

Supporting Informations

Design, simple and efficient synthesis of bio active novel pyrazolyl-isoxazoline hybrids

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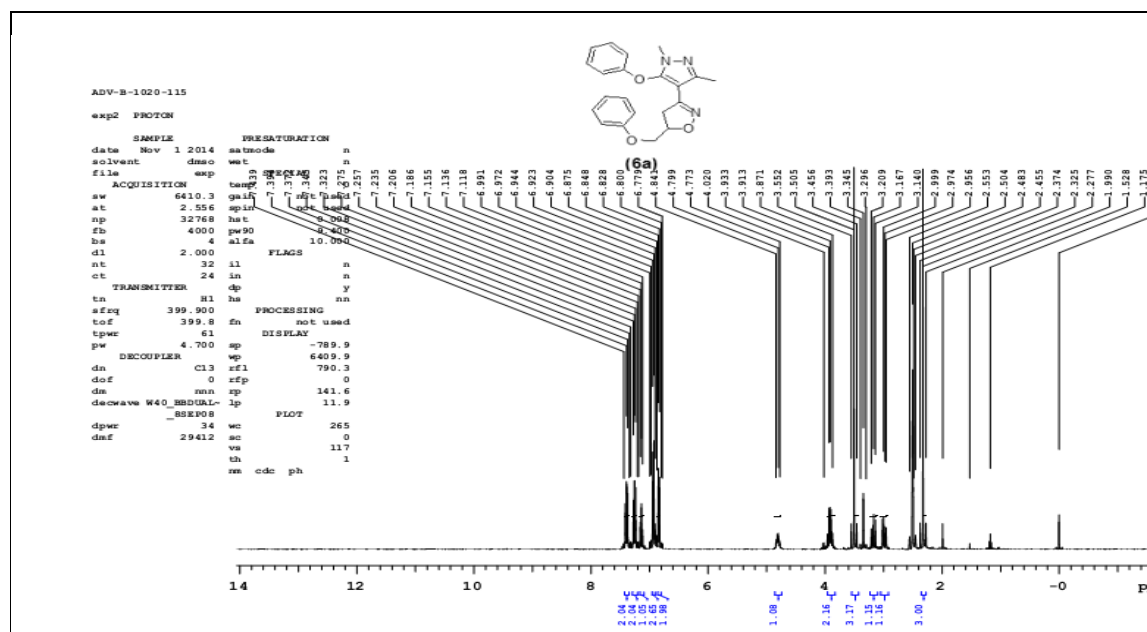


Fig. S1. ^1H NMR (300 MHz, $\text{DMSO-}d_6$): 3-(1,3-dimethyl-5-phenoxy-1H-pyrazol-4-yl)-5-(phoxymethyl)-4,5-dihydroisoxazole (6a)

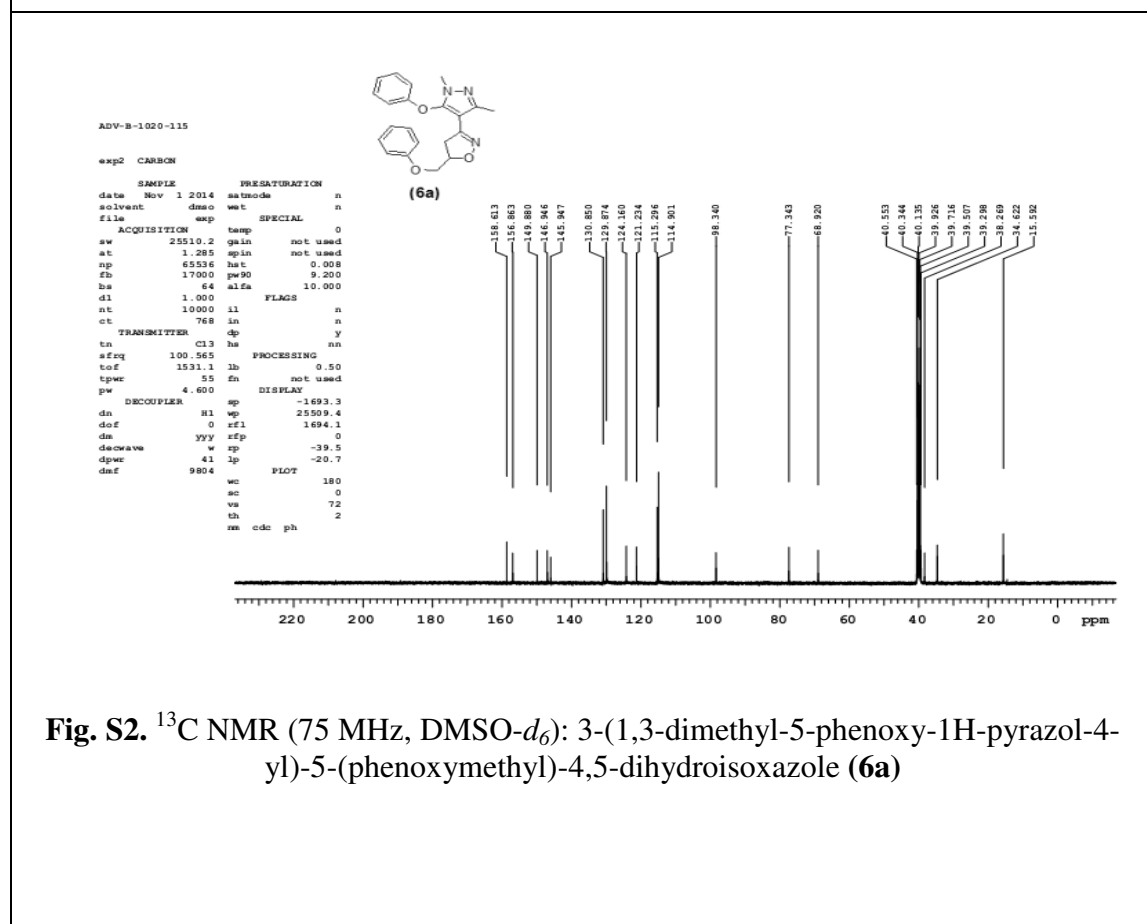


Fig. S2. ^{13}C NMR (75 MHz, $\text{DMSO-}d_6$): 3-(1,3-dimethyl-5-phenoxy-1H-pyrazol-4-yl)-5-(phoxymethyl)-4,5-dihydroisoxazole (6a)

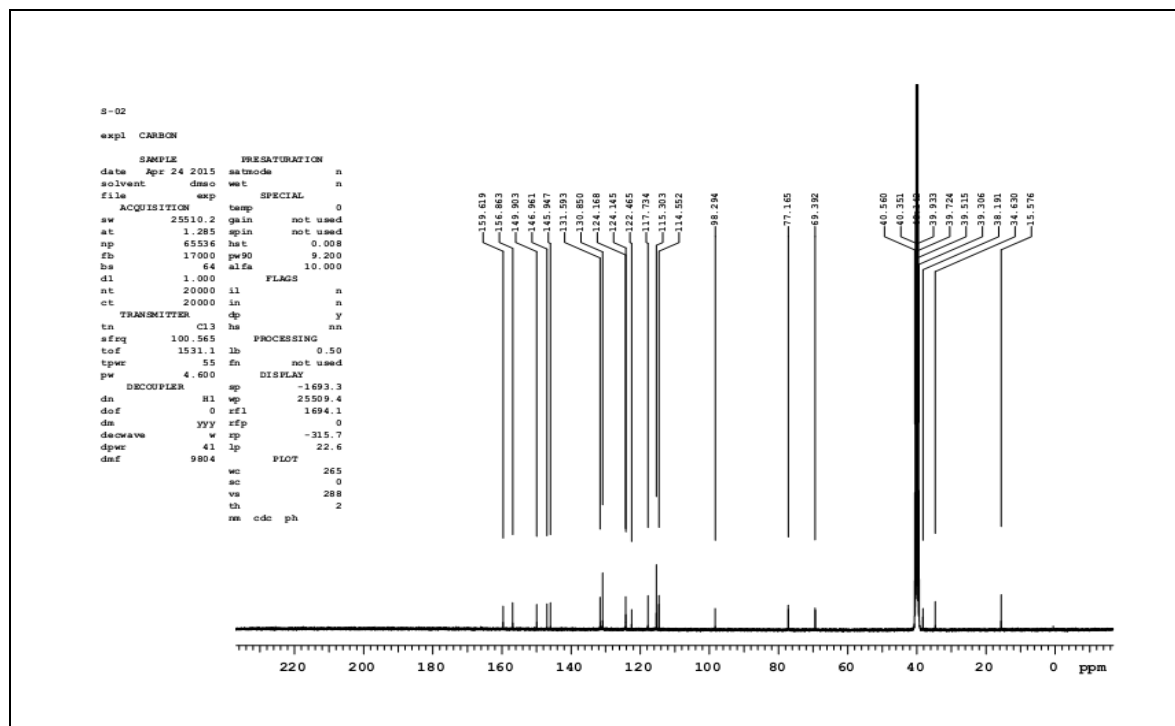


Fig. S5. ^{13}C NMR (75 MHz, DMSO- d_6): 5-((3-bromophenoxy)methyl)-3-(1,3-dimethyl-5-phenoxy-1H-pyrazol-4-yl)-4,5-dihydro isoxazole (**6b**)

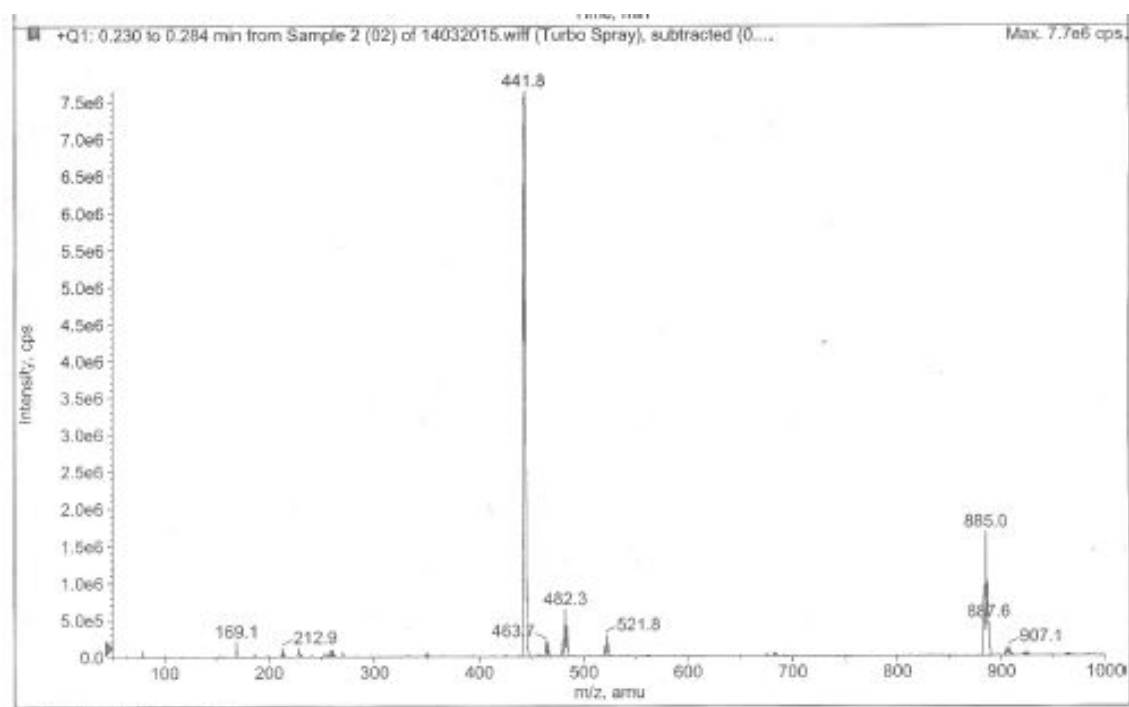


Fig. S6. ESI-MS spectra of the compound **6b**

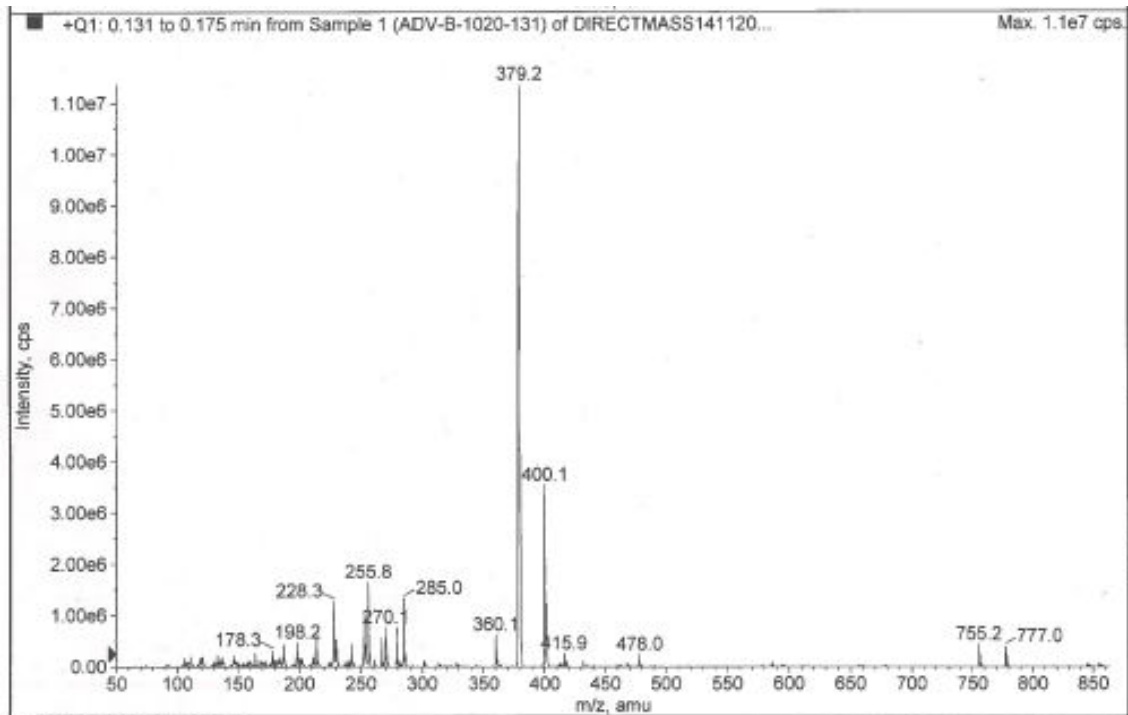


Fig. S9. ESI-MS spectra of the compound **6c**

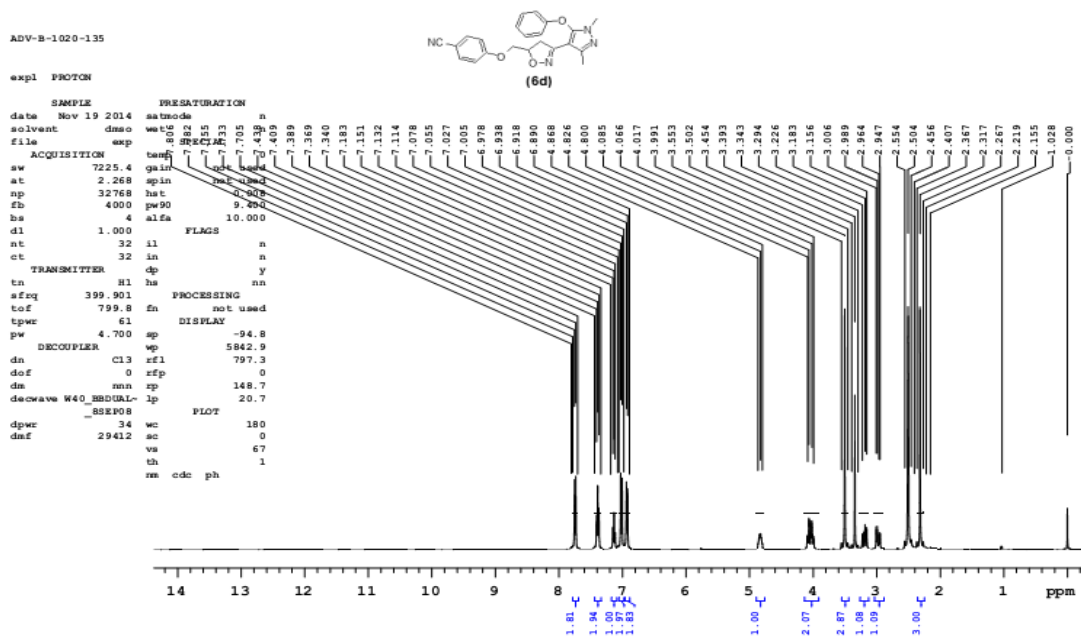


Fig. S10. ^1H NMR (300 MHz, $\text{DMSO-}d_6$): 4-((3-(1,3-dimethyl-5-phenoxy-1H-pyrazol-4-yl)-4,5-dihydroisoxazol-5-yl)methoxy) benzonitrile (**6d**)

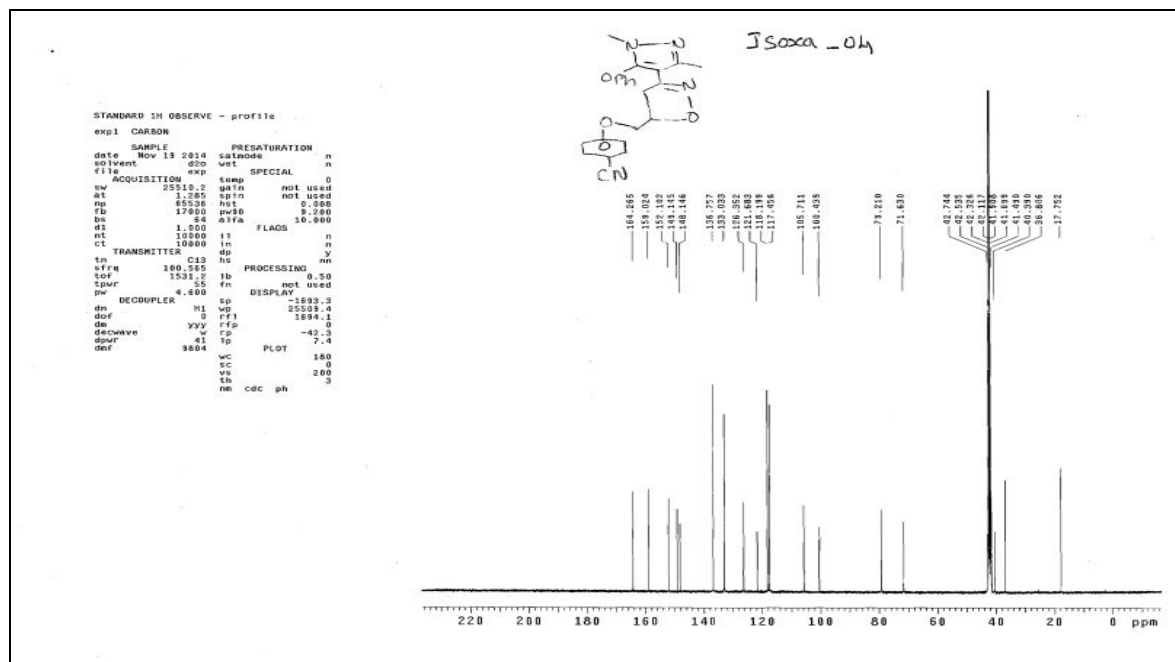


Fig. S11. ^{13}C NMR (75 MHz, $\text{DMSO-}d_6$): 4-((3-(1,3-dimethyl-5-phenoxy-1H-pyrazol-4-yl)-4,5-dihydroisoxazol-5-yl)methoxy) benzonitrile (**6d**)

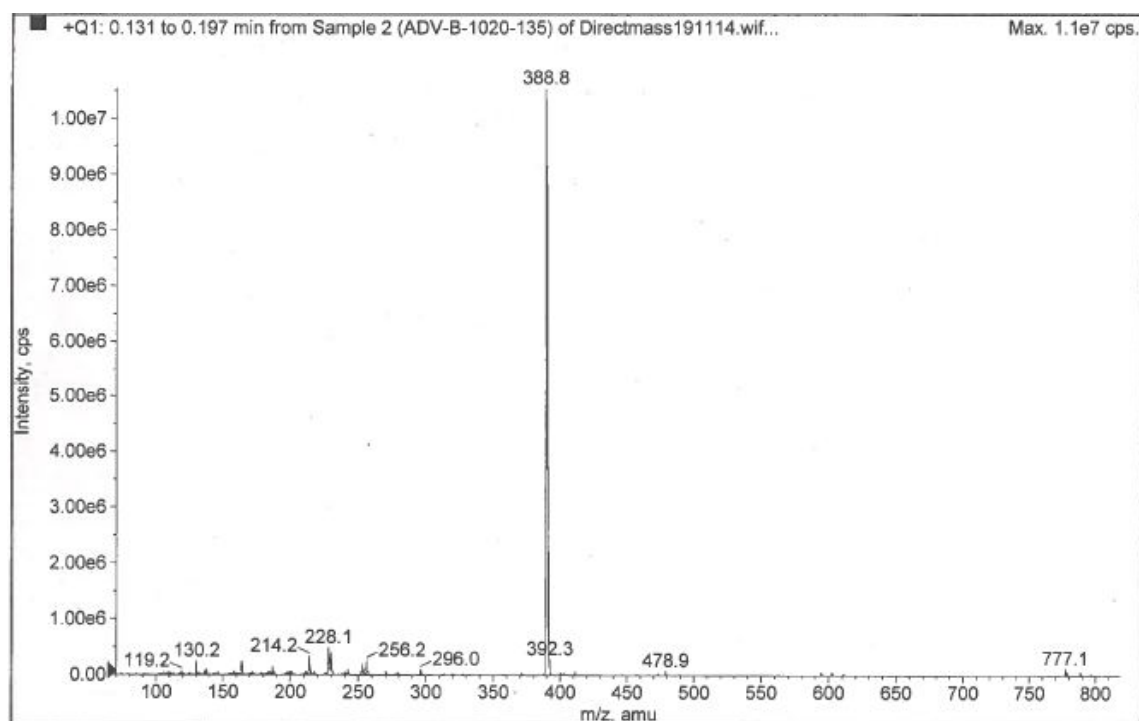


Fig. S12. ESI-MS spectra of the compound **6d**

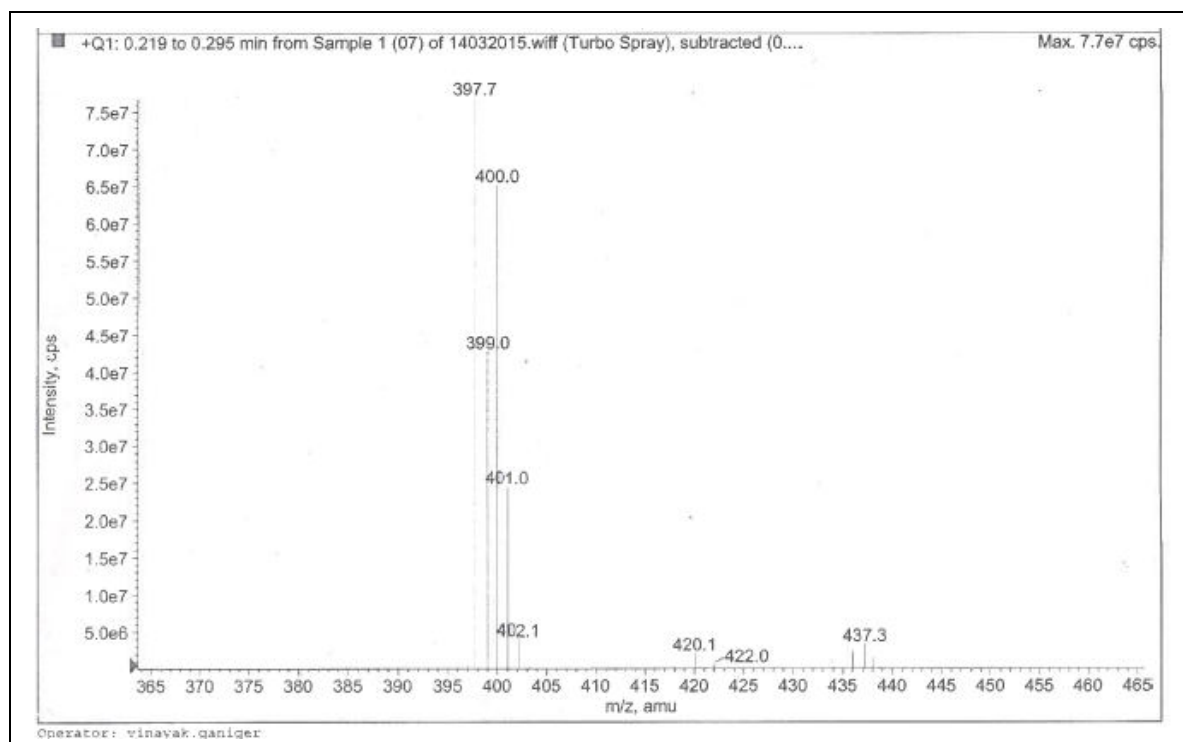


Fig. S15. ESI-MS spectra of the compound **6e**

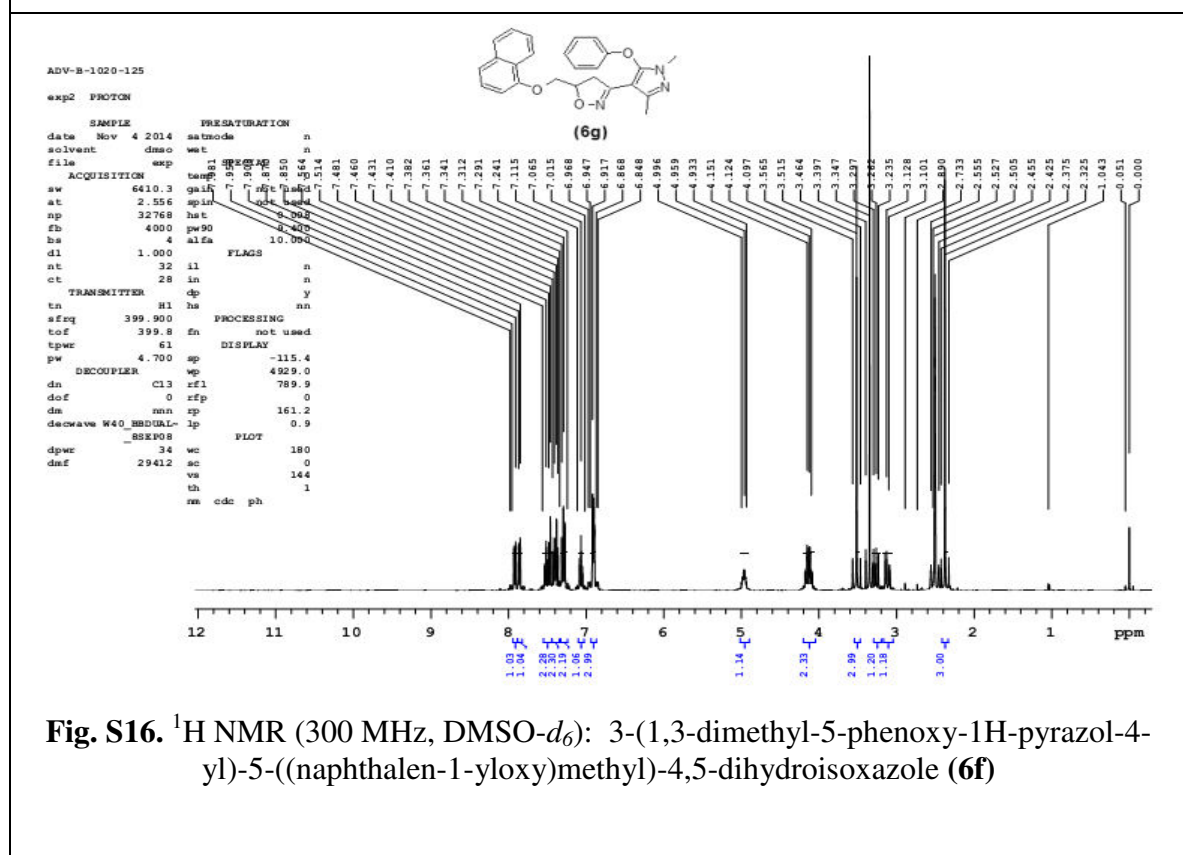


Fig. S16. ^1H NMR (300 MHz, $\text{DMSO-}d_6$): 3-(1,3-dimethyl-5-phenoxy-1H-pyrazol-4-yl)-5-((naphthalen-1-yloxy)methyl)-4,5-dihydroisoxazole (**6f**)

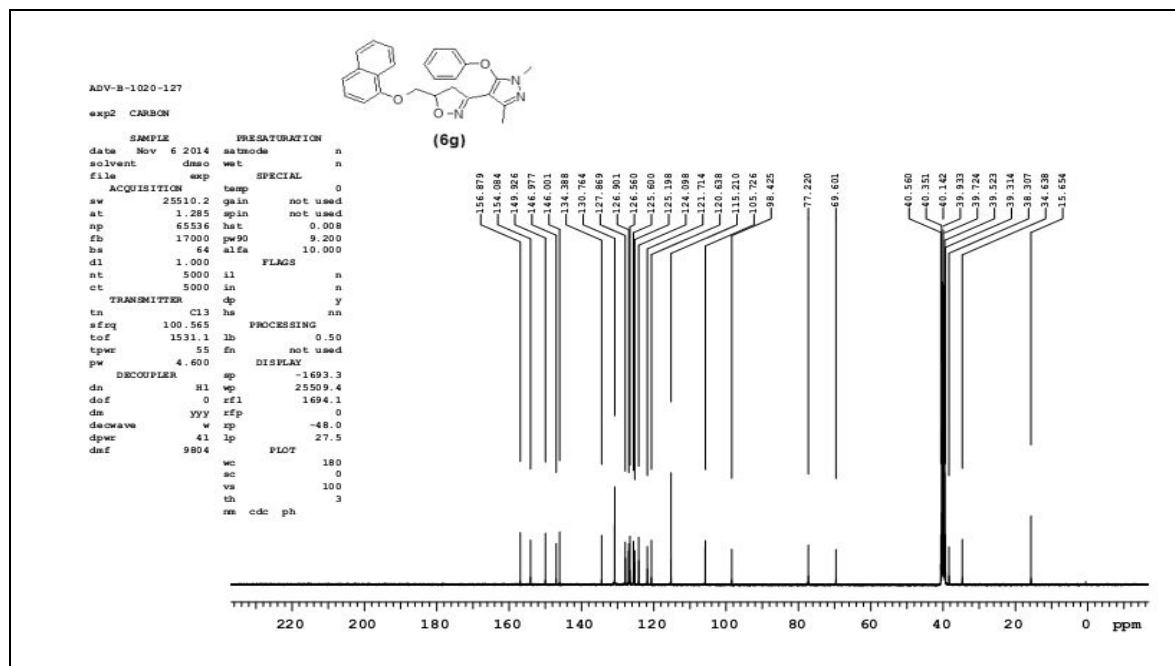


Fig. S17. ^{13}C NMR (75 MHz, $\text{DMSO-}d_6$): 3-(1,3-dimethyl-5-phenoxy-1H-pyrazol-4-yl)-5-((naphthalen-1-yloxy)methyl)-4,5-dihydroisoxazole (**6f**)

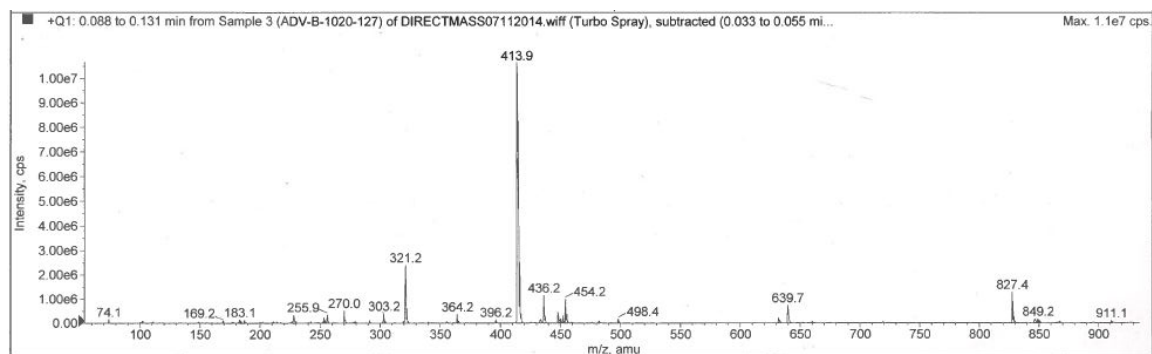


Fig. S18. ESI-MS spectra of the compound **6f**

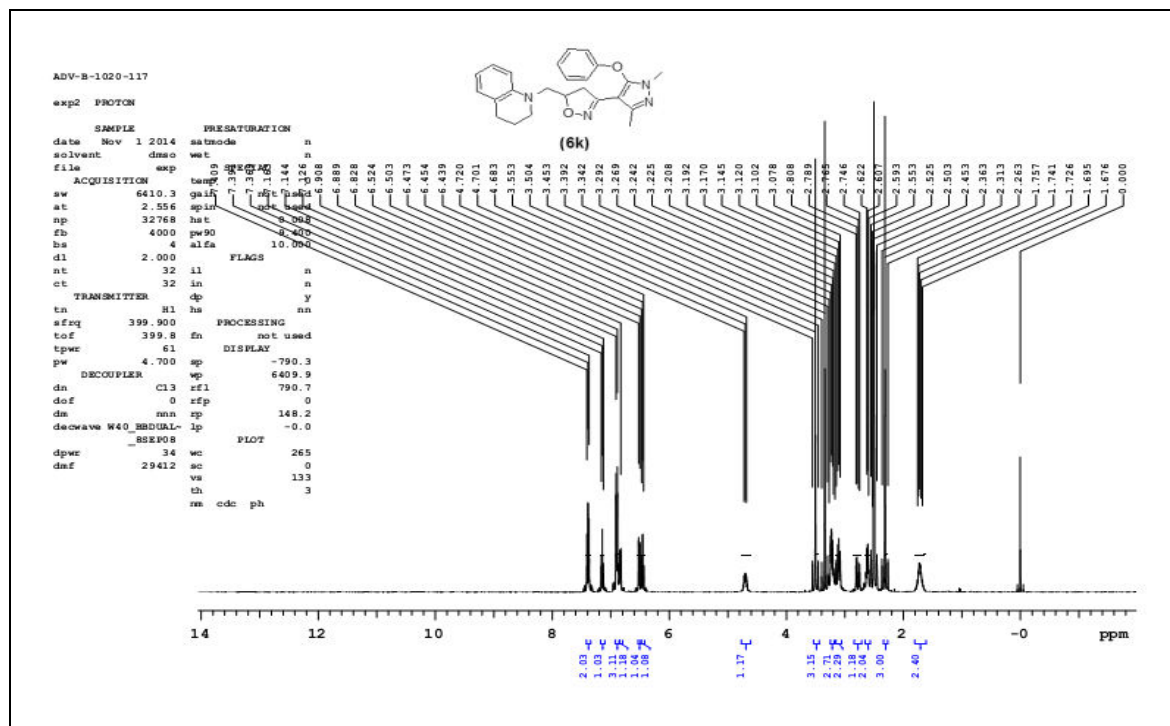


Fig. S19. ^1H NMR (300 MHz, $\text{DMSO-}d_6$): N-((3-(1,3-dimethyl-5-phenoxy-1H-pyrazol-4-yl)-4,5-dihydroisoxazol-5-yl)methyl)-1,4,4a,8a-tetrahydronaphthalen-1-amine (**6g**)

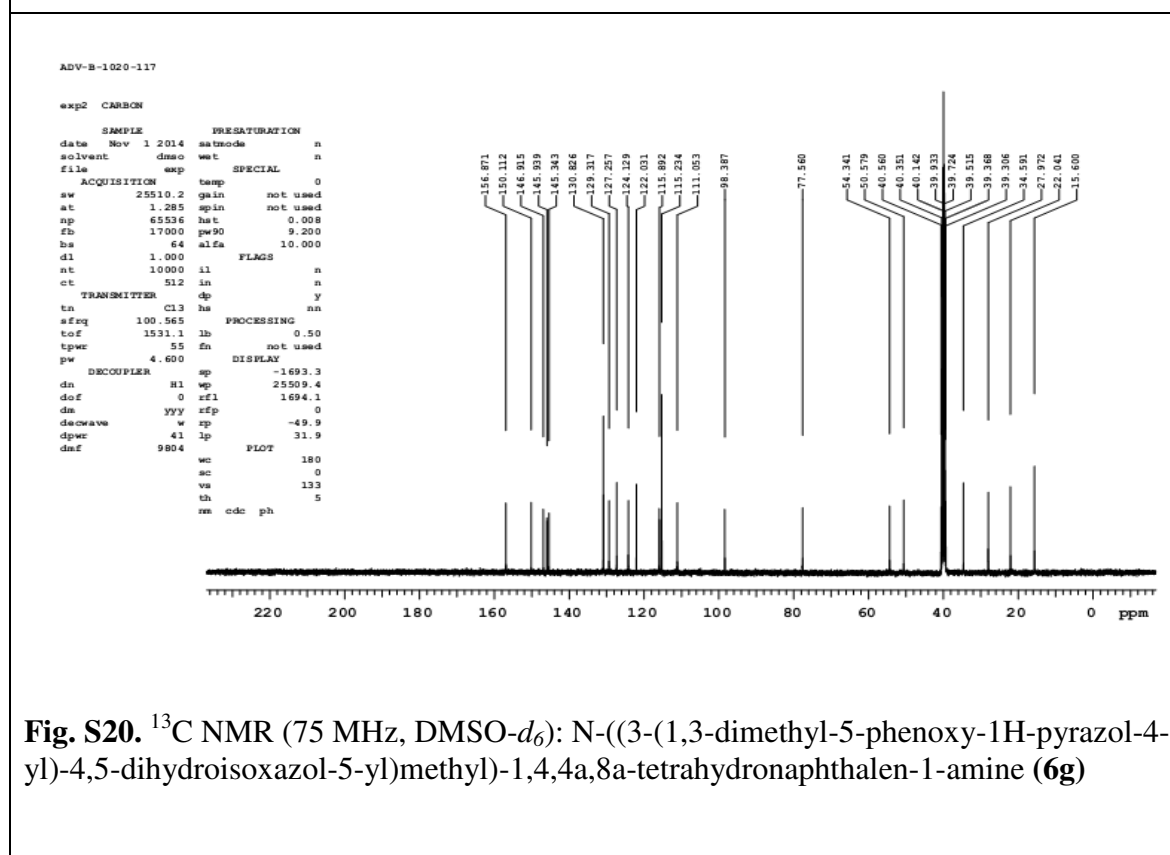


Fig. S20. ^{13}C NMR (75 MHz, $\text{DMSO-}d_6$): N-((3-(1,3-dimethyl-5-phenoxy-1H-pyrazol-4-yl)-4,5-dihydroisoxazol-5-yl)methyl)-1,4,4a,8a-tetrahydronaphthalen-1-amine (**6g**)

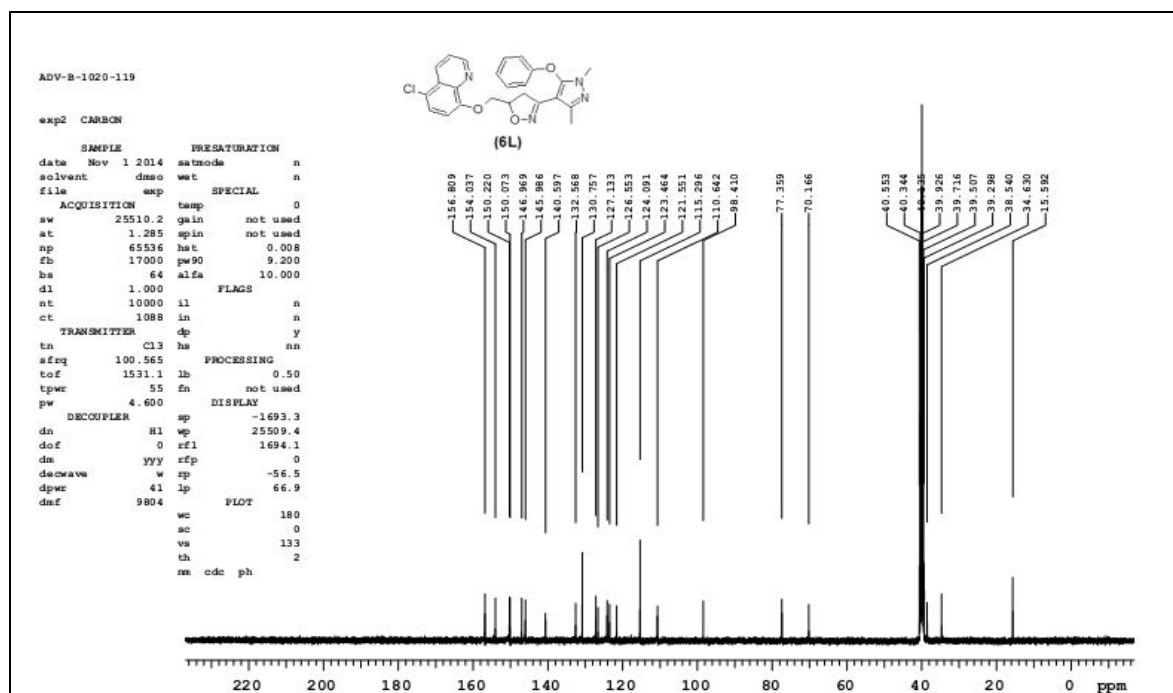


Fig. S23. ^{13}C NMR (75 MHz, $\text{DMSO-}d_6$): 5-(((5-chloroquinolin-8-yl)oxy)methyl)-3-(1,3-dimethyl-5-phenoxy-1H-pyrazol-4-yl)-4,5-dihydroisoxazole (**6h**)

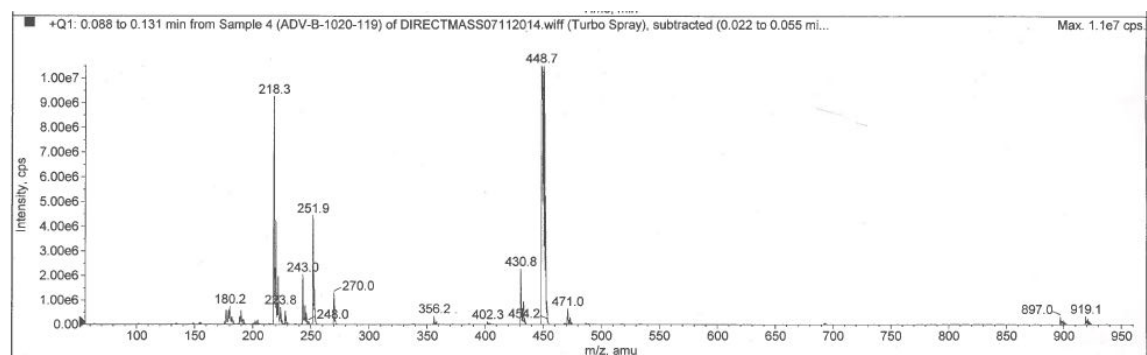


Fig. S24. ESI-MS spectra of the compound **6h**

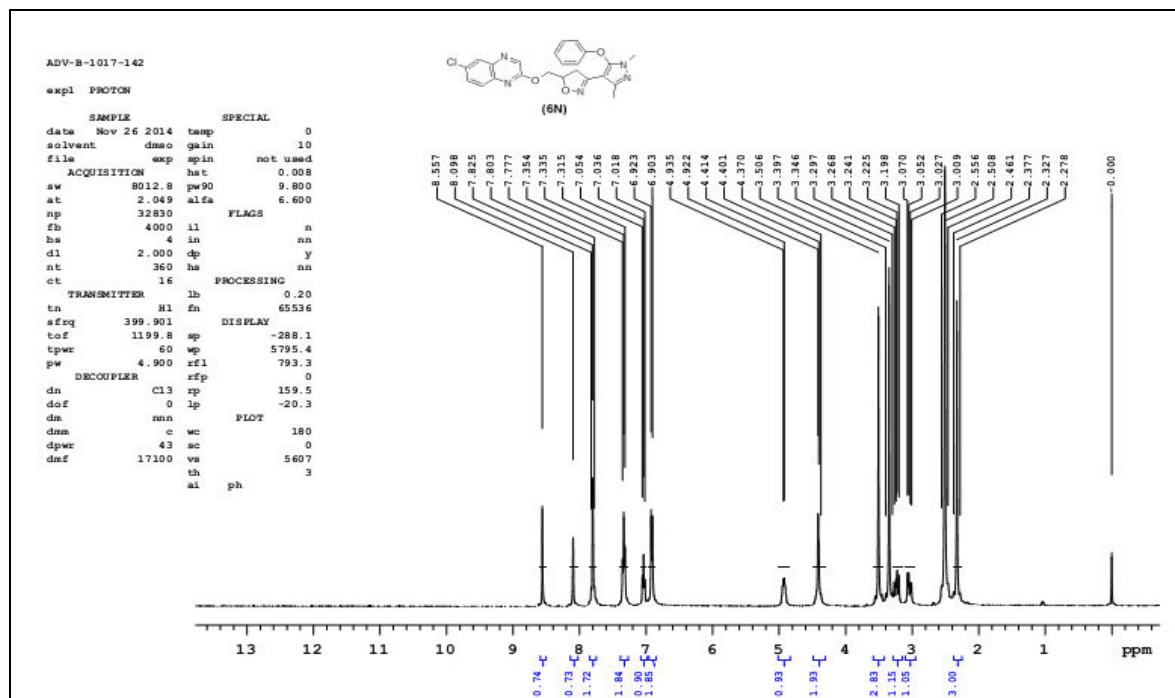


Fig. S25. ^1H NMR (300 MHz, $\text{DMSO-}d_6$): 5-(((6-chloroquinoxalin-2-yl)oxy)methyl)-3-(1,3-dimethyl-5-phenoxy-1H-pyrazol-4-yl)-4,5-dihydroisoxazole (**6i**)

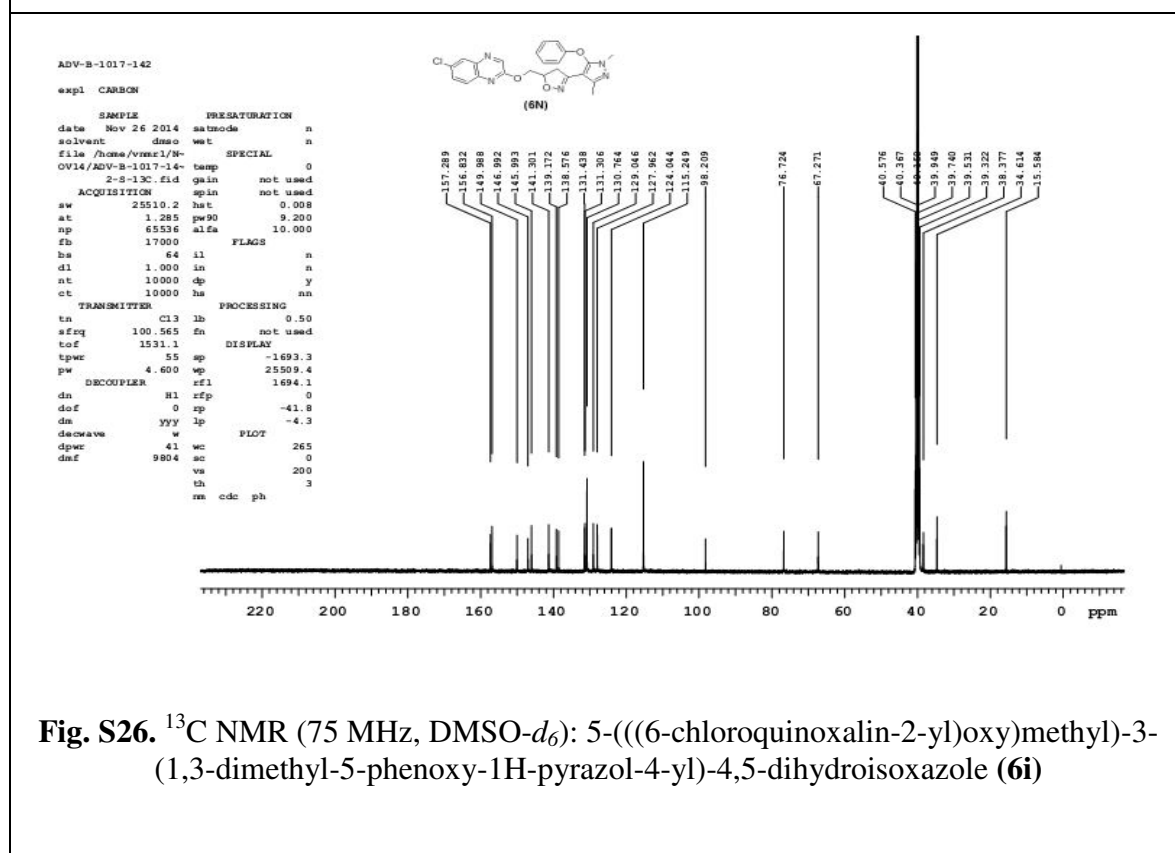


Fig. S26. ^{13}C NMR (75 MHz, $\text{DMSO-}d_6$): 5-(((6-chloroquinoxalin-2-yl)oxy)methyl)-3-(1,3-dimethyl-5-phenoxy-1H-pyrazol-4-yl)-4,5-dihydroisoxazole (**6i**)

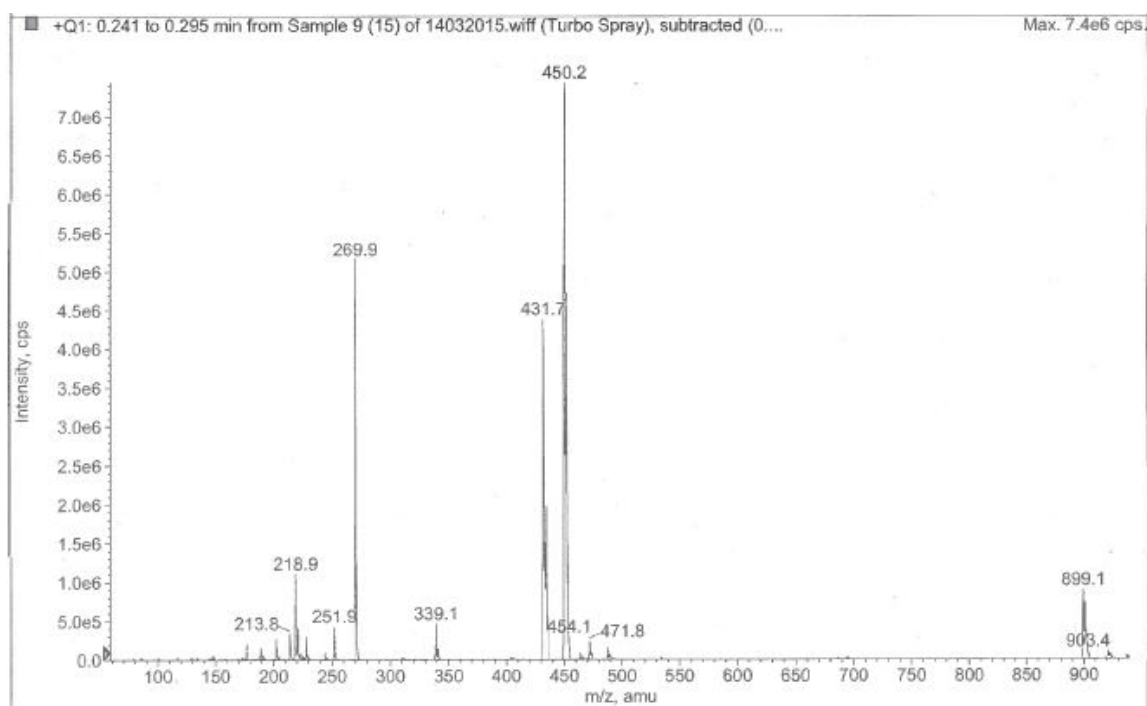


Fig. S27. ESI-MS spectra of the compound **6i**

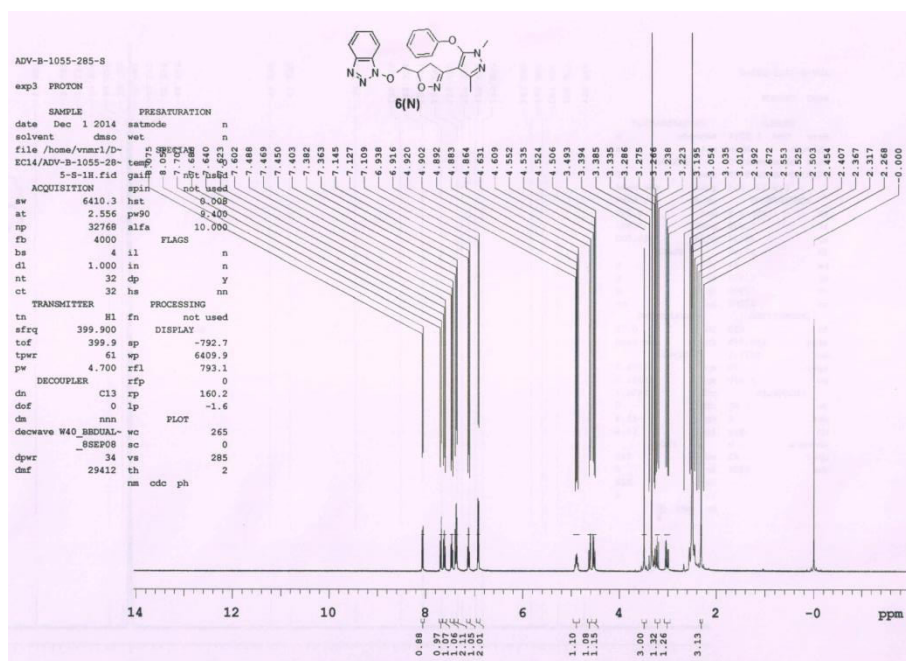


Fig. S28. ¹H NMR (300 MHz, DMSO-*d*₆): 5-((1H-benzo[d][1,2,3]triazol-1-yloxy)methyl)-3-(1,3-dimethyl-5-phenoxy-1H-pyrazol-4-yl)-4,5-dihydroisoxazole (**6j**)

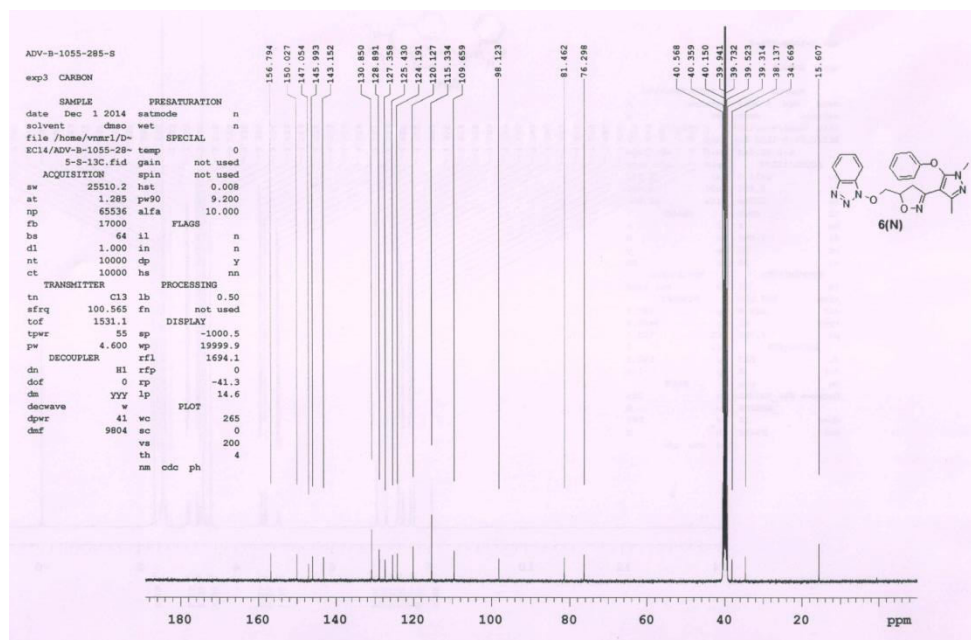


Fig. S29. ^{13}C NMR (75 MHz, $\text{DMSO-}d_6$): 5-((1H-benzo[d][1,2,3]triazol-1-yloxy)methyl)-3-(1,3-dimethyl-5-phenoxy-1H-pyrazol-4-yl)-4,5-dihydroisoxazole (**6j**)

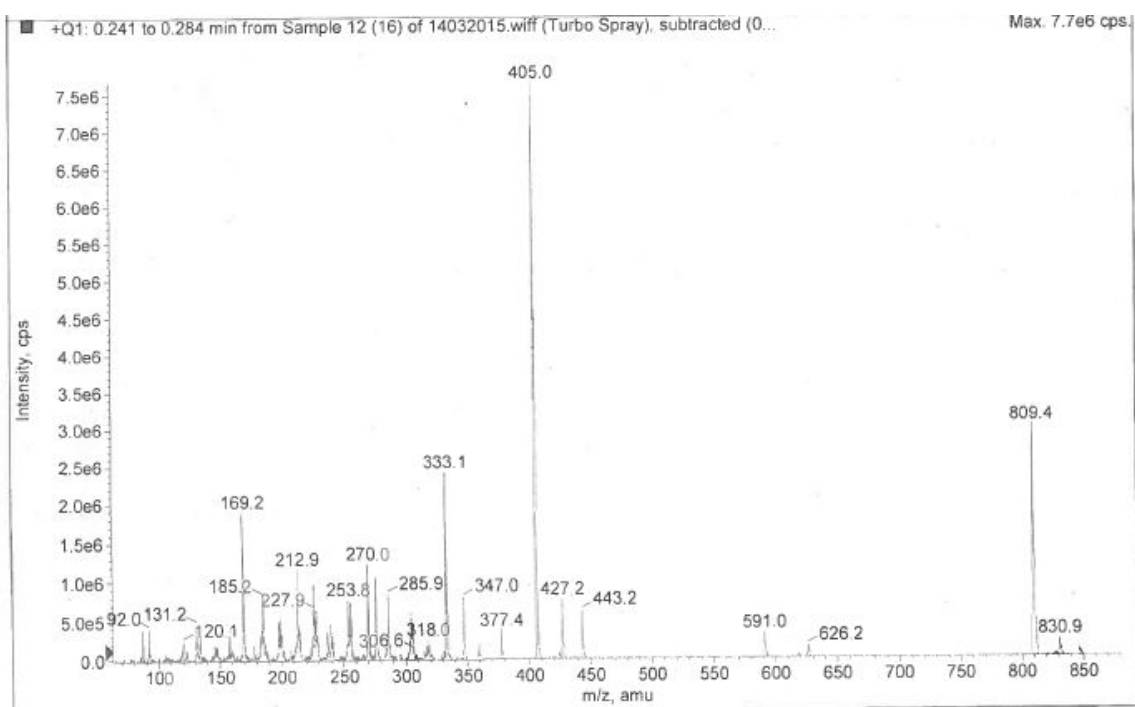
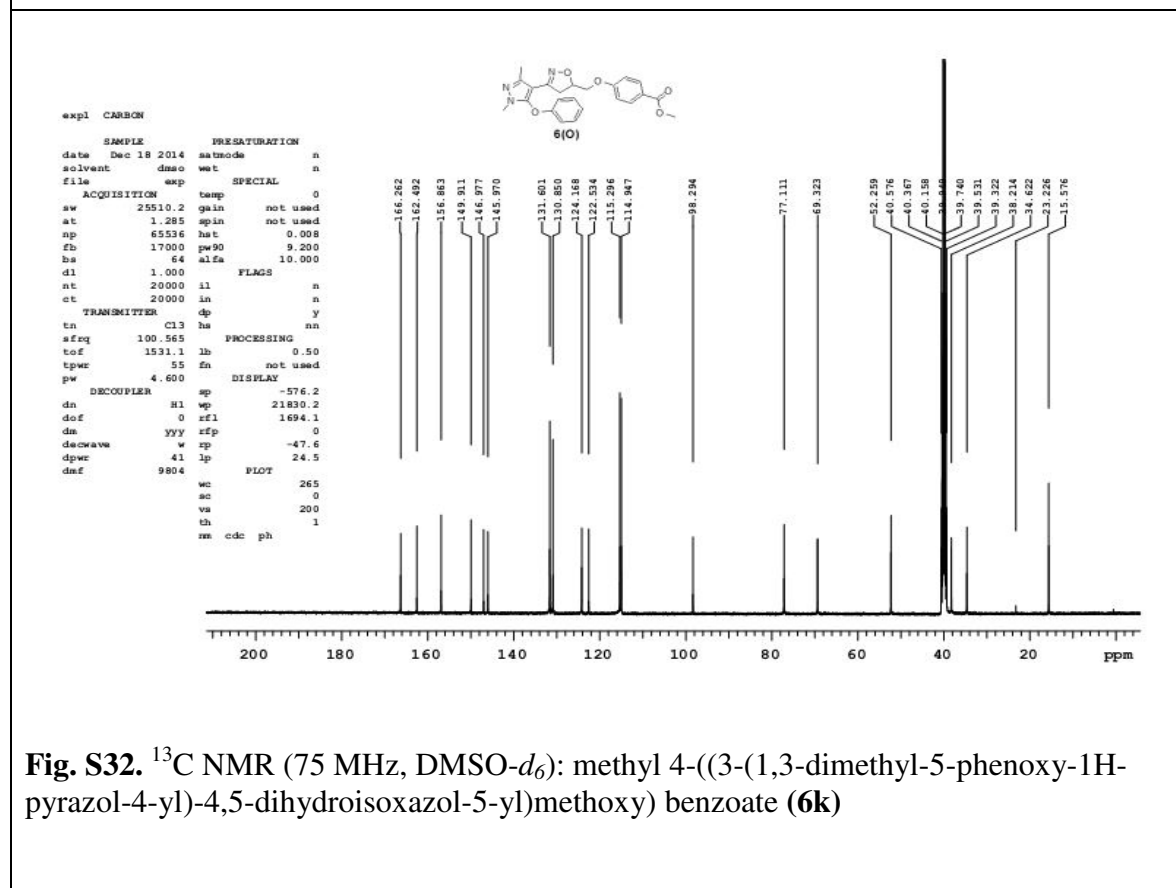
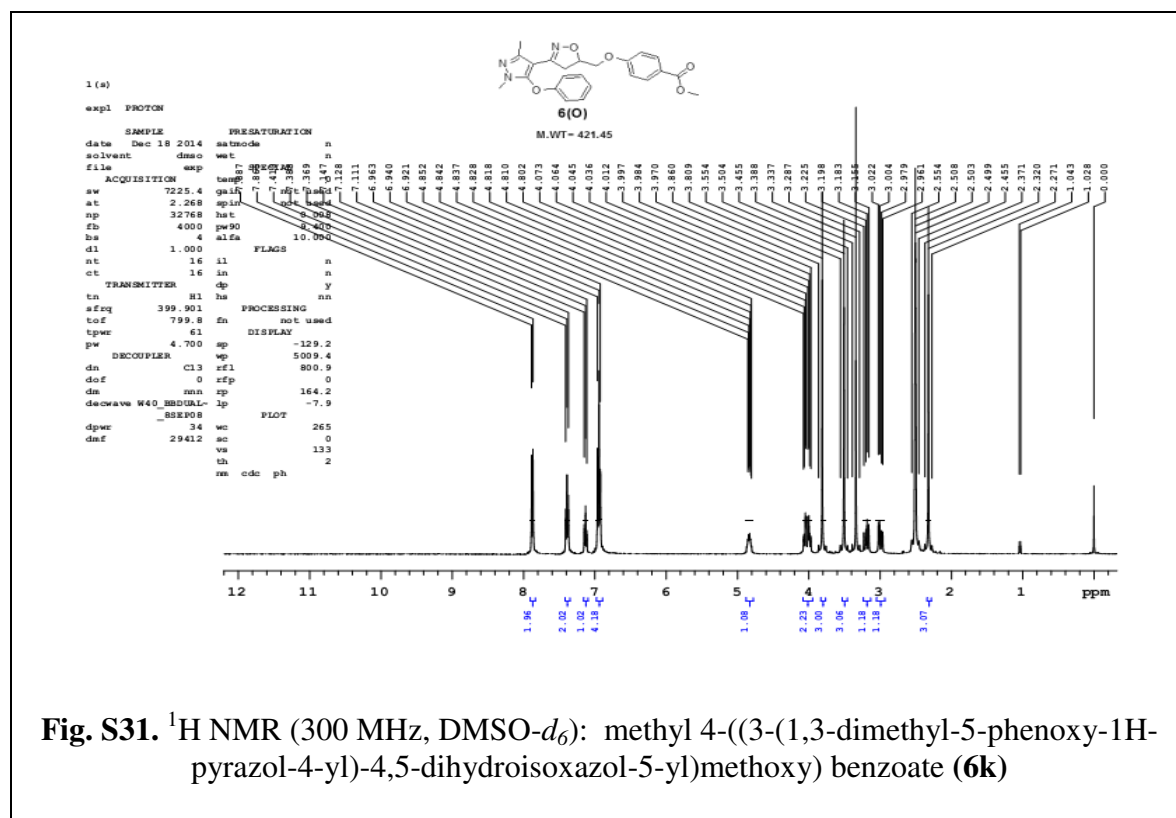


Fig. 30. ESI-MS spectra of the compound **6j**



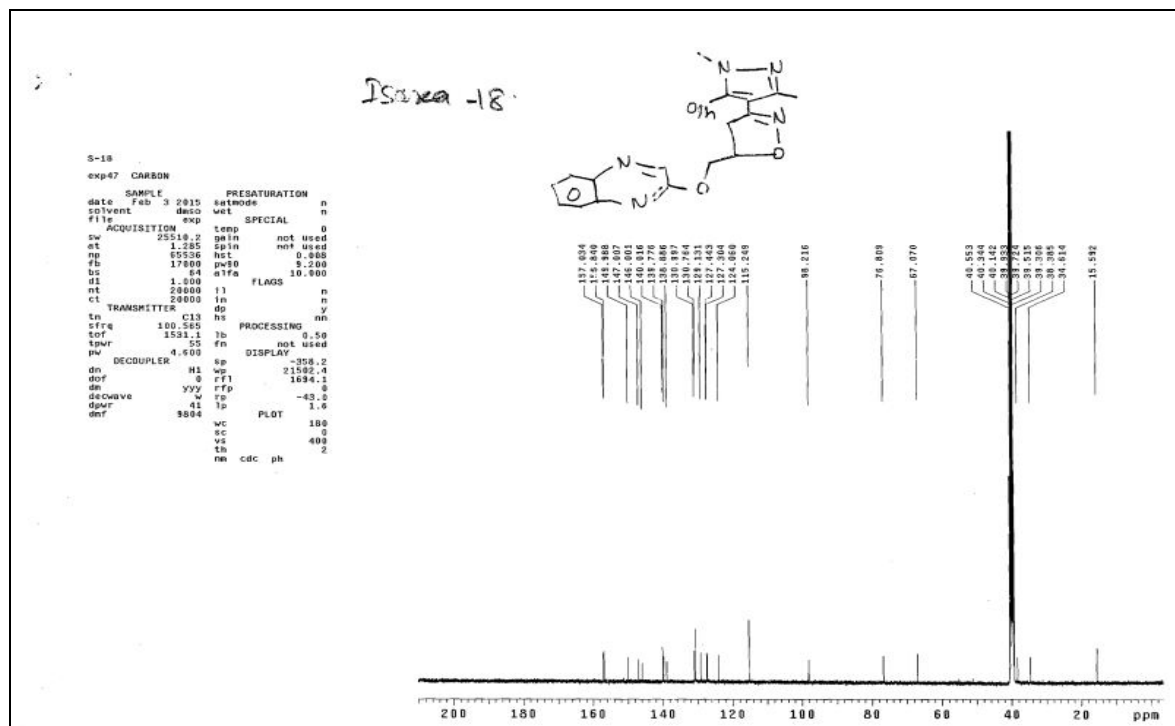


Fig. S35. ^{13}C NMR (75 MHz, $\text{DMSO-}d_6$): 3-(1,3-dimethyl-5-phenoxy-1H-pyrazol-4-yl)-5-((quinoxalin-2-yloxy)methyl)-4,5-dihydroisoxazole (**61**)

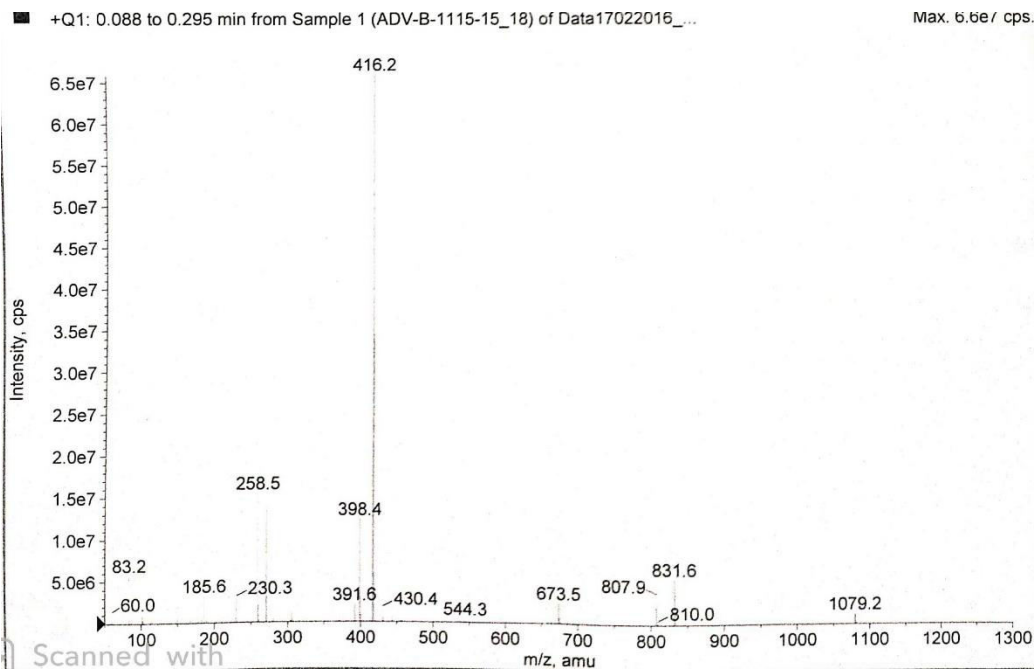


Fig. S36. ESI-MS spectra of the compound **61**

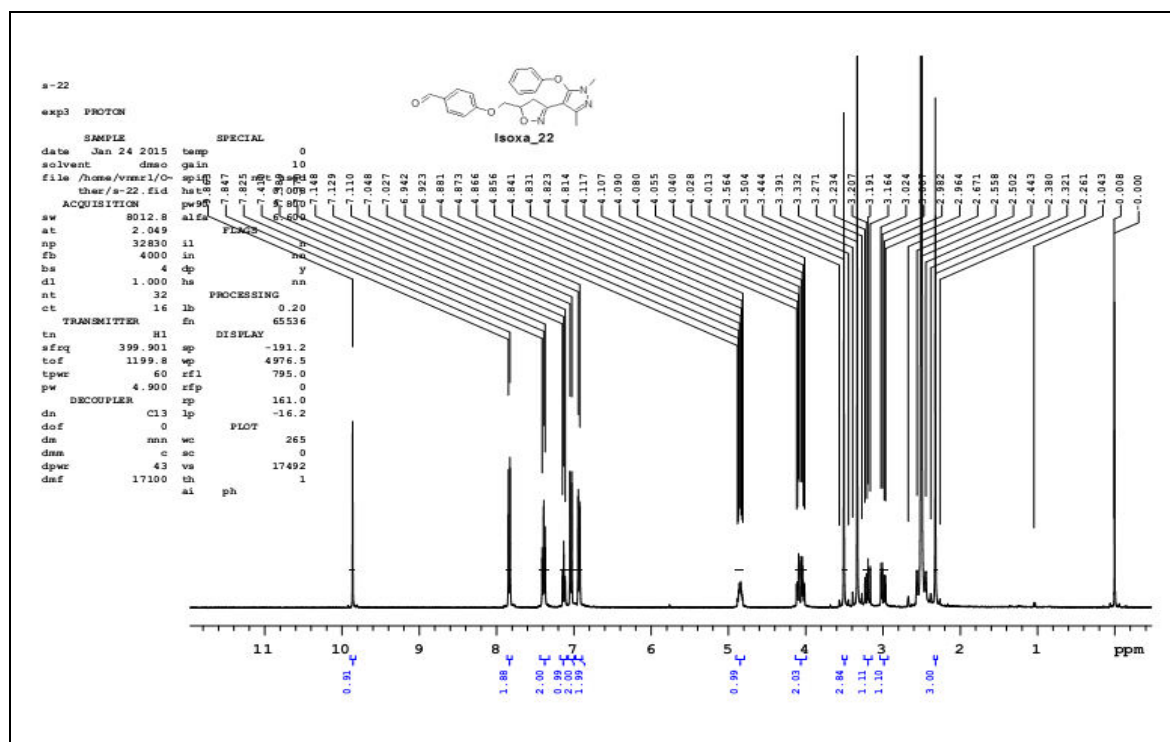


Fig. S37. ^1H NMR (300 MHz, $\text{DMSO-}d_6$): 4-((3-(1,3-dimethyl-5-phenoxy-1H-pyrazol-4-yl)-4,5-dihydroisoxazol-5-yl)methoxy) benzaldehyde (**6m**)

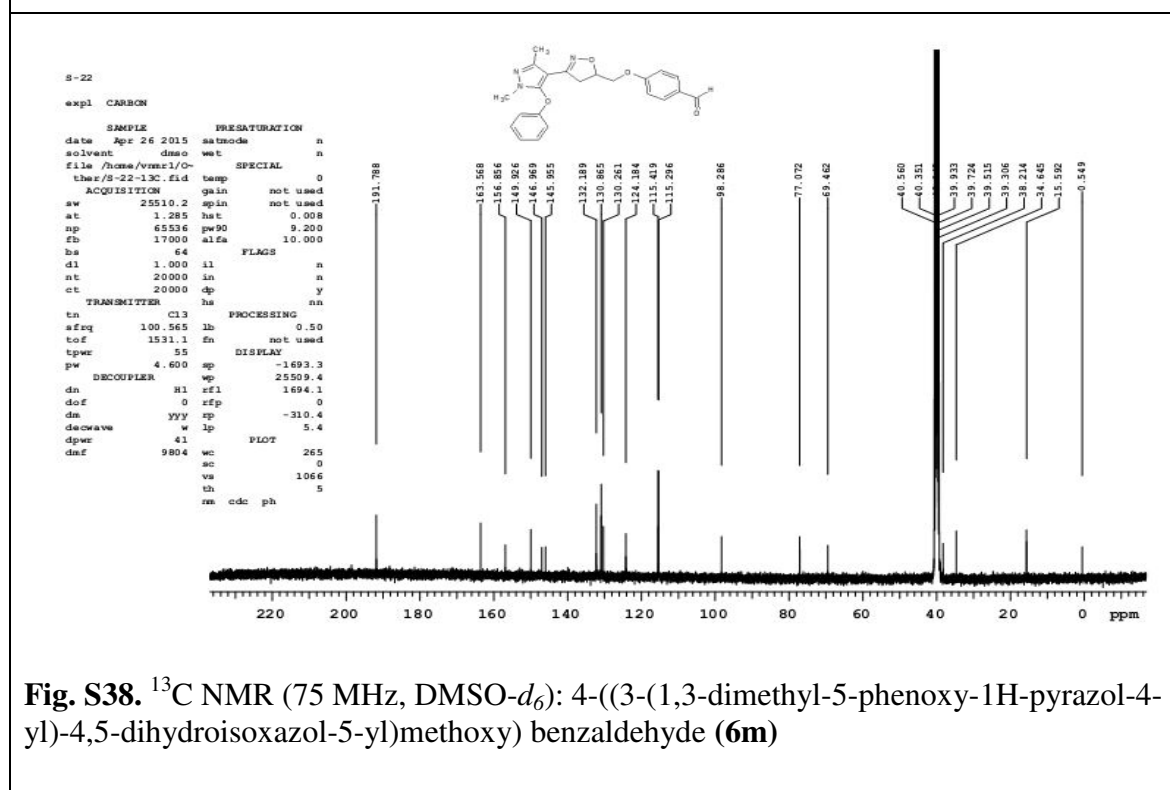


Fig. S38. ^{13}C NMR (75 MHz, $\text{DMSO-}d_6$): 4-((3-(1,3-dimethyl-5-phenoxy-1H-pyrazol-4-yl)-4,5-dihydroisoxazol-5-yl)methoxy) benzaldehyde (**6m**)

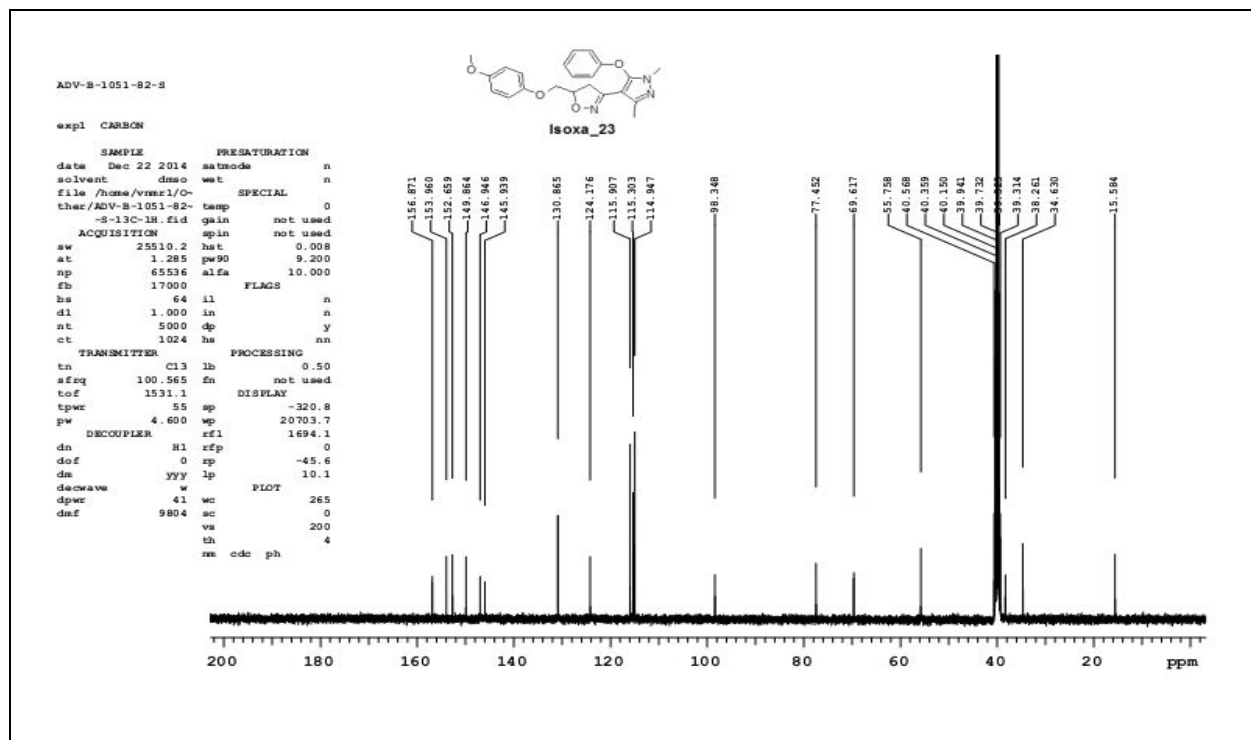


Fig. S41. ^{13}C NMR (75 MHz, $\text{DMSO-}d_6$): 3-(1,3-dimethyl-5-phenoxy-1H-pyrazol-4-yl)-5-((4-methoxyphenoxy)methyl)-4,5-dihydro isoxazole (**6n**)

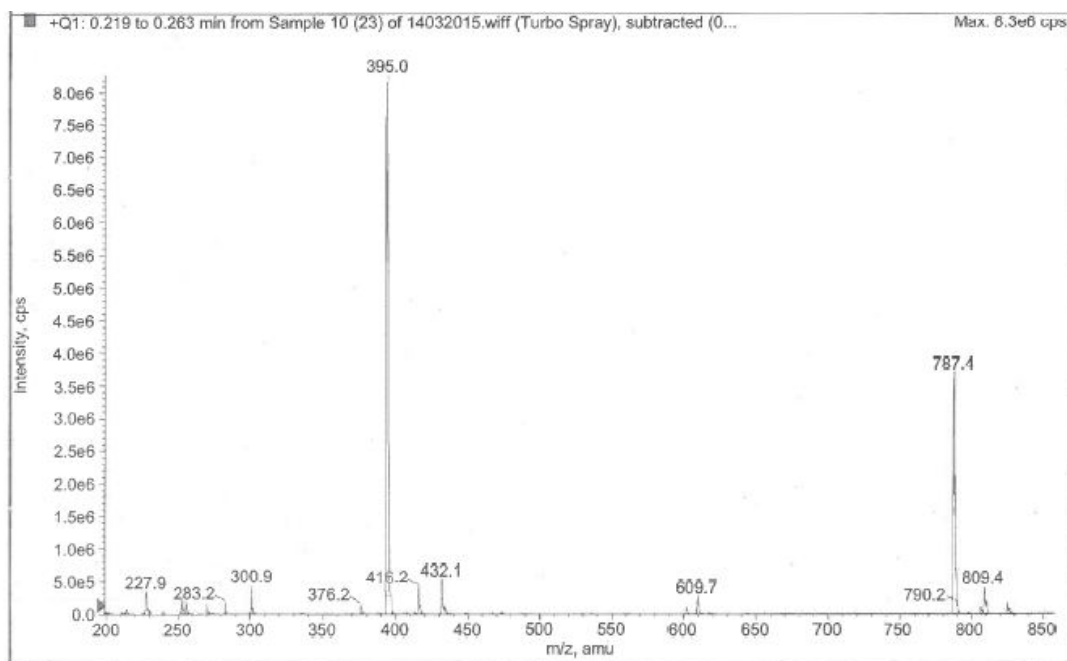


Fig. S42. ESI-MS spectra of the compound **6n**

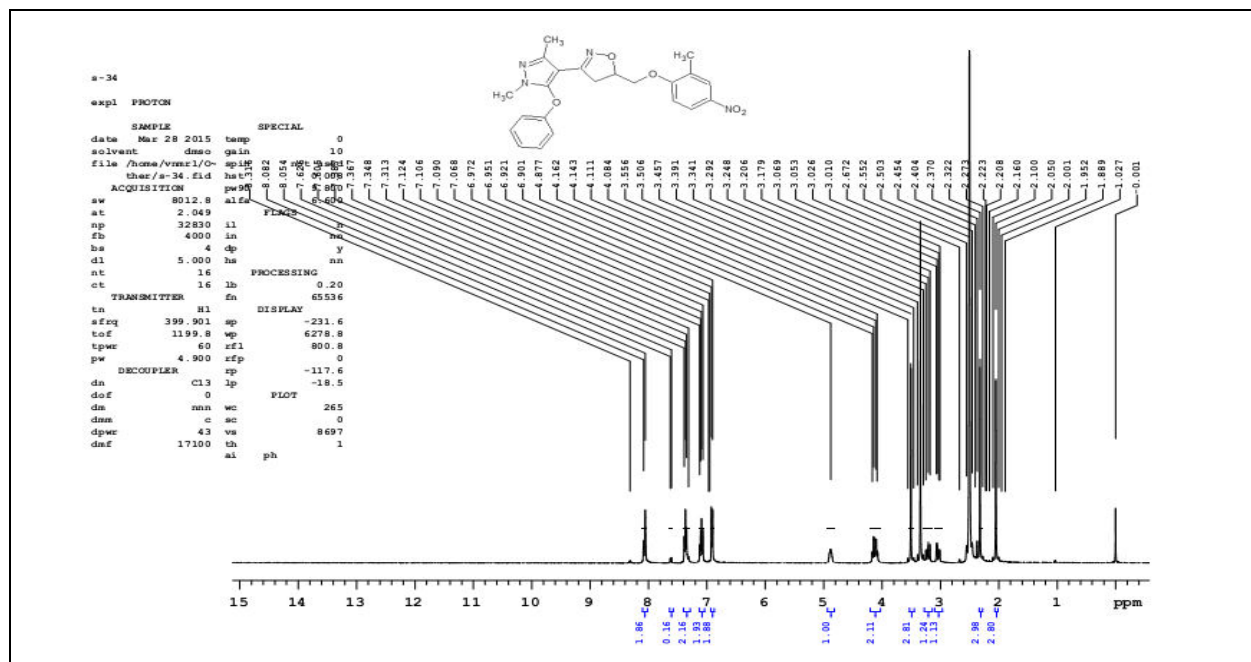


Fig. S43. ^1H NMR (300 MHz, $\text{DMSO}-d_6$): 3-(1,3-dimethyl-5-phenoxy-1H-pyrazol-4-yl)-5-((2-methyl-4-nitrophenoxy)methyl)-4,5-dihydroisoxazole (**60**)

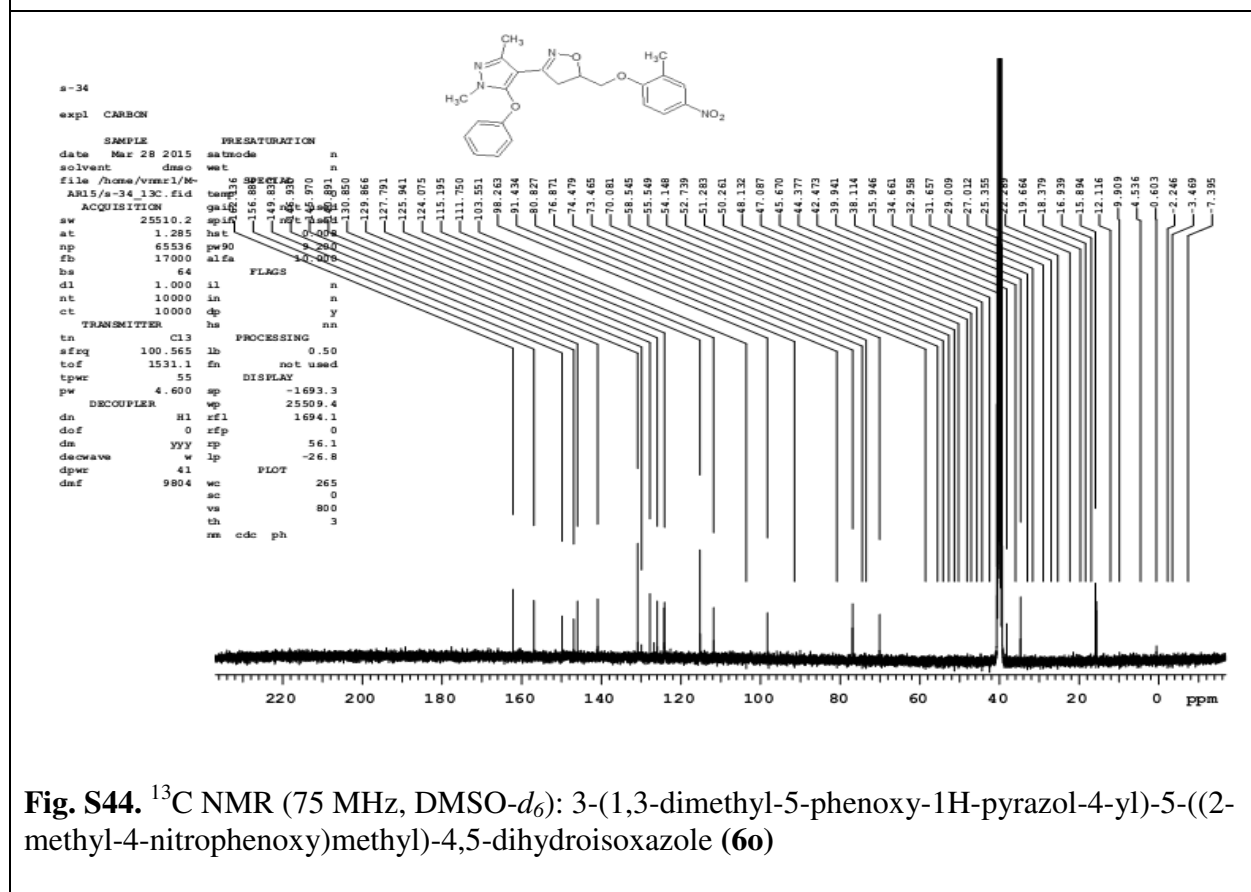


Fig. S44. ^{13}C NMR (75 MHz, $\text{DMSO}-d_6$): 3-(1,3-dimethyl-5-phenoxy-1H-pyrazol-4-yl)-5-((2-methyl-4-nitrophenoxy)methyl)-4,5-dihydroisoxazole (**60**)

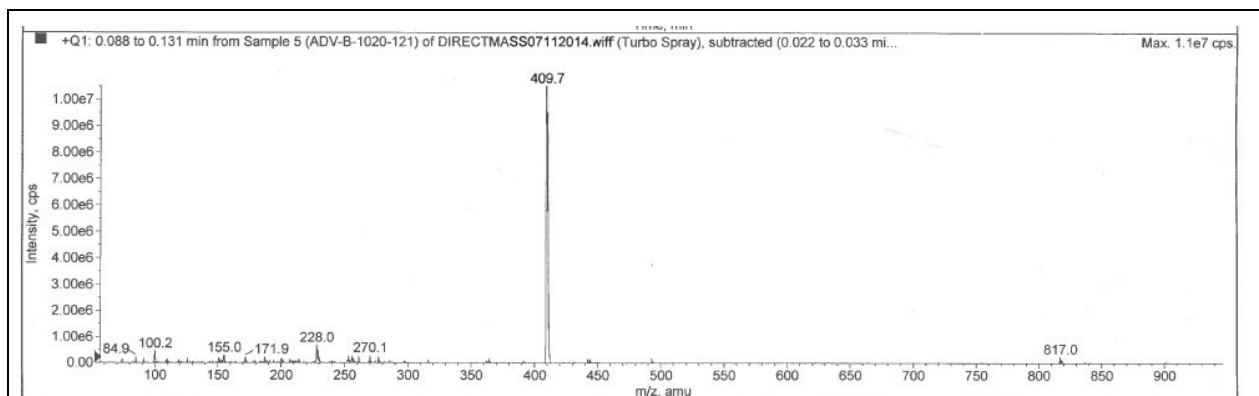


Fig. S45. ESI-MS spectra of the compound **60**

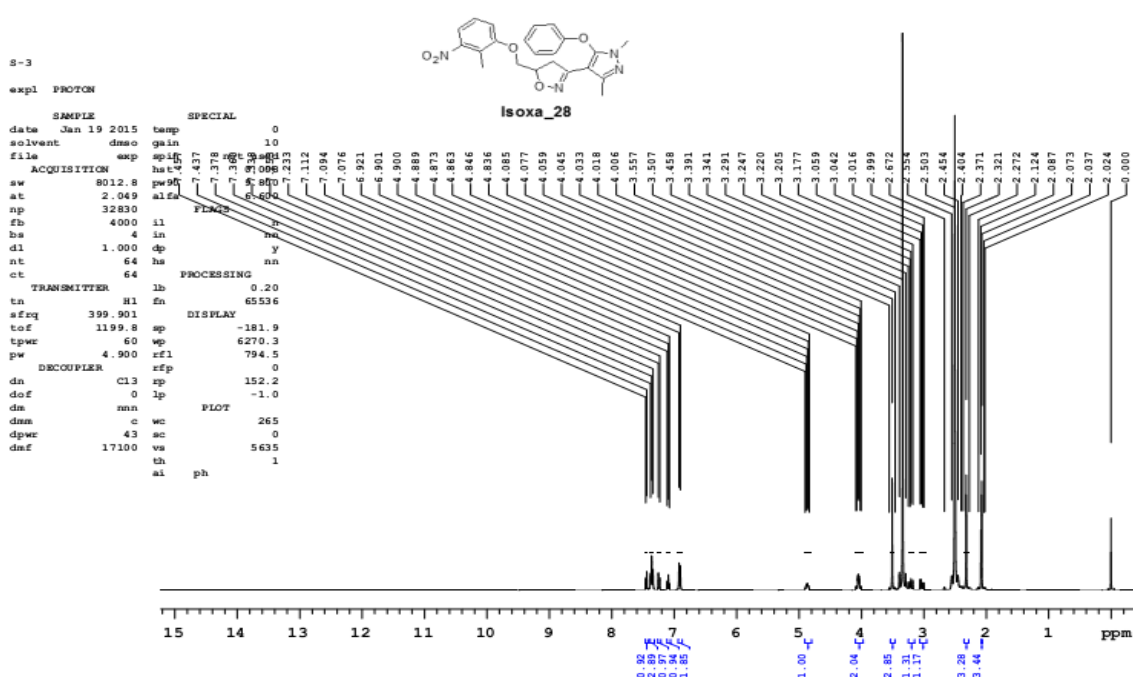


Fig. S46. ^1H NMR (300 MHz, $\text{DMSO}-d_6$): 3-(1,3-dimethyl-5-phenoxy-1H-pyrazol-4-yl)-5-((2-methyl-3-nitrophenoxy)methyl)-4,5-dihydroisoxazole (**6p**)

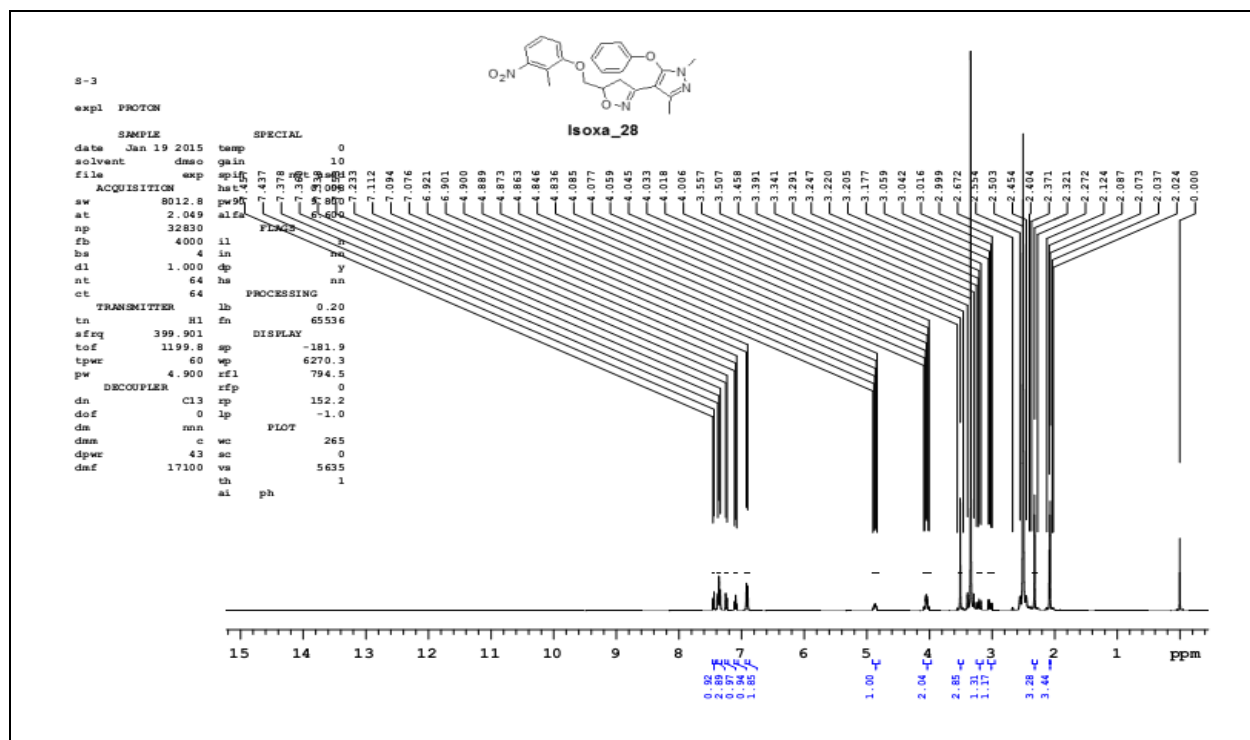


Fig. S47. ^{13}C NMR (75 MHz, $\text{DMSO}-d_6$): 3-(1,3-dimethyl-5-phenoxy-1H-pyrazol-4-yl)-5-((2-methyl-3-nitrophenoxy)methyl)-4,5-dihydroisoxazole (**6p**)

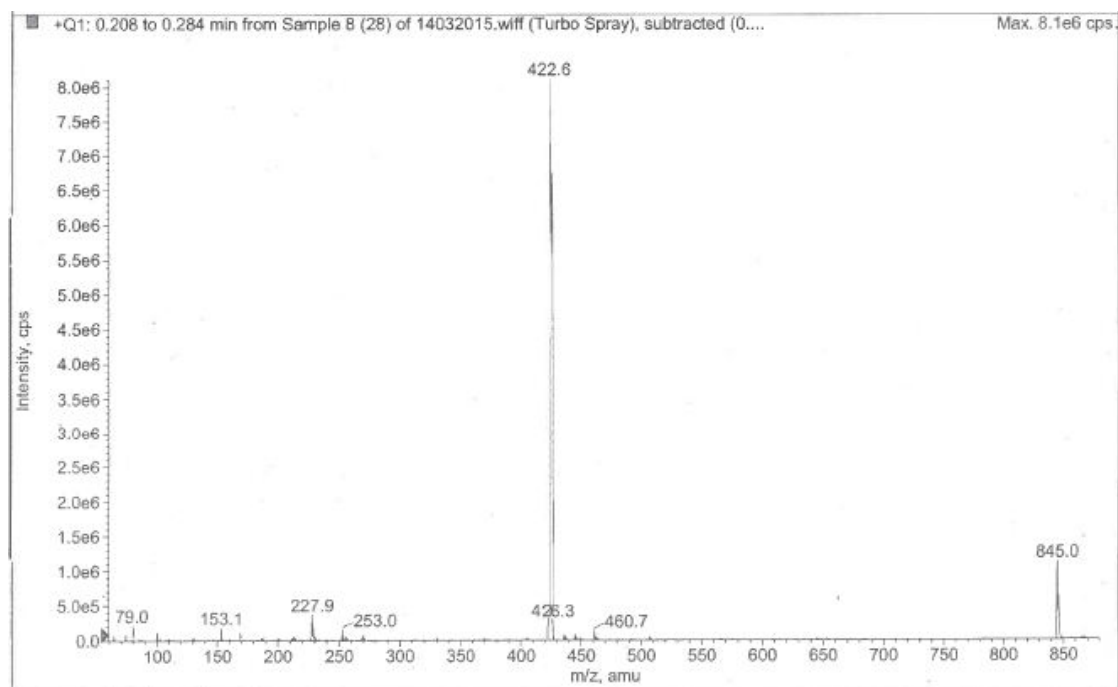


Fig. S48. ESI-MS spectra of the compound **6p**

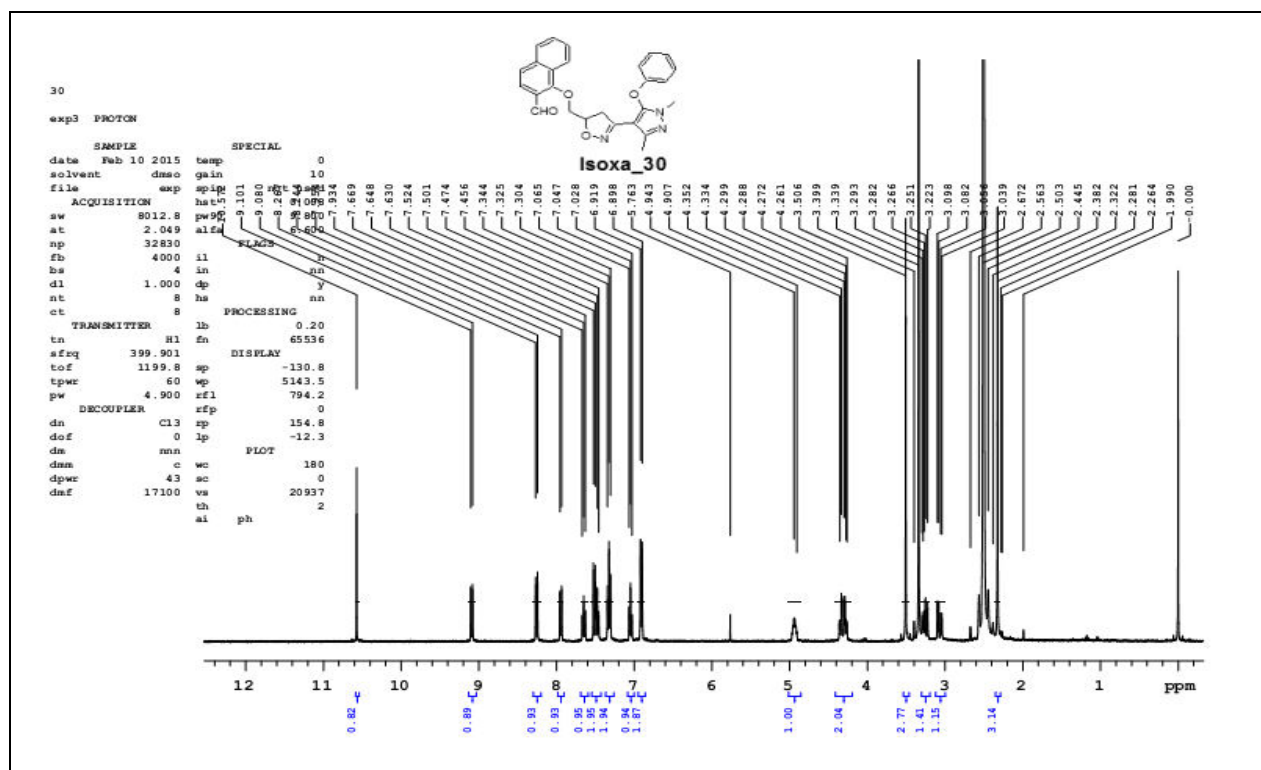


Fig. S49. ^1H NMR (300 MHz, $\text{DMSO-}d_6$): 1-((3-(1,3-dimethyl-5-phenoxy-1H-pyrazol-4-yl)-4,5-dihydroisoxazol-5-yl)methoxy)-2-naphthaldehyde (**6q**)

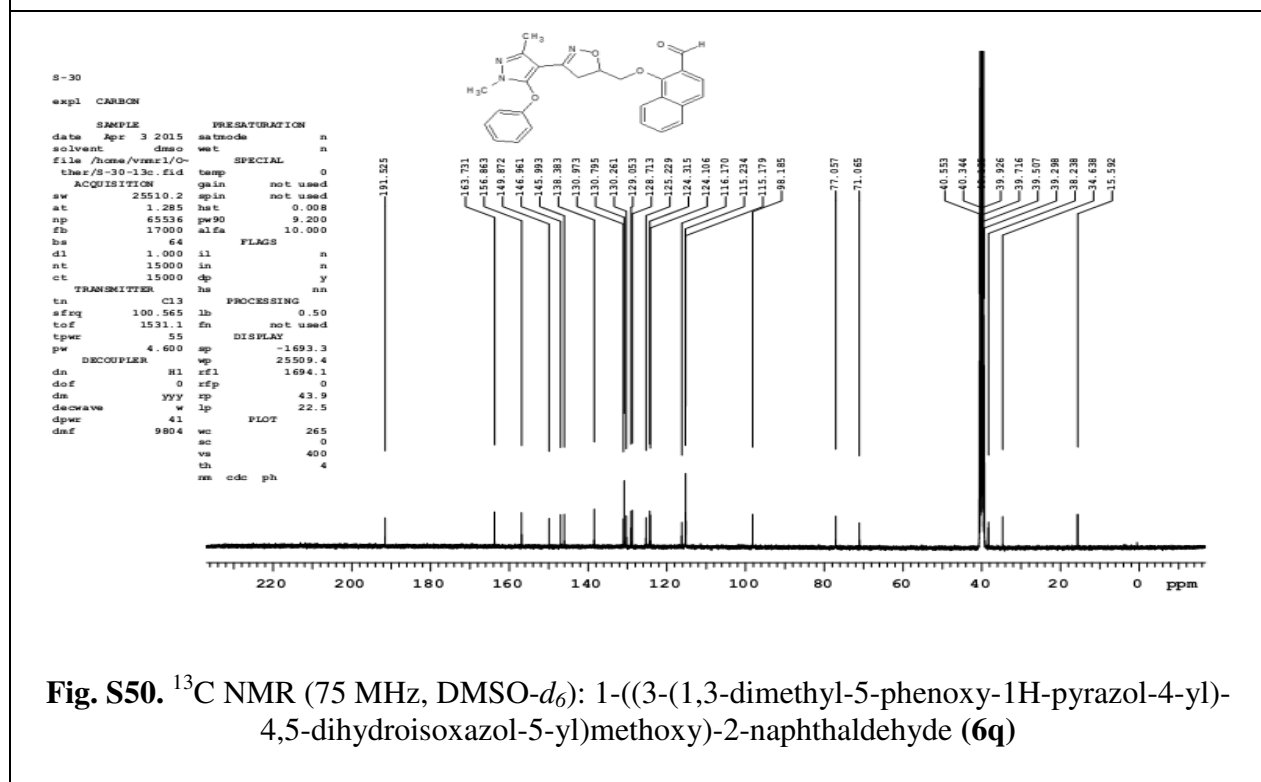
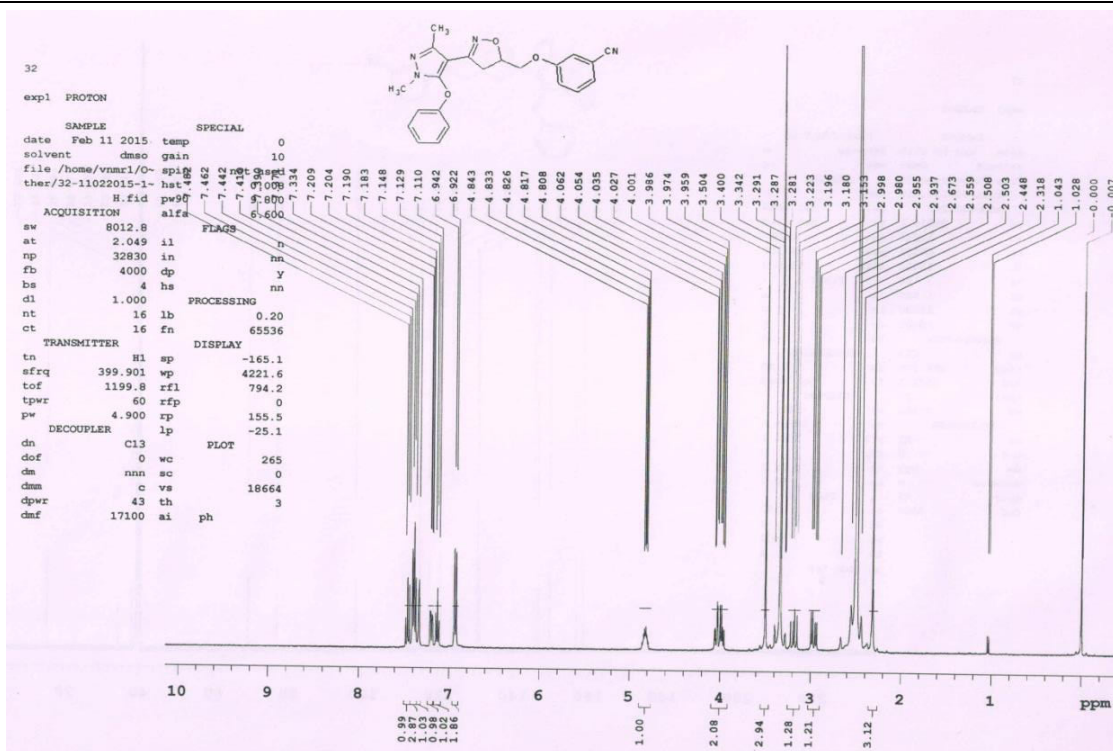
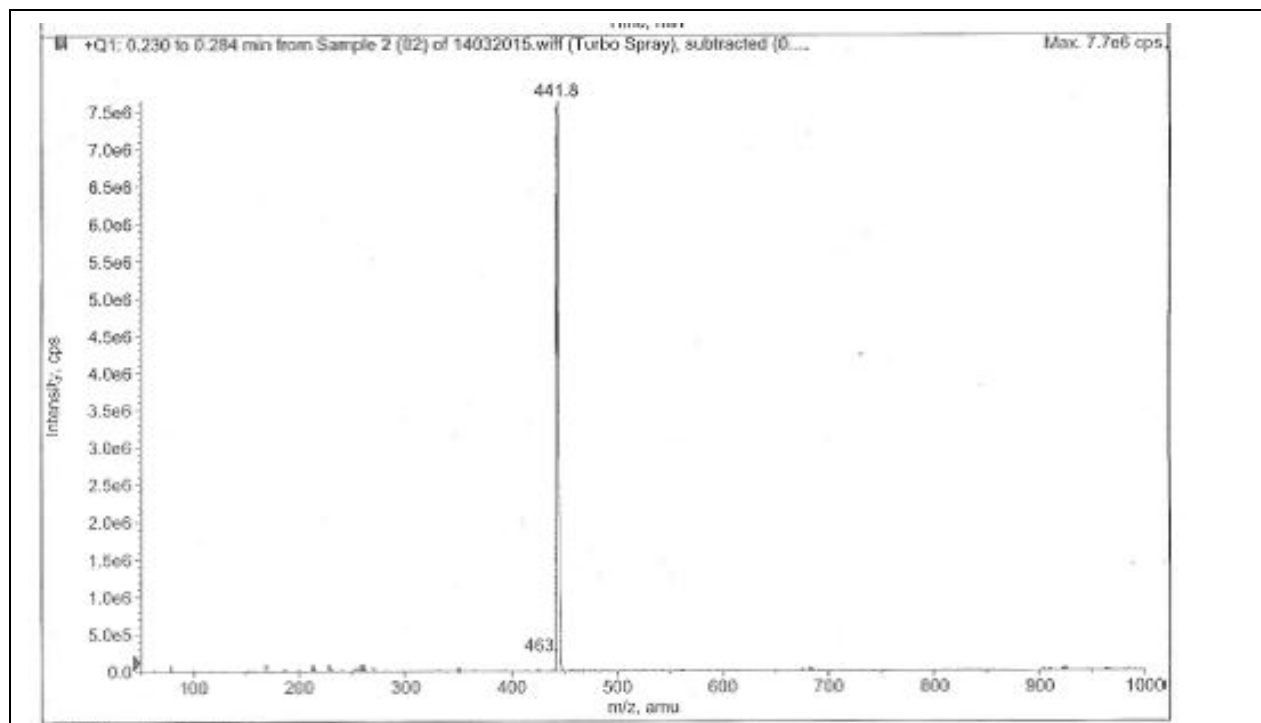


Fig. S50. ^{13}C NMR (75 MHz, $\text{DMSO-}d_6$): 1-((3-(1,3-dimethyl-5-phenoxy-1H-pyrazol-4-yl)-4,5-dihydroisoxazol-5-yl)methoxy)-2-naphthaldehyde (**6q**)



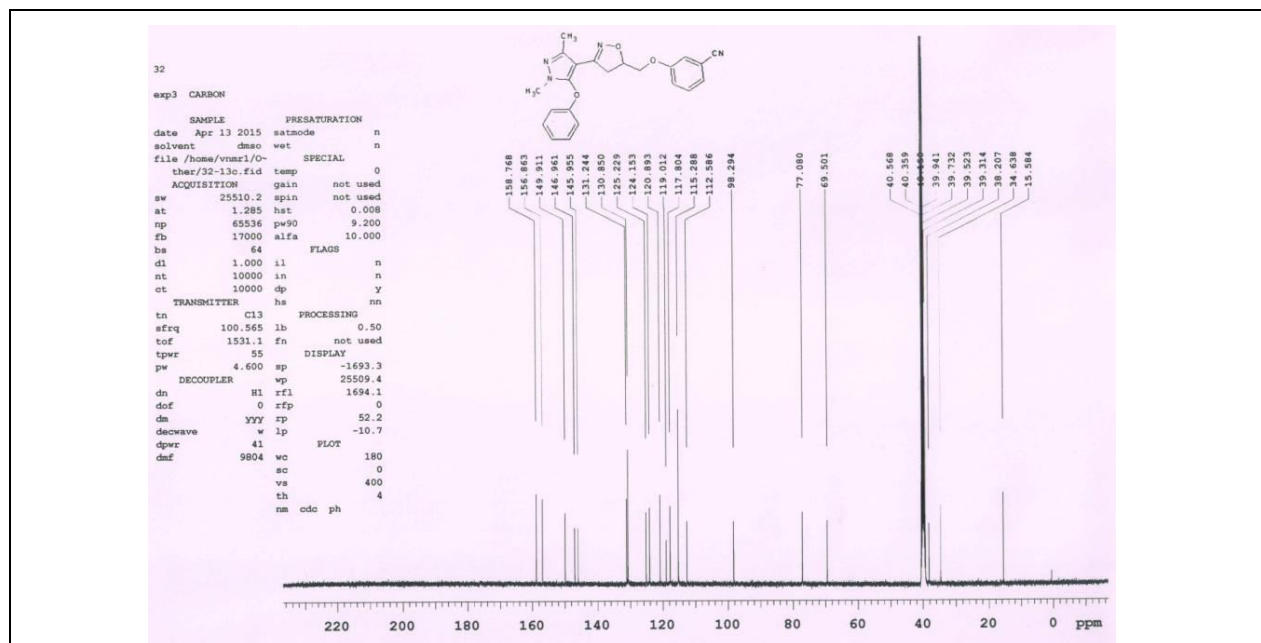


Fig. S53. ^{13}C NMR (75 MHz, $\text{DMSO-}d_6$): 3-((3-(1,3-dimethyl-5-phenoxy-1H-pyrazol-4-yl)-4,5-dihydroisoxazol-5-yl)methoxy)benzonitrile (**6r**)

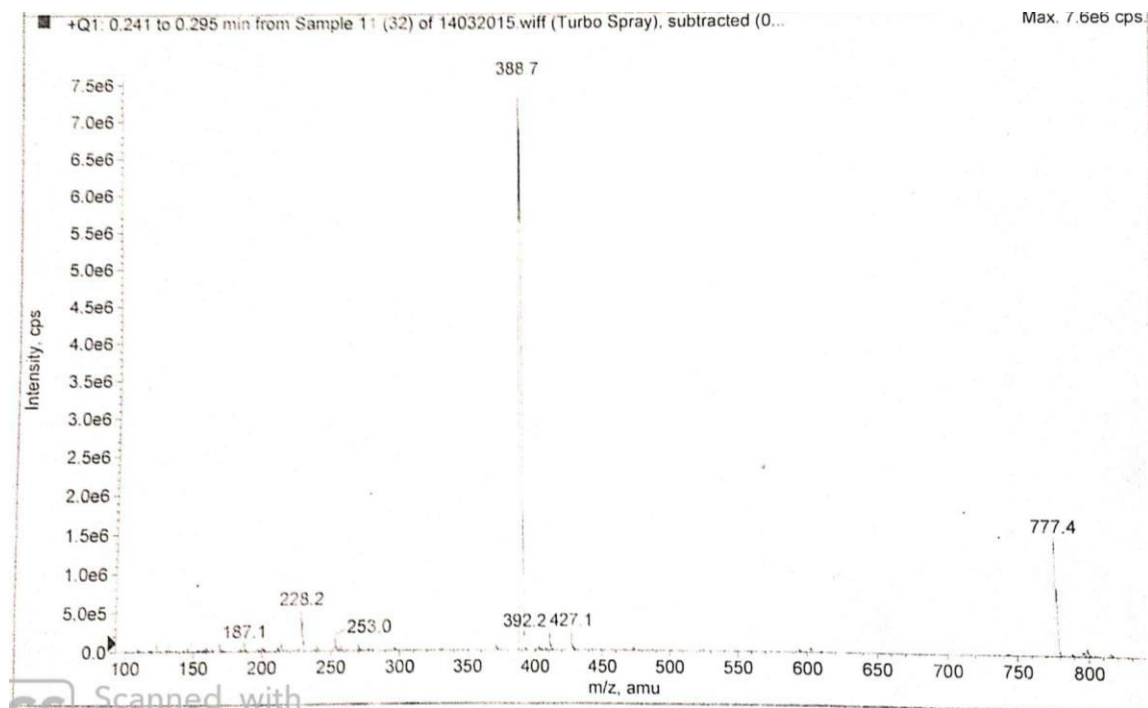


Fig. S54. ESI-MS spectra of the compound **6r**

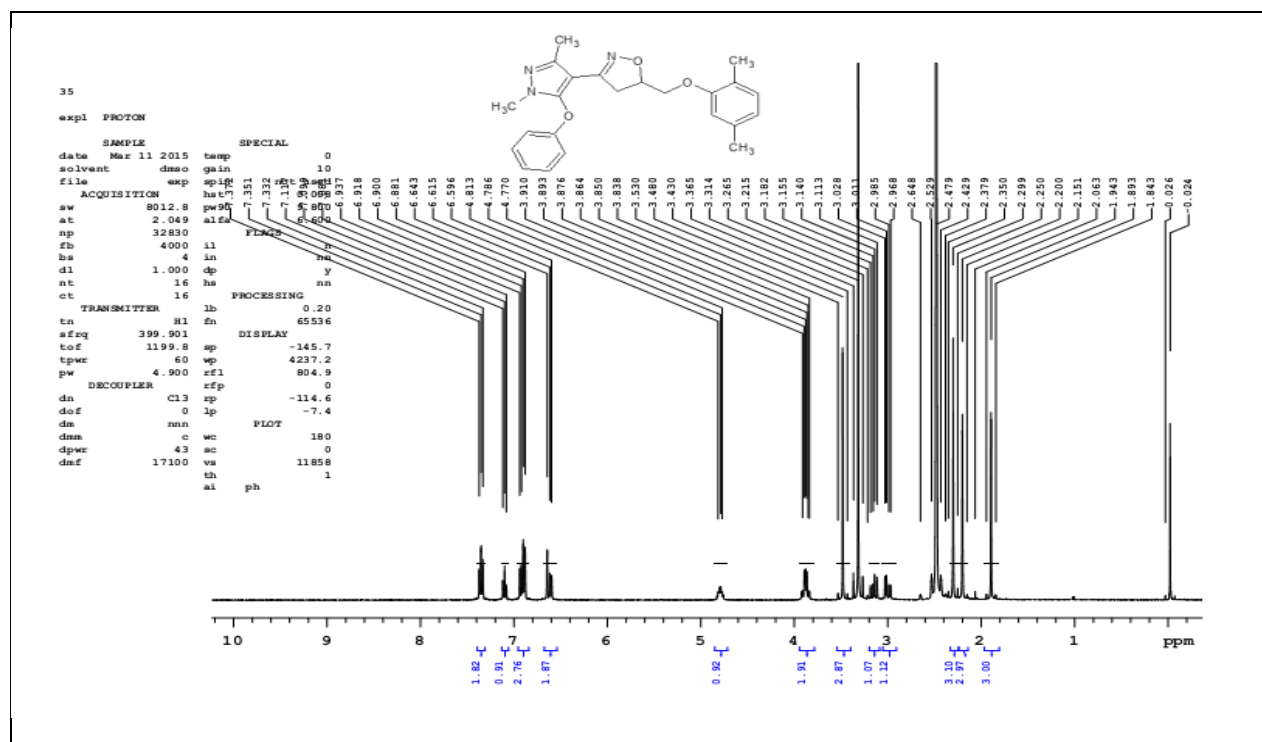


Fig. S55. ^1H NMR (300 MHz, $\text{DMSO}-d_6$): 3-(1,3-dimethyl-5-phenoxy-1H-pyrazol-4-yl)-5-((2,5-dimethylphenoxy)methyl)-4,5-dihydroisoxazole (**6s**)

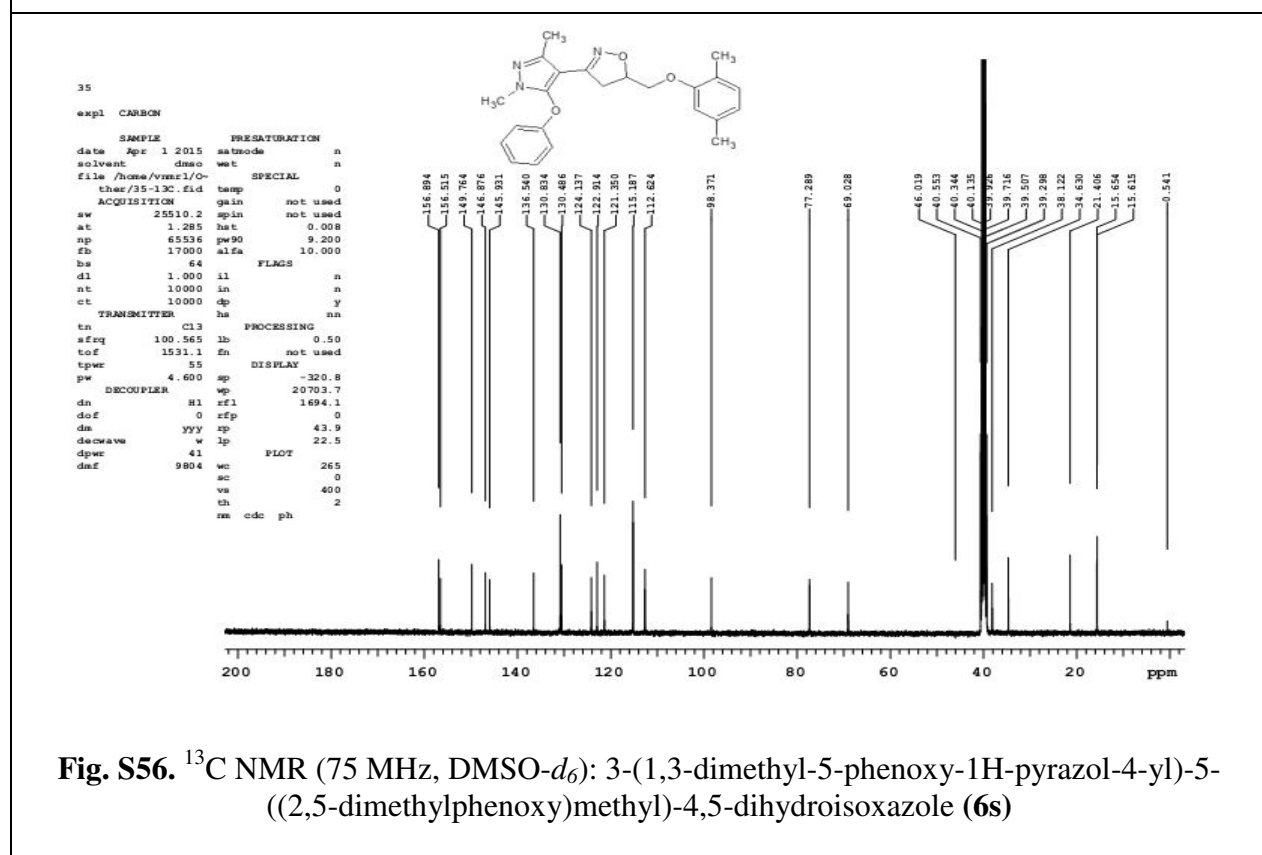


Fig. S56. ^{13}C NMR (75 MHz, $\text{DMSO}-d_6$): 3-(1,3-dimethyl-5-phenoxy-1H-pyrazol-4-yl)-5-((2,5-dimethylphenoxy)methyl)-4,5-dihydroisoxazole (**6s**)

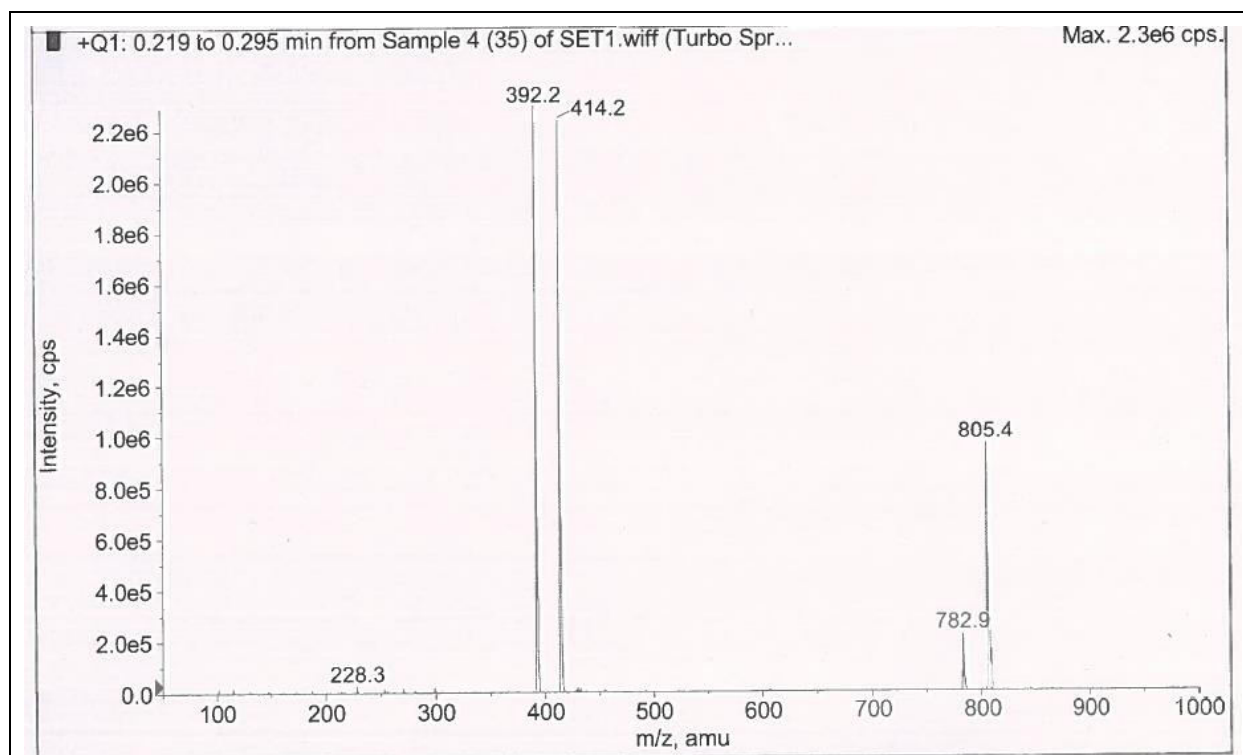
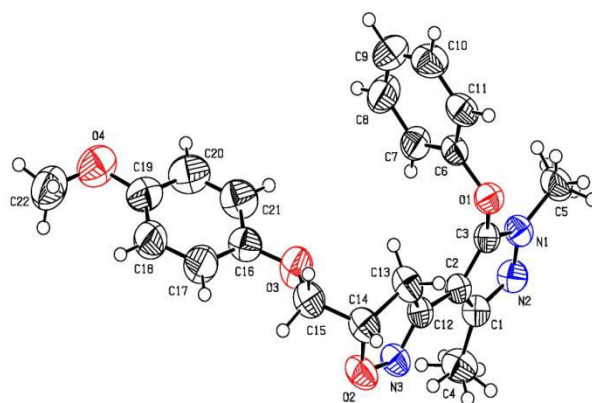


Fig. S57. ESI-MS spectra of the compound **6s**

X-ray crystallographic information



ORTEP diagram of isoxazoline derivative **6n**

Crystallographic Data for **6n** single crystal

Empirical formula	$C_{22}H_{23}N_3O_4$
Crystal shape and color	Colorless plates
Formula weight	393.43
Temperature	293K
Wavelength	0.7107 Å
Crystal system & space group	Monoclinic, $P2_1/c$
Cell dimensions	$a = 15.715 (2) \text{ \AA}$
	$b = 15.803 (2) \text{ \AA}$
	$c = 8.4108 (10) \text{ \AA}$
	$\alpha, \gamma, \beta = 100.922 (6)^\circ$
Volume	$2050.9 (4) \text{ \AA}^3$
Z, calculated density	4, 1.274Mg m ⁻³
F(000)	832
θ range for data collection	$1.3^\circ - 27.5^\circ$
Absorption coefficient	0.089 mm^{-1}
$\Delta\rho_{\max}$ and $\Delta\rho_{\min}$	0.17 e \AA^{-3} and -0.19 e \AA^{-3}
Refinement method	Full matrix least square on F^2
Data/ parameters	4716/262
Goodness-of-fit on F^2	1.03
Final R indices [$I > 2\sigma(I)$]	R1=0.047, wR2= 0.153
CCDC NO	1897410

Table.2. Bond lengths of the title molecule

O1—C3	1.3622 (18)	C14—C13	1.519 (2)
O1—C6	1.3910 (19)	C14—H14A	0.97
O2—N3	1.4138 (18)	C14—H14B	0.97
O2—C13	1.459 (2)	C13—C15	1.494 (3)
O3—C16	1.376 (2)	C13—H13	0.98
O3—C15	1.421 (2)	C15—H15A	0.97
N1—C3	1.335 (2)	C15—H15B	0.97
N1—N2	1.3629 (18)	C16—C17	1.368 (3)
N1—C5	1.451 (2)	C16—C21	1.369 (3)
N2—C1	1.328 (2)	C21—C20	1.371 (3)
N3—C12	1.2762 (19)	C21—H21	0.93
C22—O4	1.416 (3)	C20—C19	1.376 (3)
C22—H22A	0.96	C20—H20	0.93
C22—H22B	0.96	C19—C18	1.366 (3)
C22—H22C	0.96	C19—O4	1.375 (2)
C1—C2	1.410 (2)	C18—C17	1.381 (3)
C1—C4	1.490 (2)	C18—H18	0.93
C2—C3	1.377 (2)	C17—H17	0.93
C2—C12	1.449 (2)	C5—H5A	0.96
C6—C7	1.370 (2)	C5—H5B	0.96
C6—C11	1.376 (2)	C5—H5C	0.96
C7—C8	1.382 (3)	C5—H5D	0.96
C7—H7	0.93	C5—H5E	0.96
C8—C9	1.379 (3)	C5—H5F	0.96
C8—H8	0.93	C4—H4A	0.96
C9—C10	1.367 (3)	C4—H4B	0.96
C9—H9	0.93	C4—H4C	0.96
C10—C11	1.377 (3)	C4—H4D	0.96
C10—H10	0.93	C4—H4E	0.96
C12—C14	1.495 (2)	C4—H4F	0.96

Table.3. Bond Angles of the title compound

C3—O1—C6	118.12 (11)	C17—C16—C21	118.74 (19)
N3—O2—C13	109.72 (11)	C17—C16—O3	125.14 (17)
C16—O3—C15	117.72 (13)	C21—C16—O3	116.10 (17)
C3—N1—N2	110.91 (12)	C16—C21—C20	120.6 (2)
C3—N1—C5	128.05 (15)	C16—C21—H21	119.7
N2—N1—C5	121.04 (14)	C20—C21—H21	119.7
C1—N2—N1	105.31 (13)	C21—C20—C19	120.88 (19)
C12—N3—O2	109.28 (12)	C21—C20—H20	119.6
O4—C22—H22A	109.5	C19—C20—H20	119.6
O4—C22—H22B	109.5	C18—C19—O4	125.2 (2)
H22A—C22—H22B	109.5	C18—C19—C20	118.6 (2)
O4—C22—H22C	109.5	O4—C19—C20	116.15 (19)
H22A—C22—H22C	109.5	C19—C18—C17	120.4 (2)
H22B—C22—H22C	109.5	C19—C18—H18	119.8
N2—C1—C2	111.45 (14)	C17—C18—H18	119.8
N2—C1—C4	119.88 (14)	C16—C17—C18	120.82 (19)
C2—C1—C4	128.67 (14)	C16—C17—H17	119.6
C3—C2—C1	103.61 (13)	C18—C17—H17	119.6
C3—C2—C12	125.86 (14)	C19—O4—C22	117.64 (18)
C1—C2—C12	130.52 (14)	N1—C5—H5A	109.5
N1—C3—O1	120.28 (13)	N1—C5—H5B	109.5
N1—C3—C2	108.73 (13)	H5A—C5—H5B	109.5
O1—C3—C2	130.89 (14)	N1—C5—H5C	109.5
C7—C6—C11	121.52 (16)	H5A—C5—H5C	109.5
C7—C6—O1	123.35 (14)	H5B—C5—H5C	109.5
C11—C6—O1	115.13 (14)	N1—C5—H5D	109.5
C6—C7—C8	118.60 (17)	H5A—C5—H5D	141.1
C6—C7—H7	120.7	H5B—C5—H5D	56.3
C8—C7—H7	120.7	H5C—C5—H5D	56.3
C9—C8—C7	120.6 (2)	N1—C5—H5E	109.5
C9—C8—H8	119.7	H5A—C5—H5E	56.3
C7—C8—H8	119.7	H5B—C5—H5E	141.1
C10—C9—C8	119.6 (2)	H5C—C5—H5E	56.3
C10—C9—H9	120.2	H5D—C5—H5E	109.5
C8—C9—H9	120.2	N1—C5—H5F	109.5
C9—C10—C11	120.66 (18)	H5A—C5—H5F	56.3
C9—C10—H10	119.7	H5B—C5—H5F	56.3
C11—C10—H10	119.7	H5C—C5—H5F	141.1
C6—C11—C10	118.93 (18)	H5D—C5—H5F	109.5
C6—C11—H11	120.5	H5E—C5—H5F	109.5

C10—C11—H11	120.5	C1—C4—H4A	109.5
N3—C12—C2	121.50 (14)	C1—C4—H4B	109.5
N3—C12—C14	114.36 (14)	H4A—C4—H4B	109.5
C2—C12—C14	124.14 (13)	C1—C4—H4C	109.5
C12—C14—C13	101.54 (13)	H4A—C4—H4C	109.5
C12—C14—H14A	111.5	H4B—C4—H4C	109.5
C13—C14—H14A	111.5	C1—C4—H4D	109.5
C12—C14—H14B	111.5	H4A—C4—H4D	141.1
C13—C14—H14B	111.5	H4B—C4—H4D	56.3
H14A—C14—H14B	109.3	H4C—C4—H4D	56.3
O2—C13—C15	108.69 (14)	C1—C4—H4E	109.5
O2—C13—C14	104.80 (13)	H4A—C4—H4E	56.3
C15—C13—C14	116.14 (16)	H4B—C4—H4E	141.1
O2—C13—H13	109	H4C—C4—H4E	56.3
C15—C13—H13	109	H4D—C4—H4E	109.5
C14—C13—H13	109	C1—C4—H4F	109.5
O3—C15—C13	108.44 (14)	H4A—C4—H4F	56.3
O3—C15—H15A	110	H4B—C4—H4F	56.3
C13—C15—H15A	110	H4C—C4—H4F	141.1
O3—C15—H15B	110	H4D—C4—H4F	109.5
C13—C15—H15B	110	H4E—C4—H4F	109.5

Table.4. Torsion angles of the compound

C3—N1—N2—C1	-0.04 (17)	O2—N3—C12—C2	179.59 (14)
C5—N1—N2—C1	179.47 (15)	O2—N3—C12—C14	0.62 (19)
C13—O2—N3—C12	3.02 (18)	C3—C2—C12—N3	179.79 (15)
N1—N2—C1—C2	-0.16 (18)	C1—C2—C12—N3	-1.8 (3)
N1—N2—C1—C4	-179.59 (14)	C3—C2—C12—C14	-1.3 (3)
N2—C1—C2—C3	0.29 (18)	C1—C2—C12—C14	177.10 (16)
C4—C1—C2—C3	179.66 (16)	N3—C12—C14—C13	-3.7 (2)
N2—C1—C2—C12	-178.41 (15)	C2—C12—C14—C13	177.34 (15)
C4—C1—C2—C12	1.0 (3)	N3—O2—C13—C15	119.60 (14)
N2—N1—C3—O1	176.84 (13)	N3—O2—C13—C14	-5.17 (18)
C5—N1—C3—O1	-2.6 (2)	C12—C14—C13—O2	5.06 (18)
N2—N1—C3—C2	0.23 (17)	C12—C14—C13—C15	-114.87 (16)
C5—N1—C3—C2	-179.24 (15)	C16—O3—C15—C13	174.63 (15)
C6—O1—C3—N1	90.33 (17)	O2—C13—C15—O3	-72.19 (18)
C6—O1—C3—C2	-93.91 (19)	C14—C13—C15—O3	45.6 (2)
C1—C2—C3—N1	-0.31 (17)	C15—O3—C16—C17	-22.5 (3)
C12—C2—C3—N1	178.48 (14)	C15—O3—C16—C21	159.36 (18)
C1—C2—C3—O1	-176.44 (15)	C17—C16—C21—C20	-0.1 (3)
C12—C2—C3—O1	2.3 (3)	O3—C16—C21—C20	178.15 (19)
C3—O1—C6—C7	6.1 (2)	C16—C21—C20—C19	-0.5 (3)
C3—O1—C6—C11	-174.30 (14)	C21—C20—C19—C18	0.1 (3)
C11—C6—C7—C8	0.6 (3)	C21—C20—C19—O4	179.71 (19)
O1—C6—C7—C8	-179.77 (17)	O4—C19—C18—C17	-178.6 (2)
C6—C7—C8—C9	-0.6 (3)	C20—C19—C18—C17	0.9 (3)
C7—C8—C9—C10	0.3 (4)	C21—C16—C17—C18	1.2 (3)
C8—C9—C10—C11	0.0 (3)	O3—C16—C17—C18	-176.9 (2)
C7—C6—C11—C10	-0.3 (3)	C19—C18—C17—C16	-1.6 (4)
O1—C6—C11—C10	-179.95 (15)	C18—C19—O4—C22	-4.1 (3)
C9—C10—C11—C6	0.0 (3)	C20—C19—O4—C22	176.29 (19)

Table.5. Hydrogen bonding geometry of the molecule.

D—H...A (Å, °)	(D—H) (Å)	(H...A) (Å)	(D...A) (Å)	(D—H...A) (°)
C11—H11...N3	0.93	2.46	3.306	151
C7—H7...O4	0.93	2.62	3.398	140