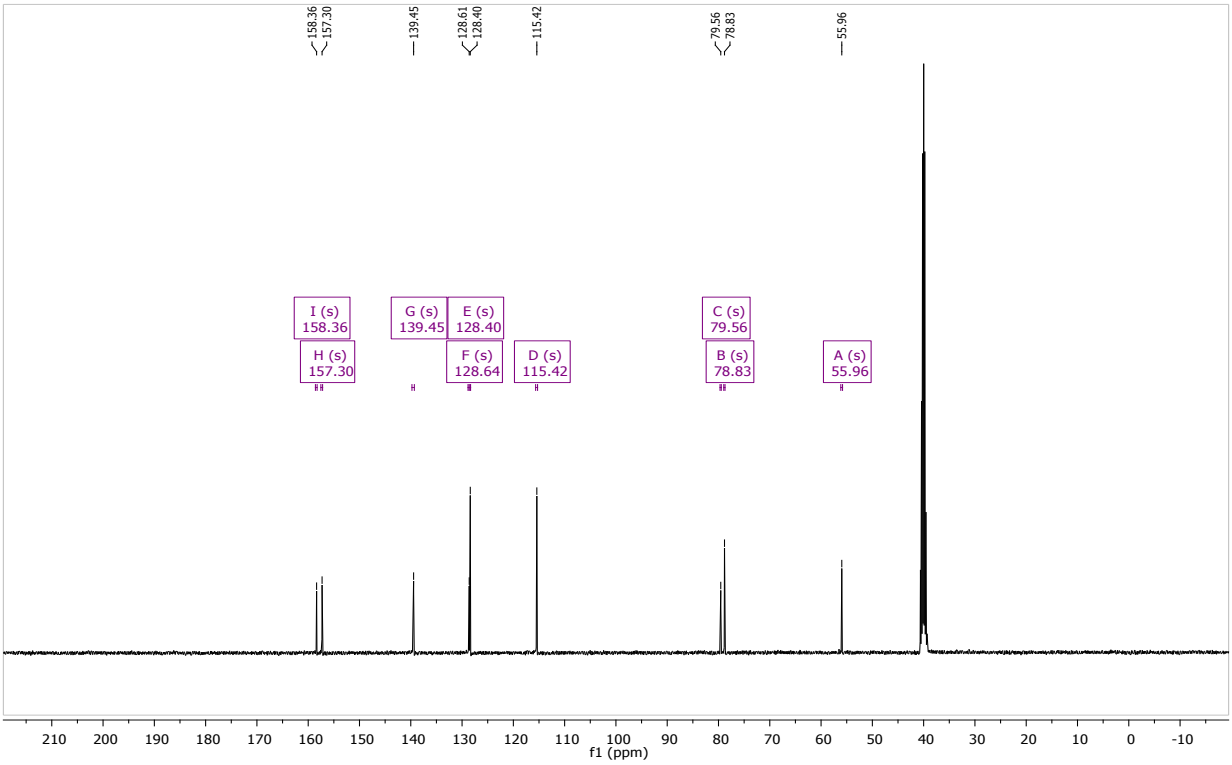


HRMS $[M+Na]^+$: m/z cal. for $C_{18}H_{18}N_6O_3Na$ 389.1333, found 389.1352.

Physical Data (^{1}H-NMR & ^{13}C-NMR spectra of **8**)

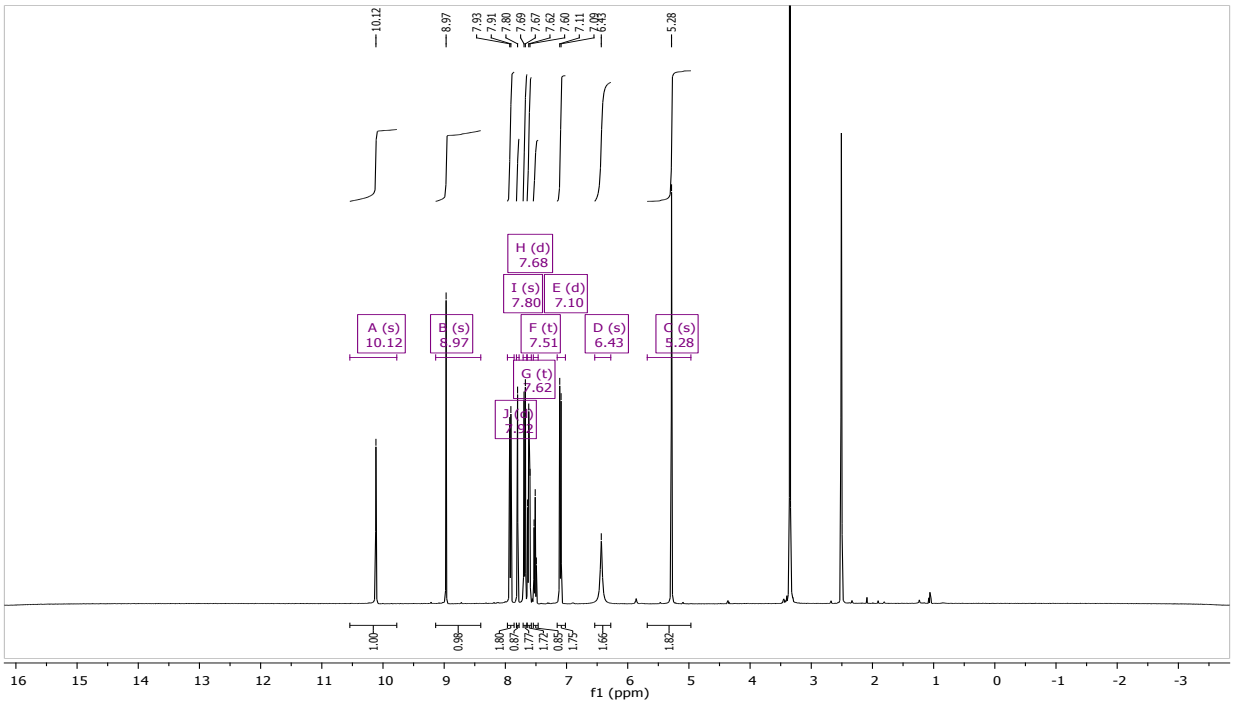


^{1}H-NMR (**8**)

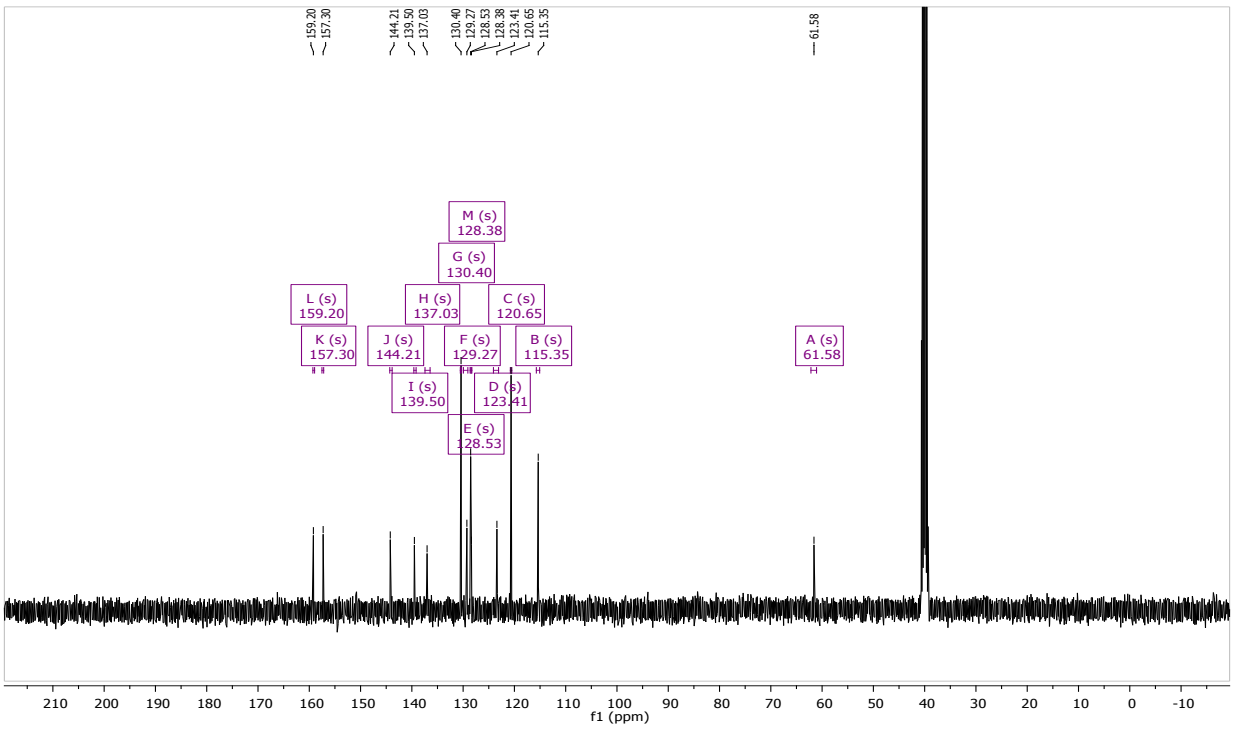


^{13}C-NMR (**8**)

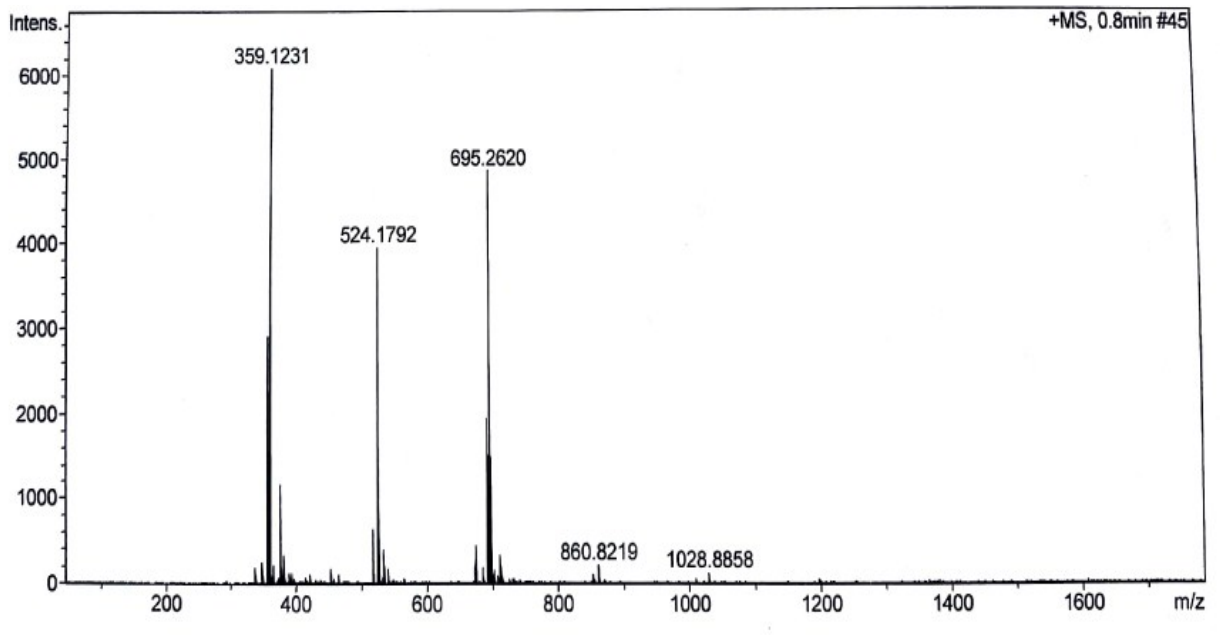
Physical Data (^{1}H-NMR, ^{13}C-NMR & HRMS spectra of **9a-f**)



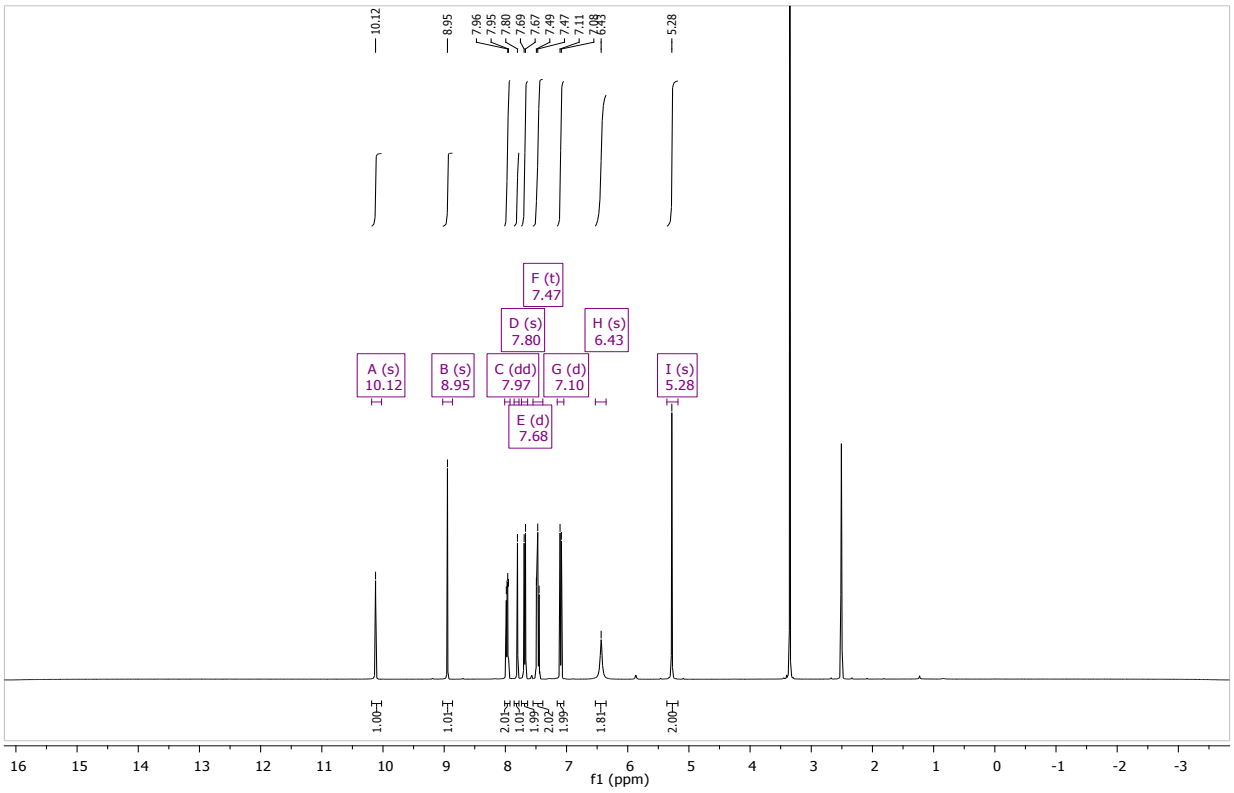
^{1}H-NMR (**9a**)



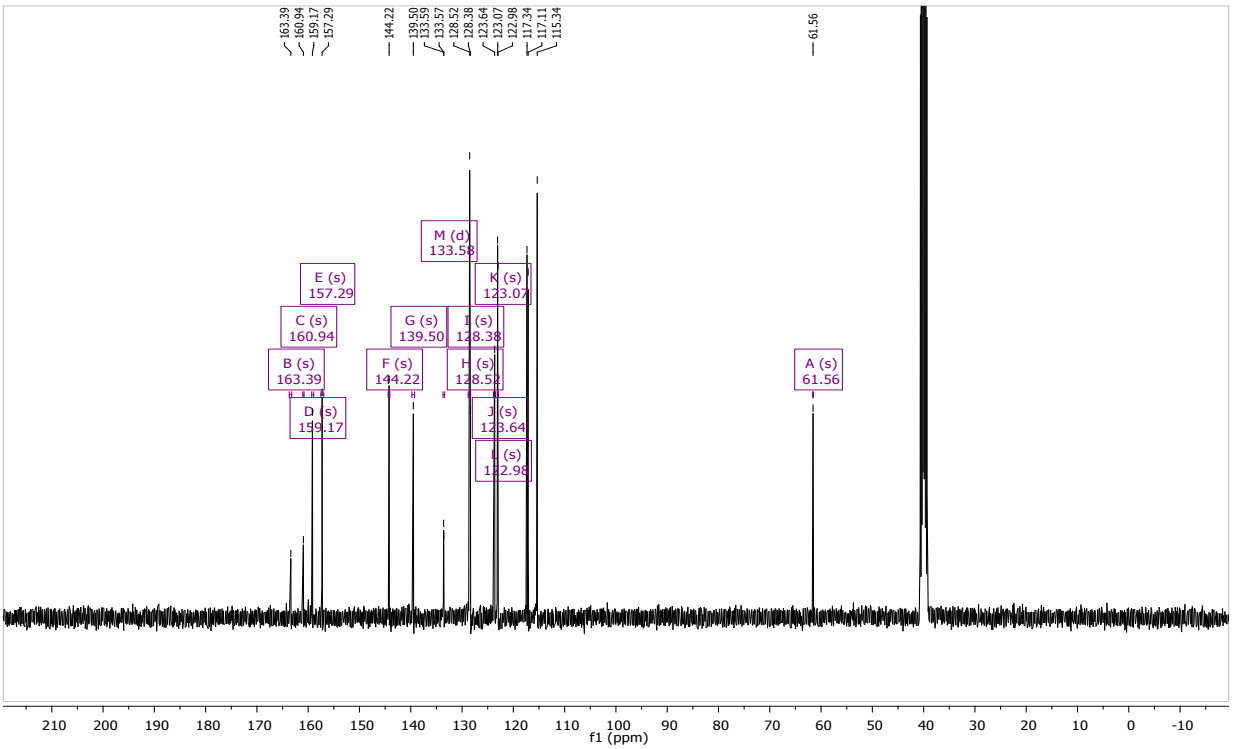
^{13}C-NMR (**9a**)



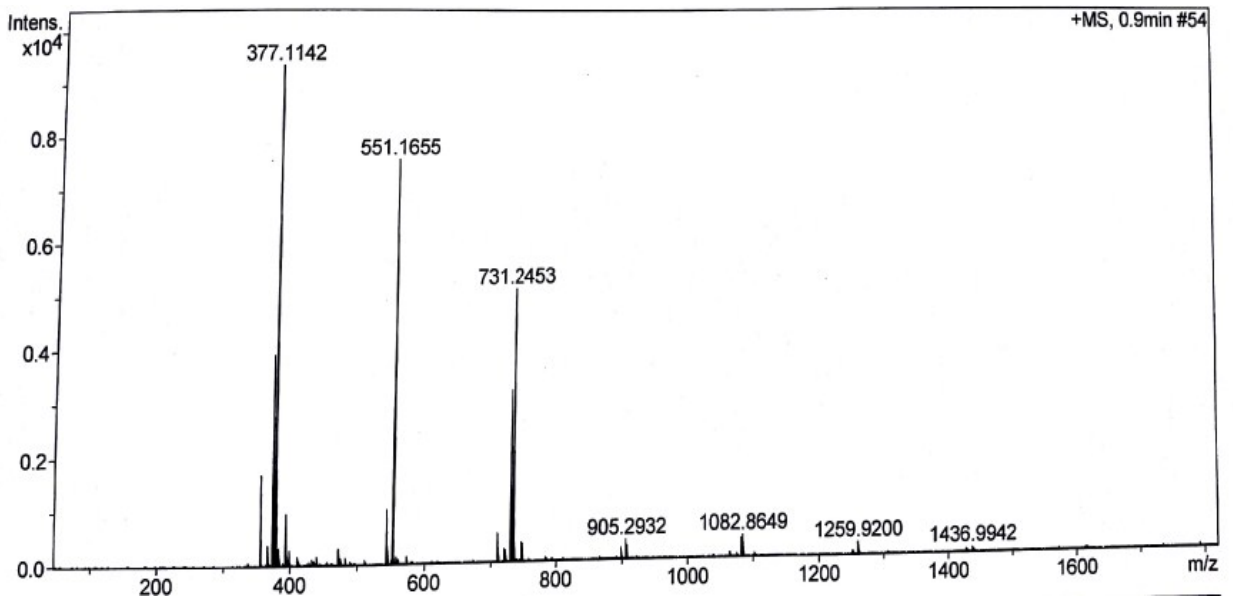
HRMS [M+Na]+: m/z cal. for $C_{17}H_{16}N_6O_2Na$ 359.1227, found 359.1231.



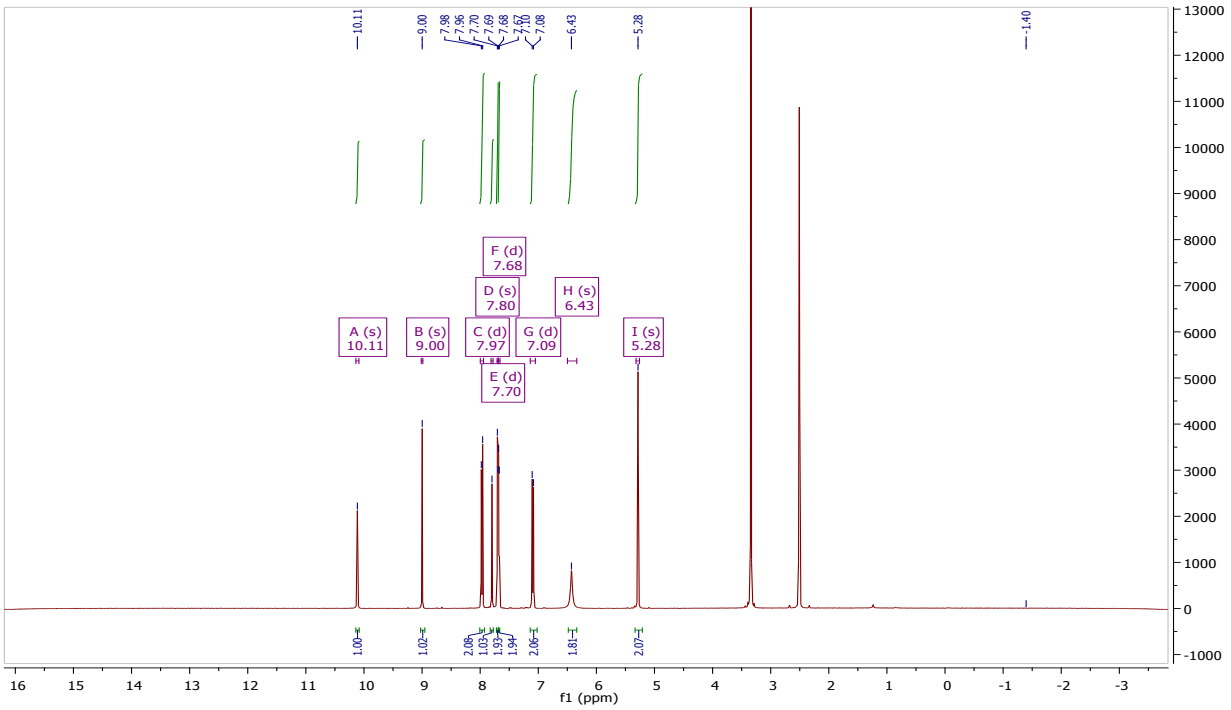
^{1}H NMR (**9b**)



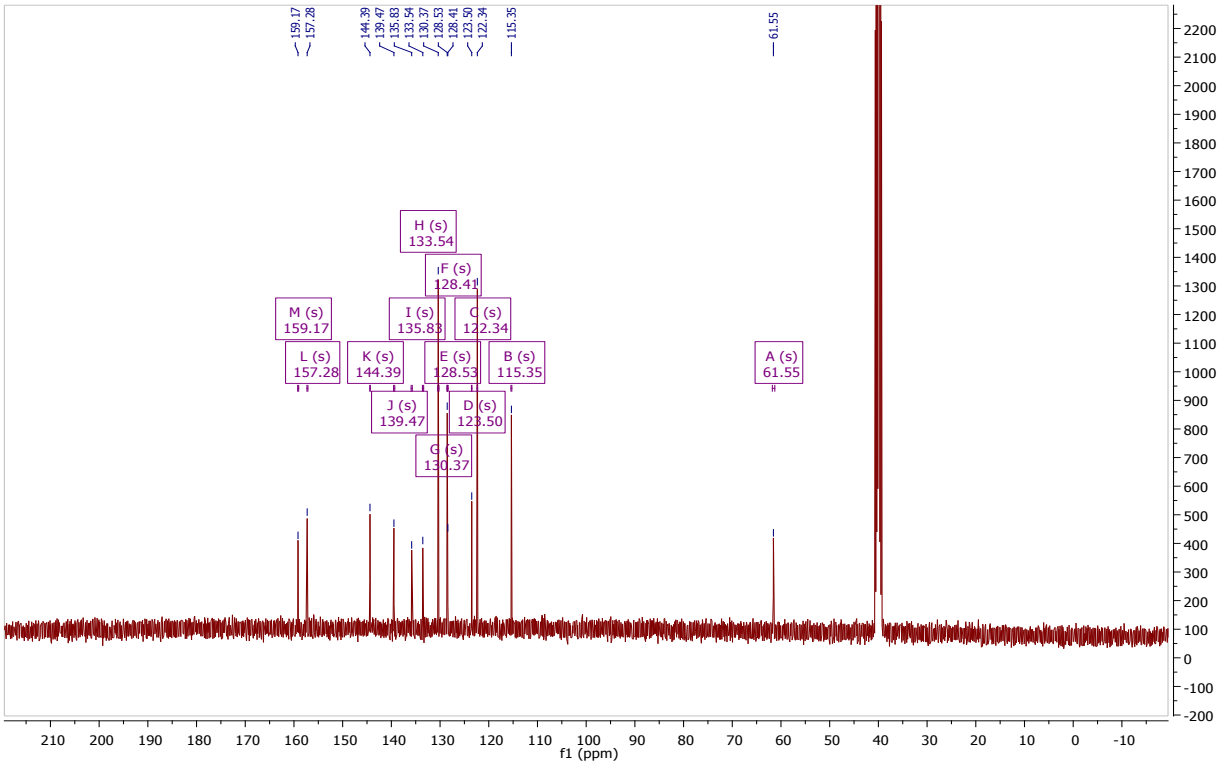
^{13}C-NMR (**9b**)



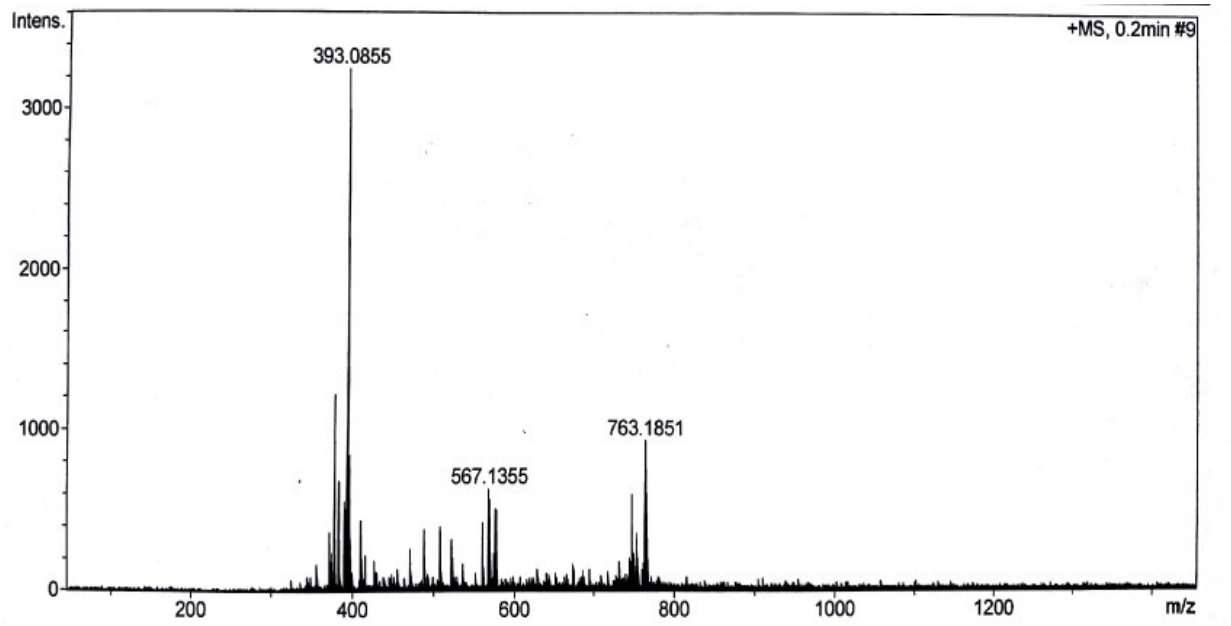
HRMS [M+Na]+: m/z cal. for $C_{17}H_{15}N_6O_2FNa$ 377.1133, found 377.1142.



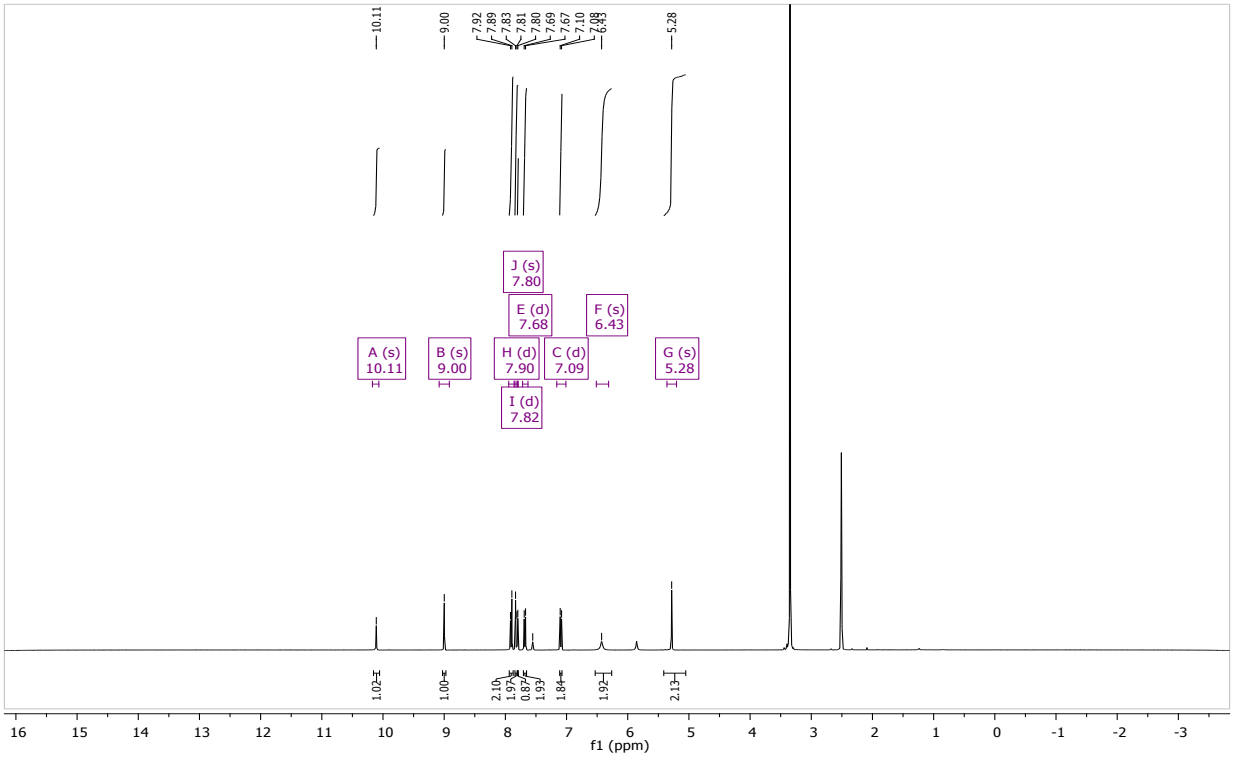
^{1}H-NMR (**9c**)



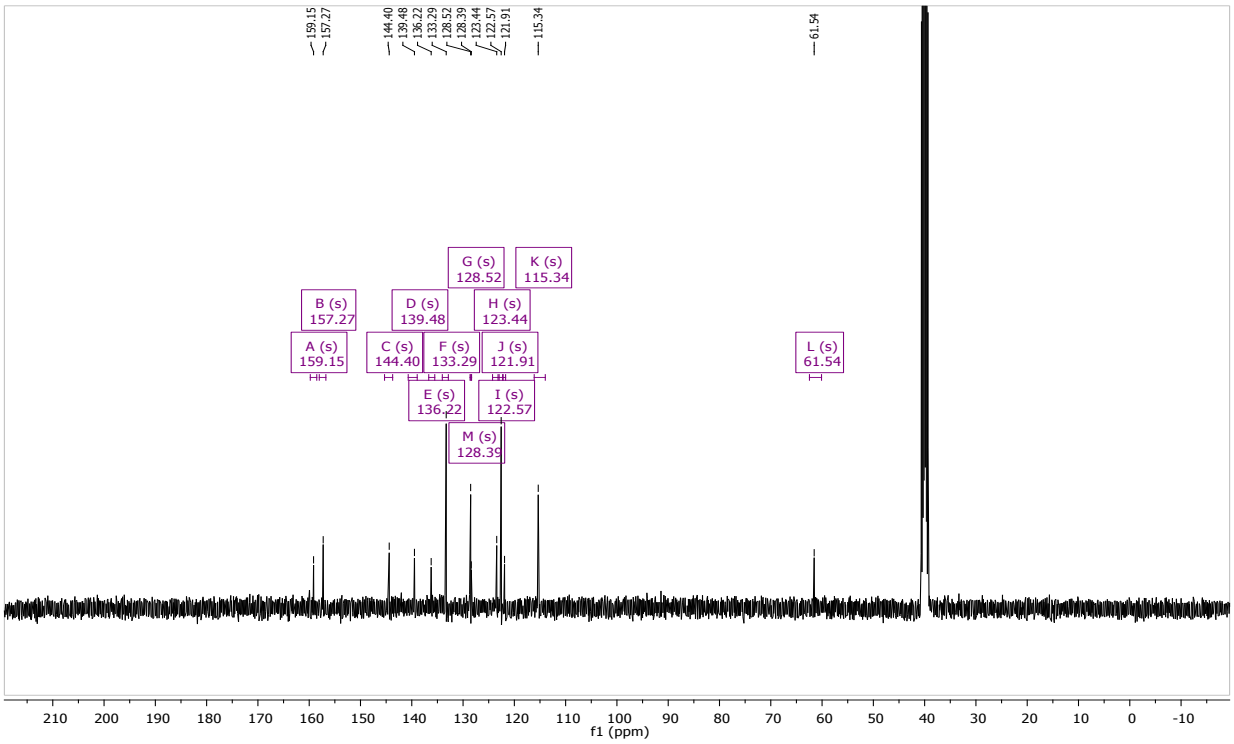
^{13}C-NMR (**9c**)



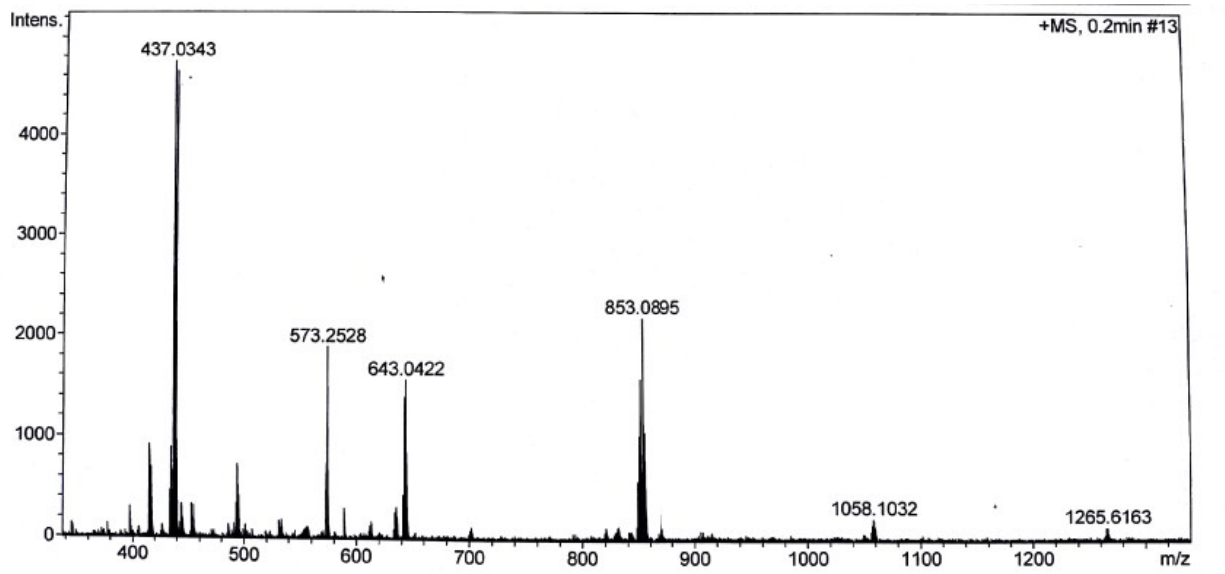
HRMS $[M+Na]^+$: m/z cal. for $C_{17}H_{15}N_6O_2FNa$ 393.0837, found 393.0855.



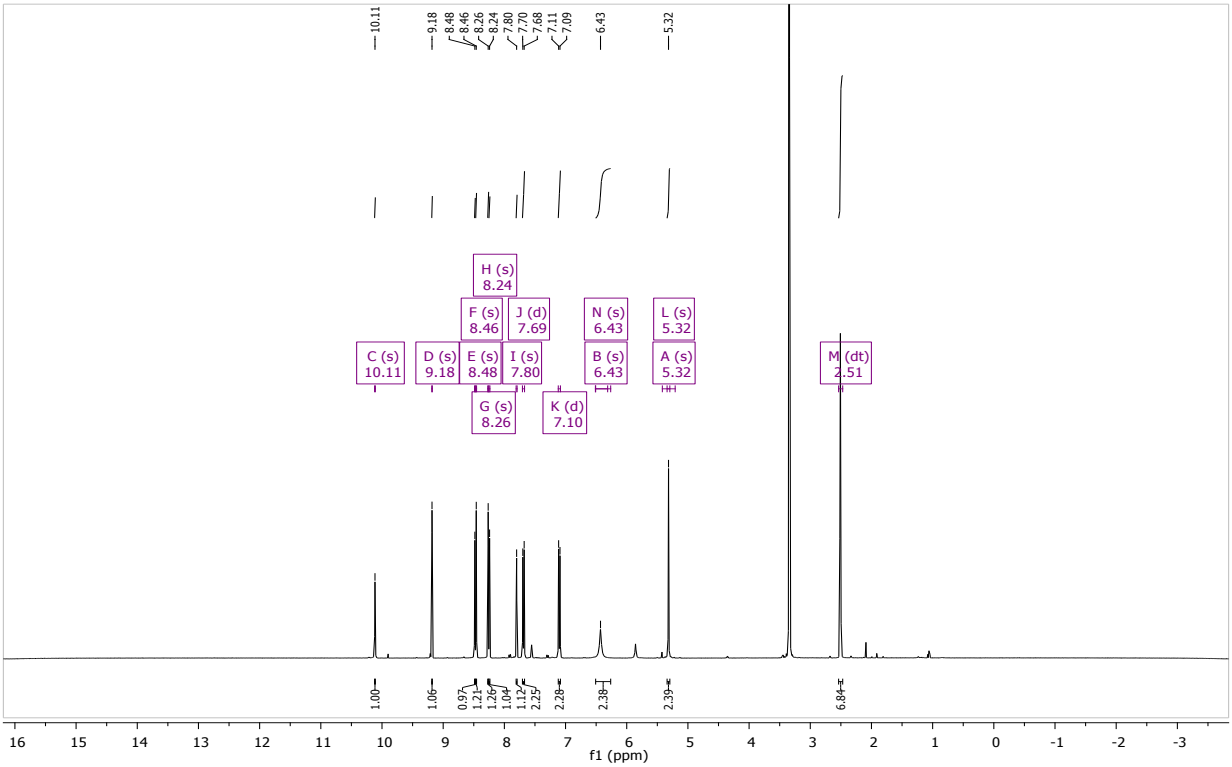
^{1}H-NMR (**9d**)



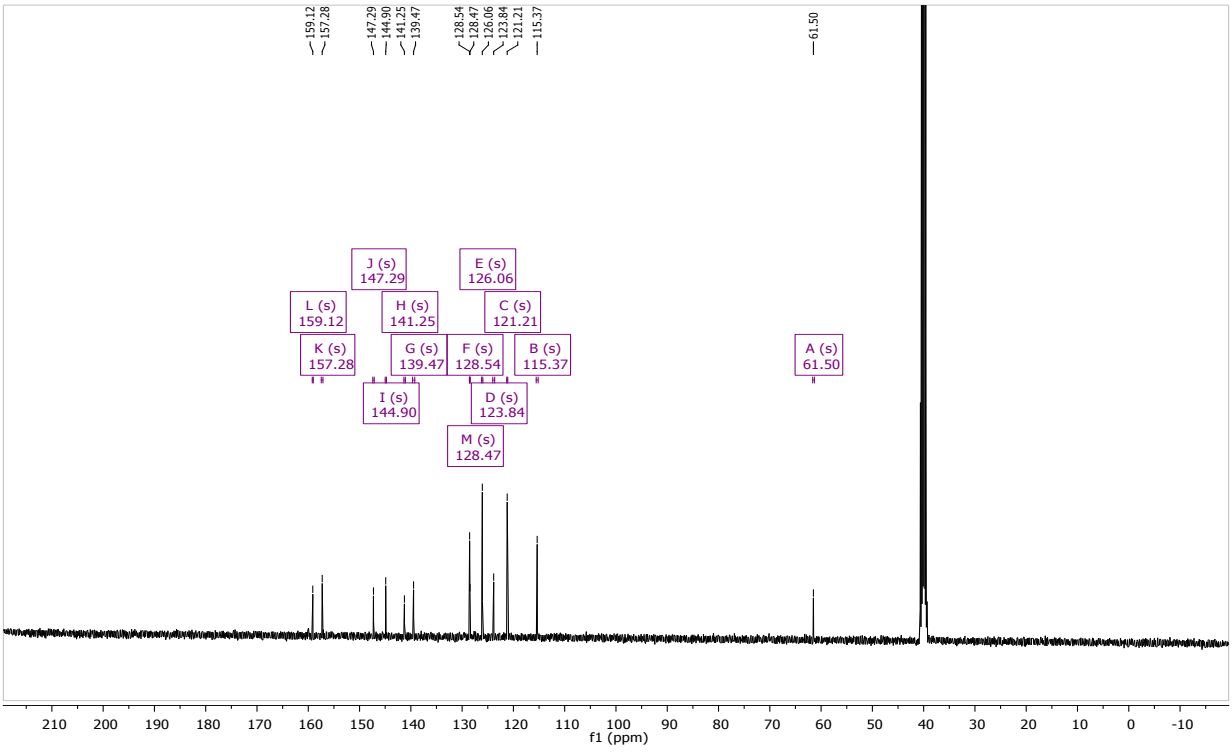
^{13}C-NMR (**9d**)



HRMS $[M+Na]^+$: m/z cal. for $C_{17}H_{15}N_6O_2FNa$ 437.0332, found 437.0343.

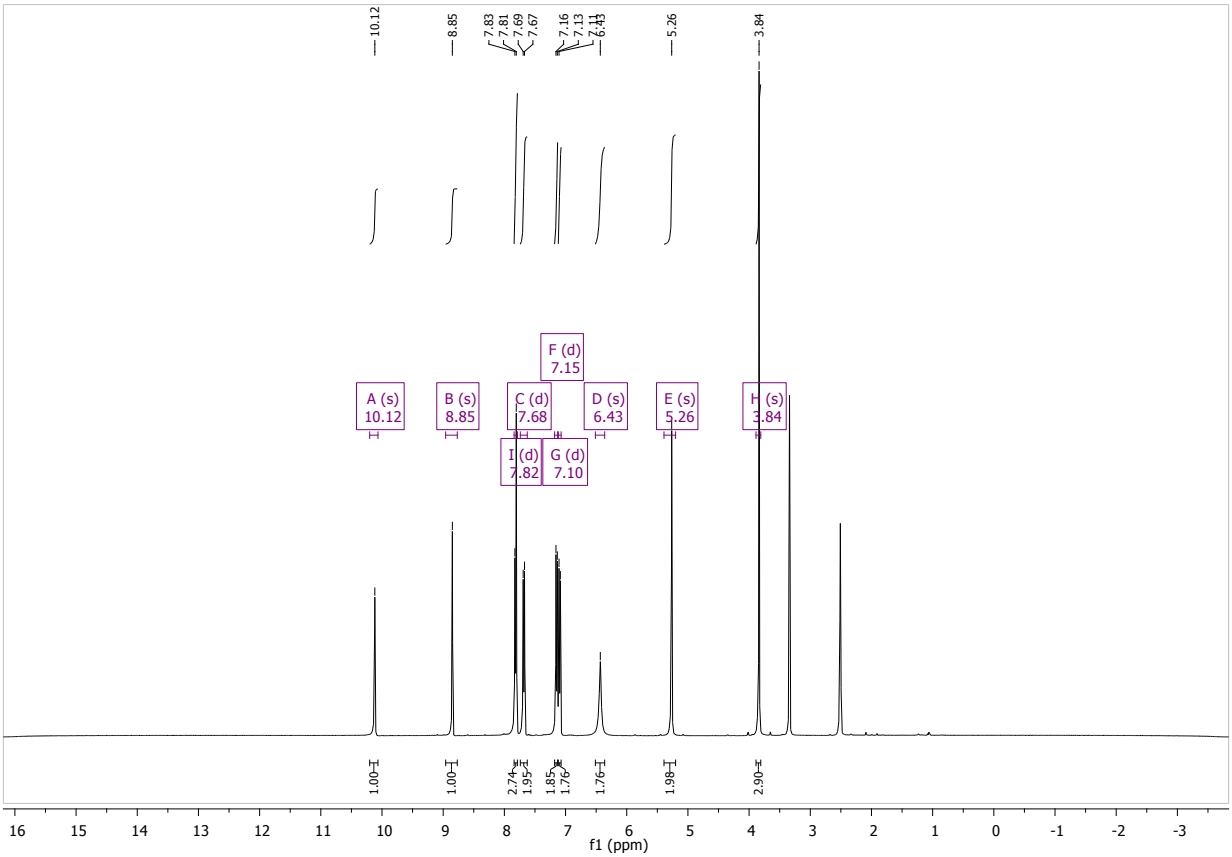


^{1}H-NMR (**9e**)

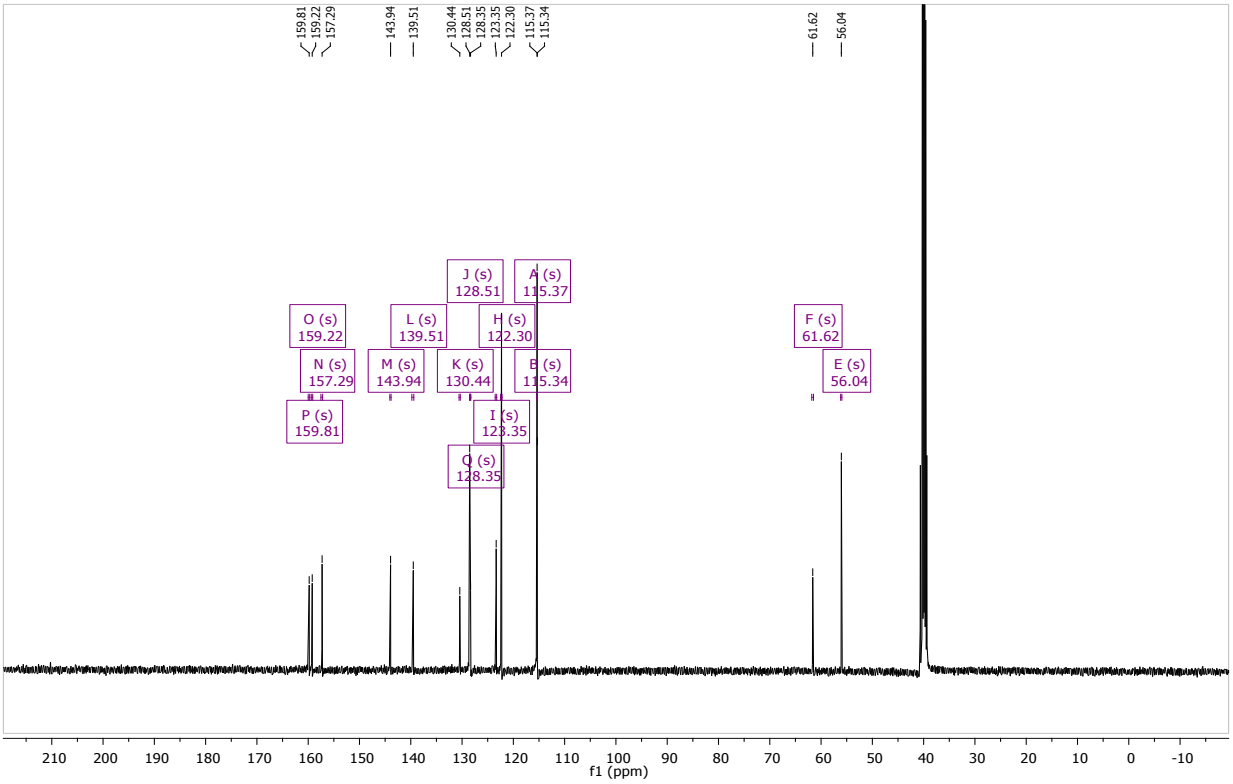


^{13}C-NMR (**9e**)

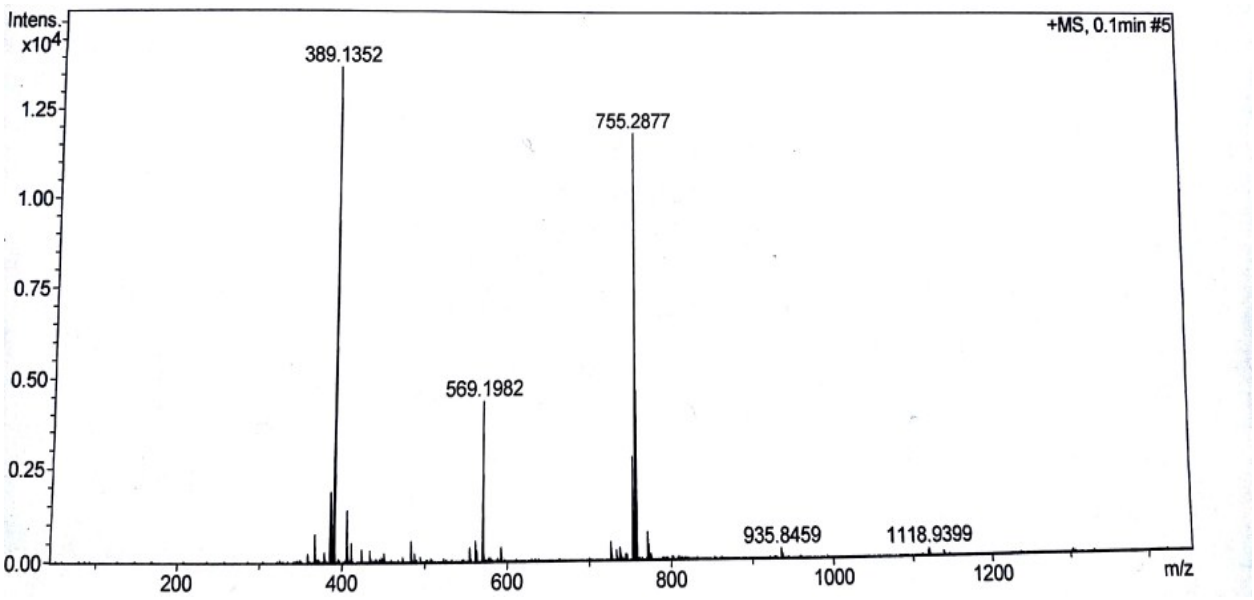
HRMS $[M+Na]^+$: m/z cal. for $C_{17}H_{15}N_7O_4Na$ 404.1078, found 404.1094.



^{1}H-NMR (**9f**)



^{13}C-NMR (**9f**)



HRMS $[M+Na]^+$: m/z cal. for $C_{18}H_{18}N_6O_3Na$ 389.1333, found 389.1352.

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