Copper-catalyzed cascade three-component azide-alkyne cycloaddition/condensation/transesterification: easy access to 3-triazolylcoumarins

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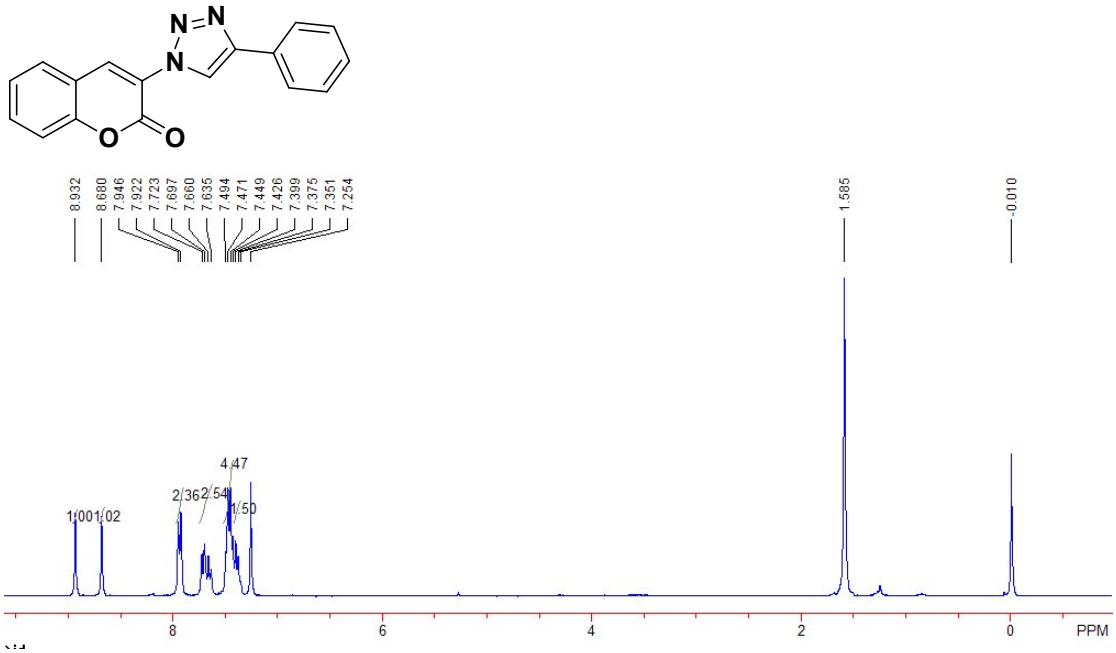
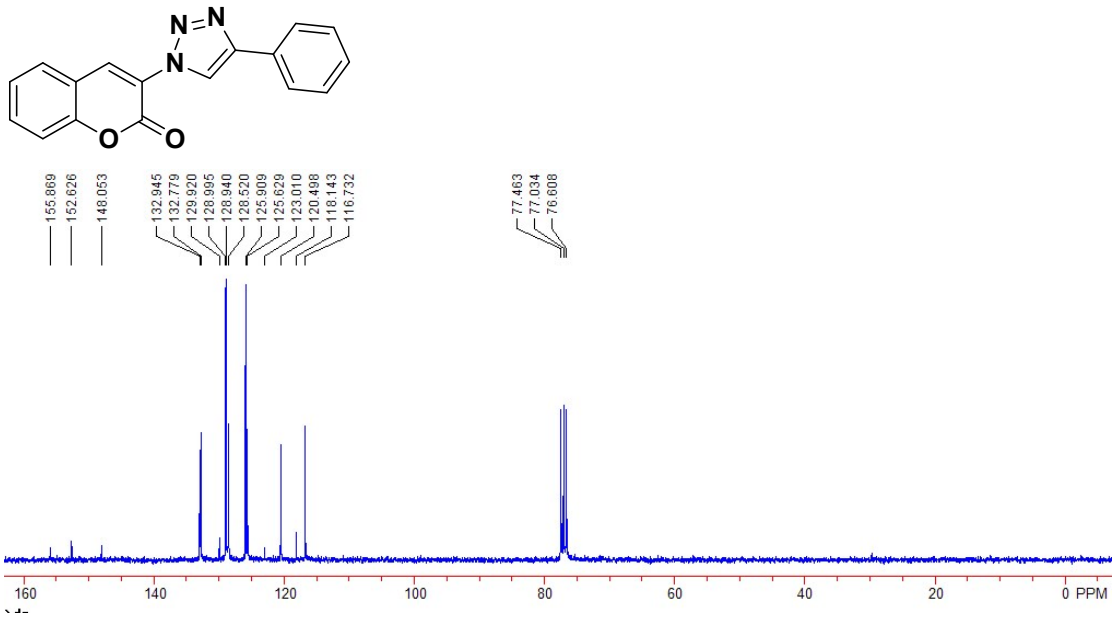
^{1}H and ^{13}C NMR spectra of compound 4a





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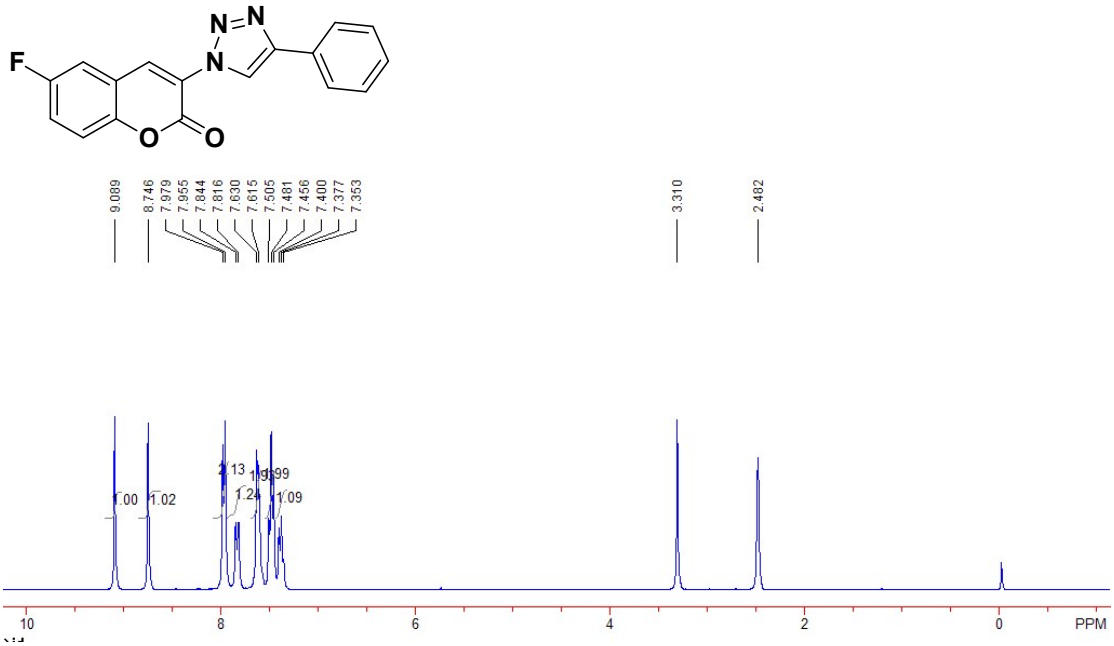

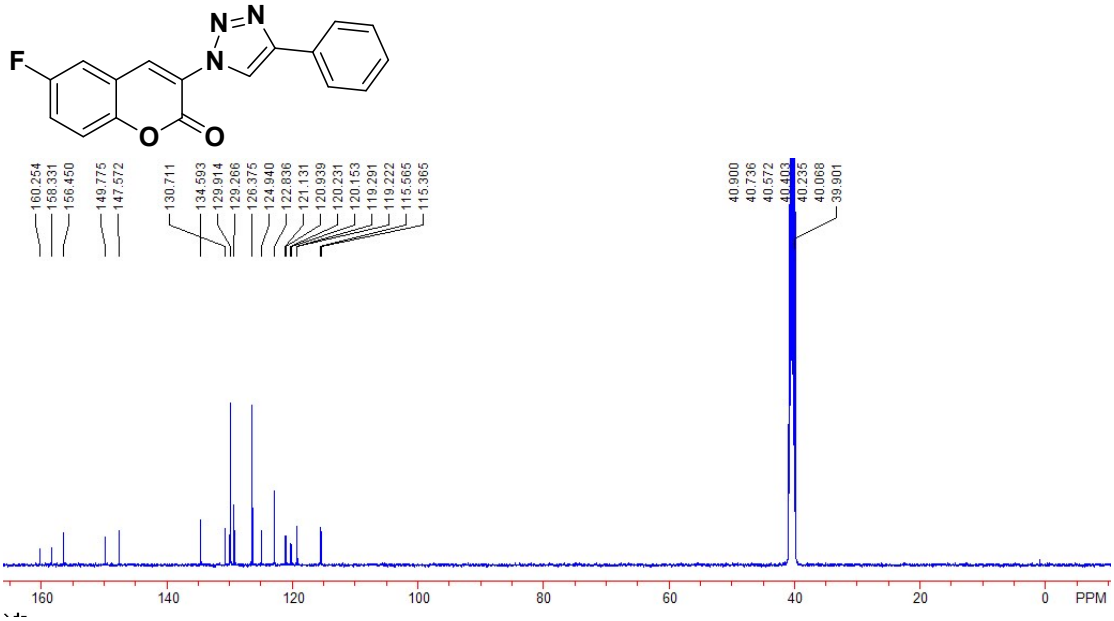

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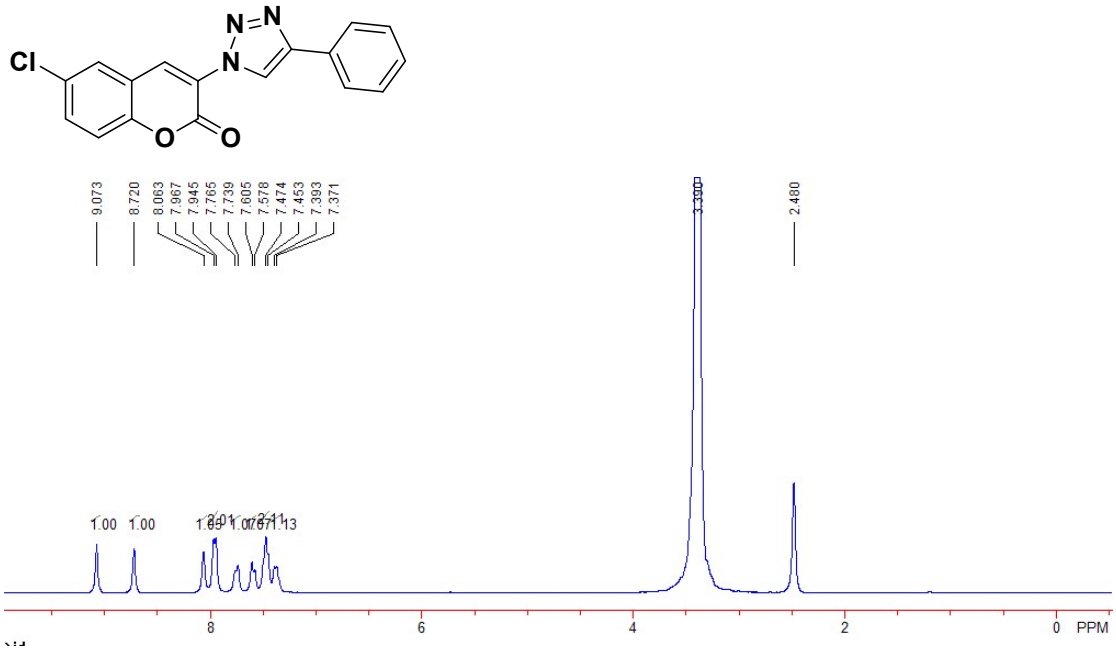

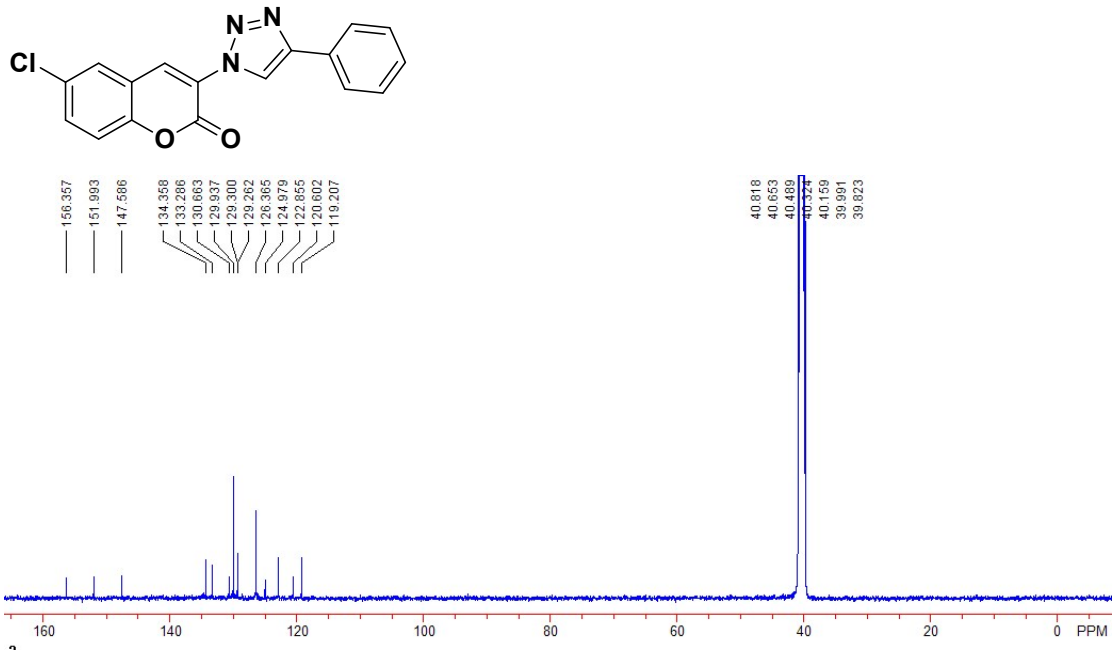

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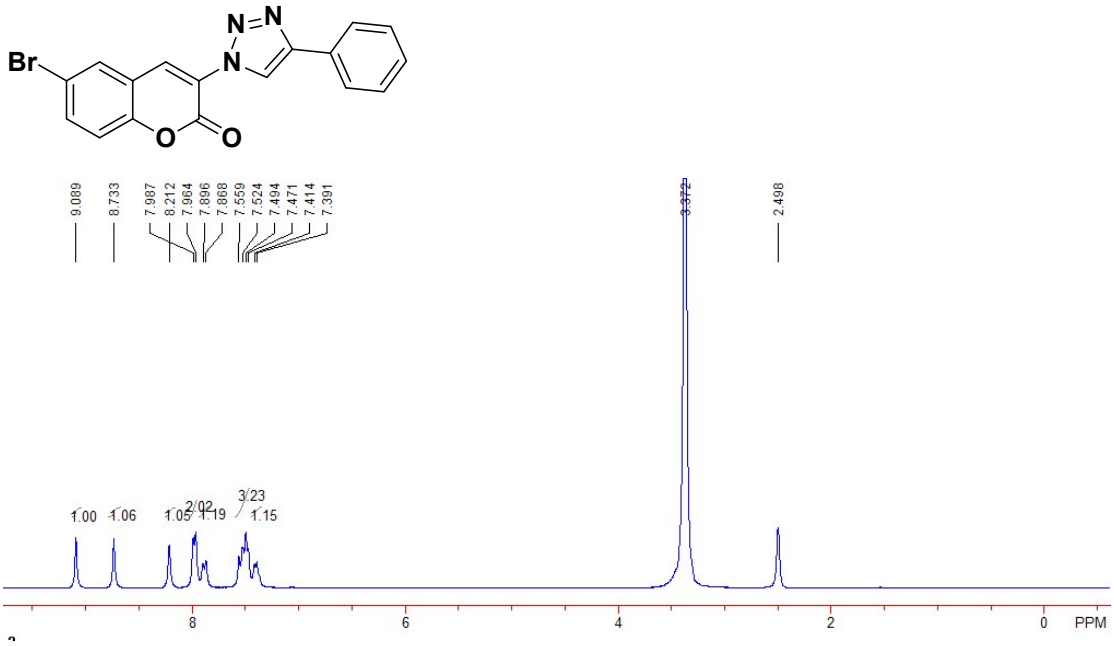

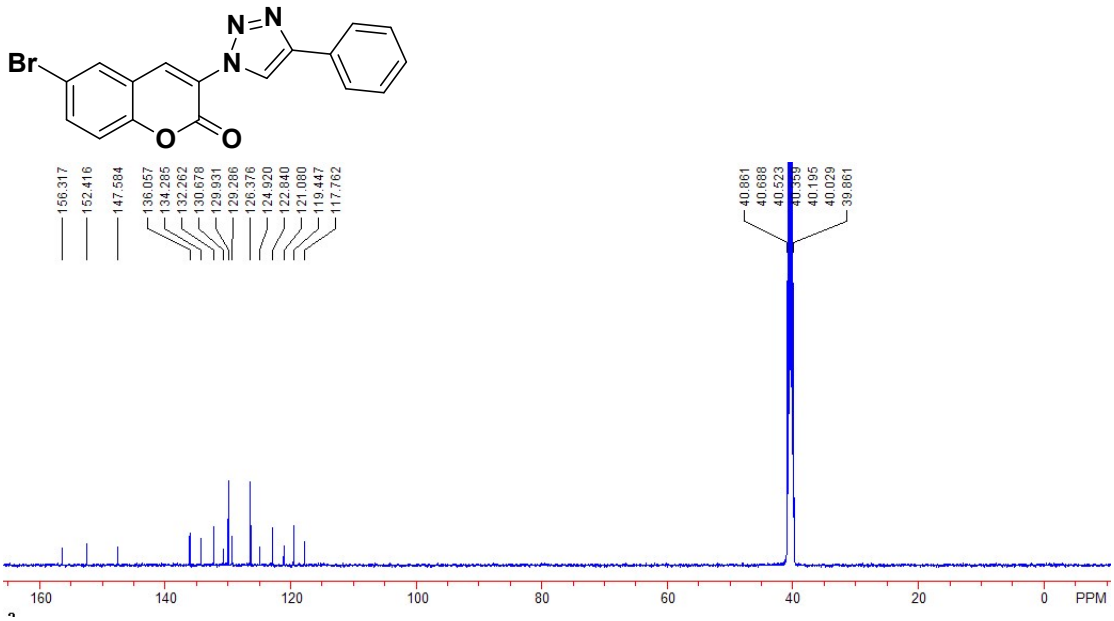

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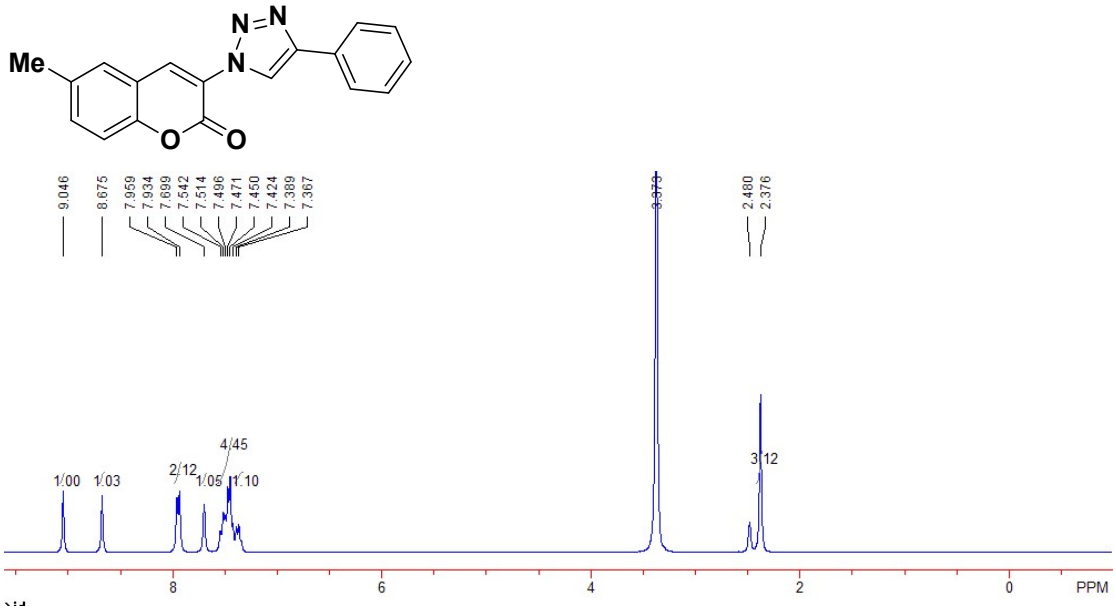

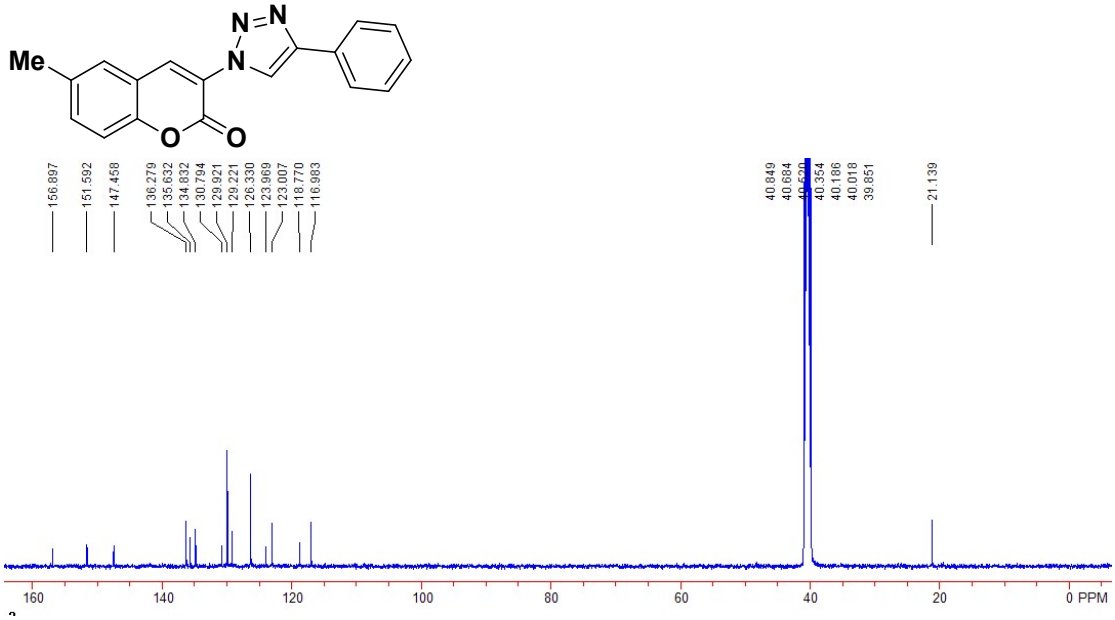

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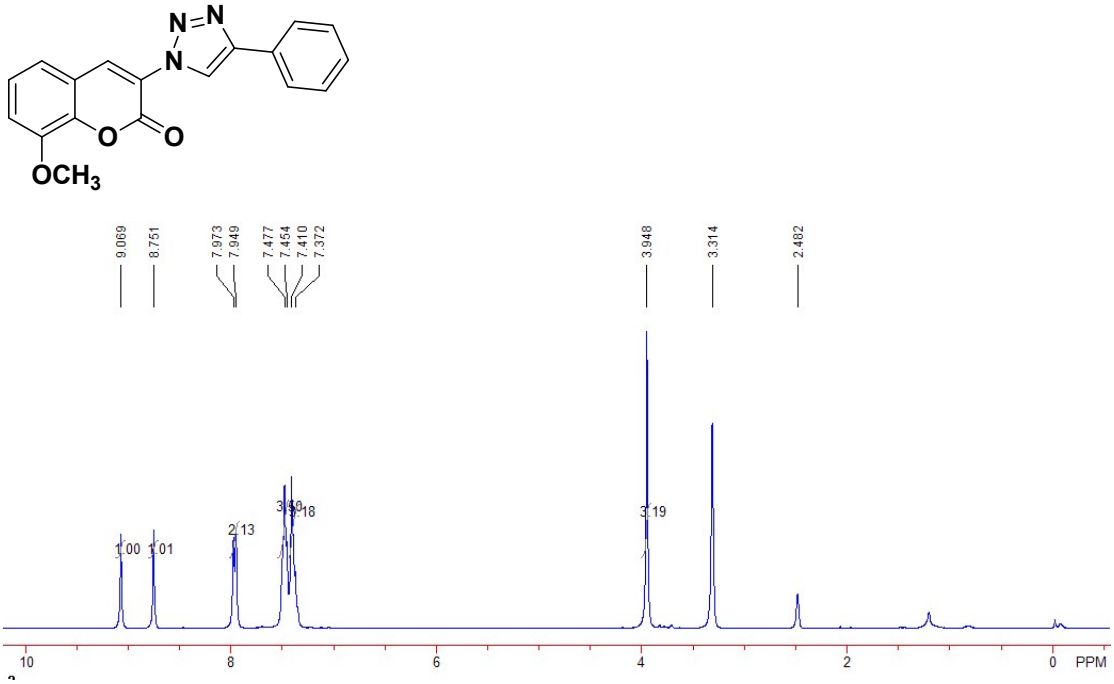

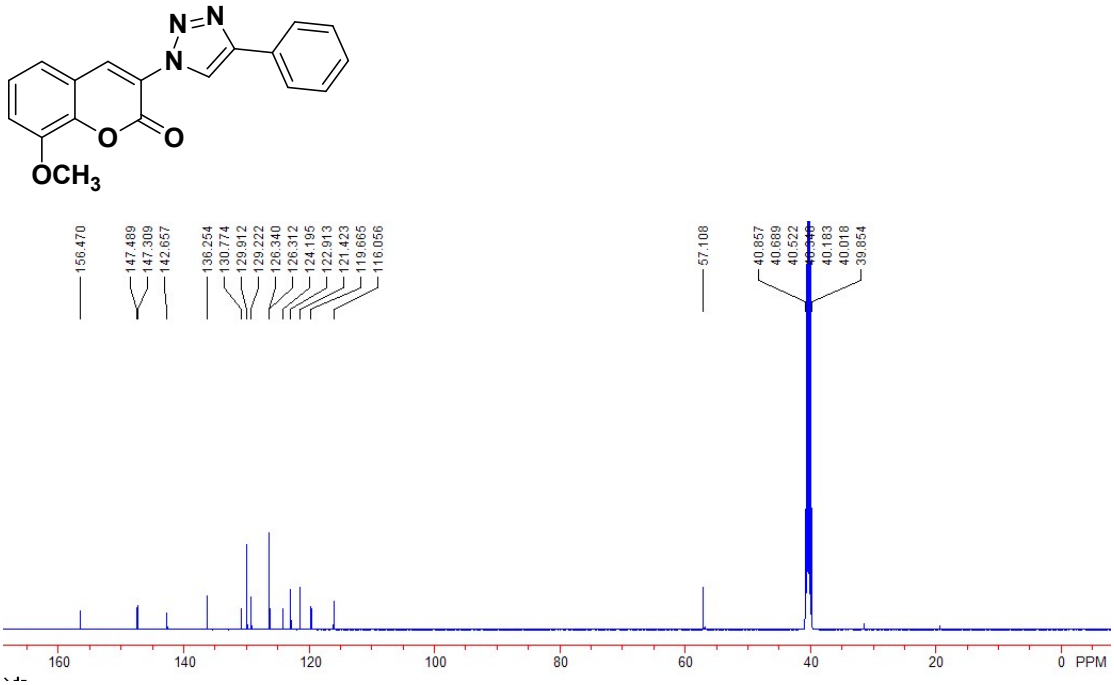

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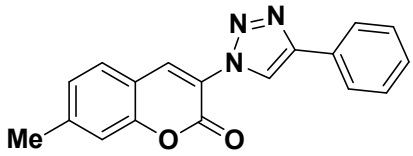
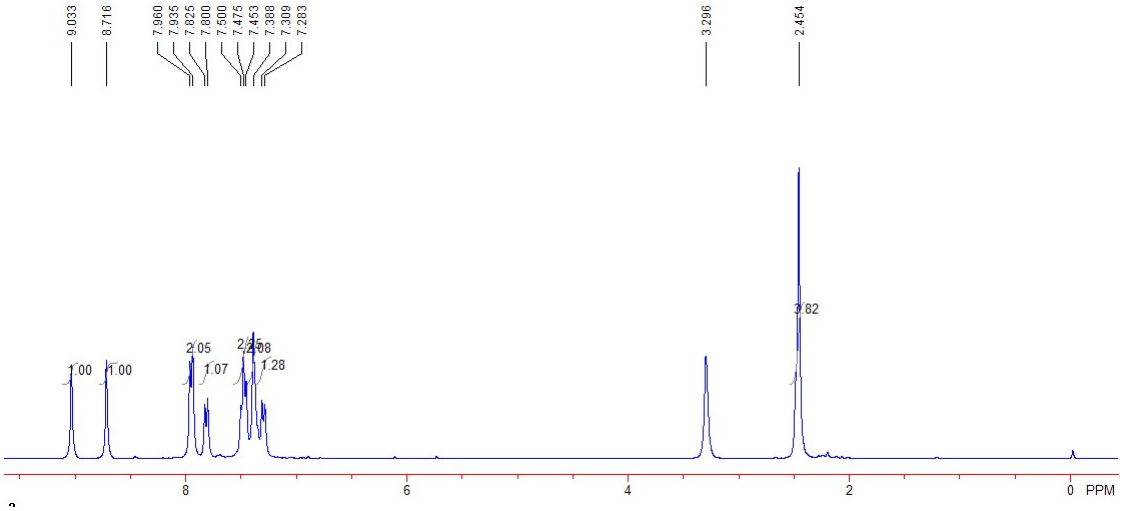
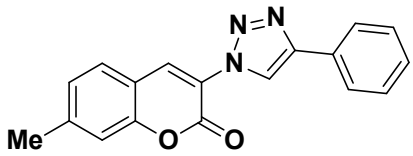
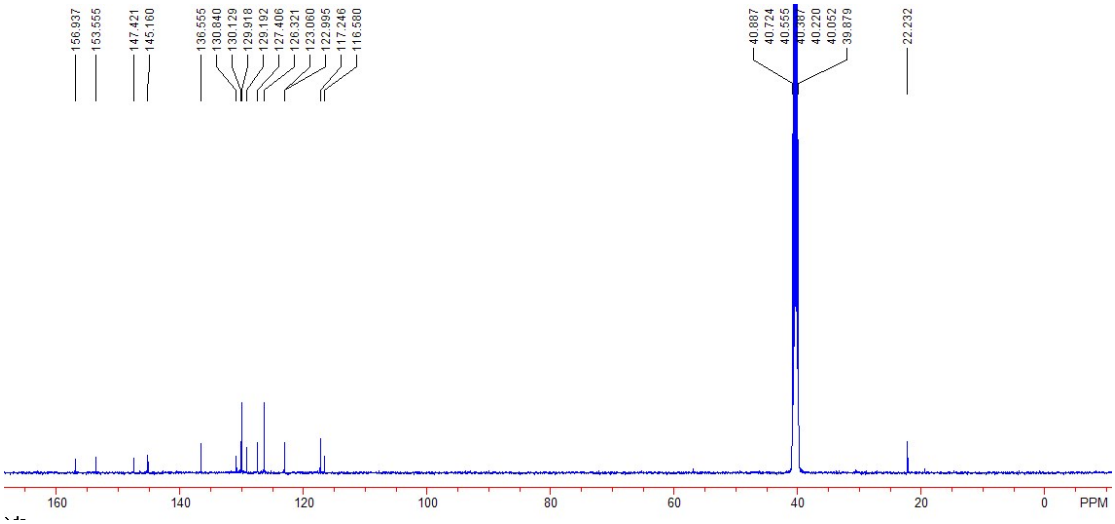
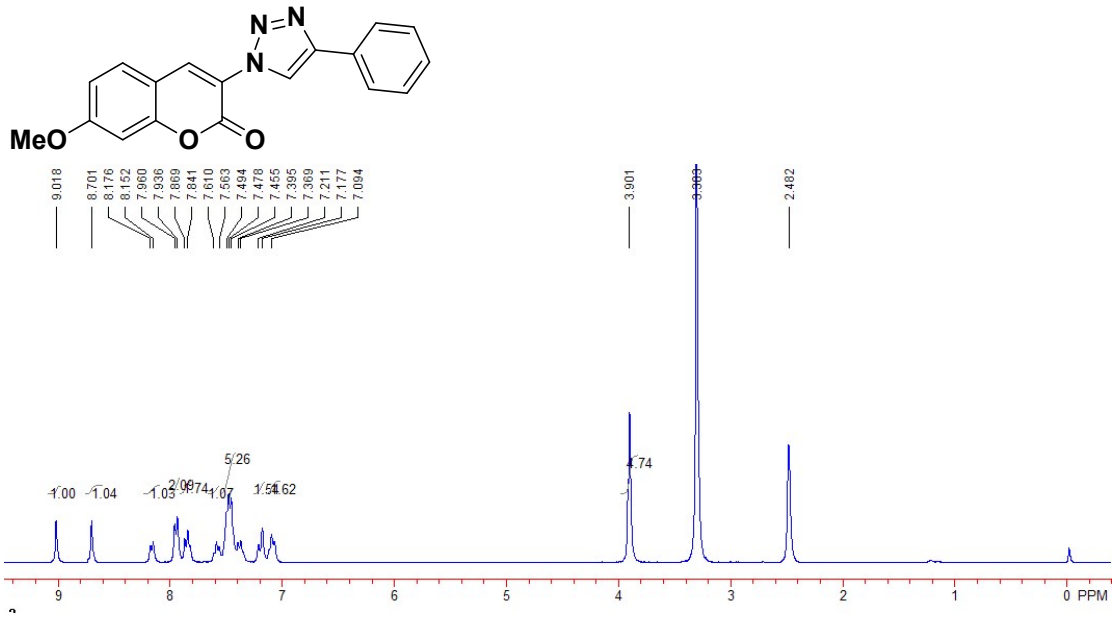


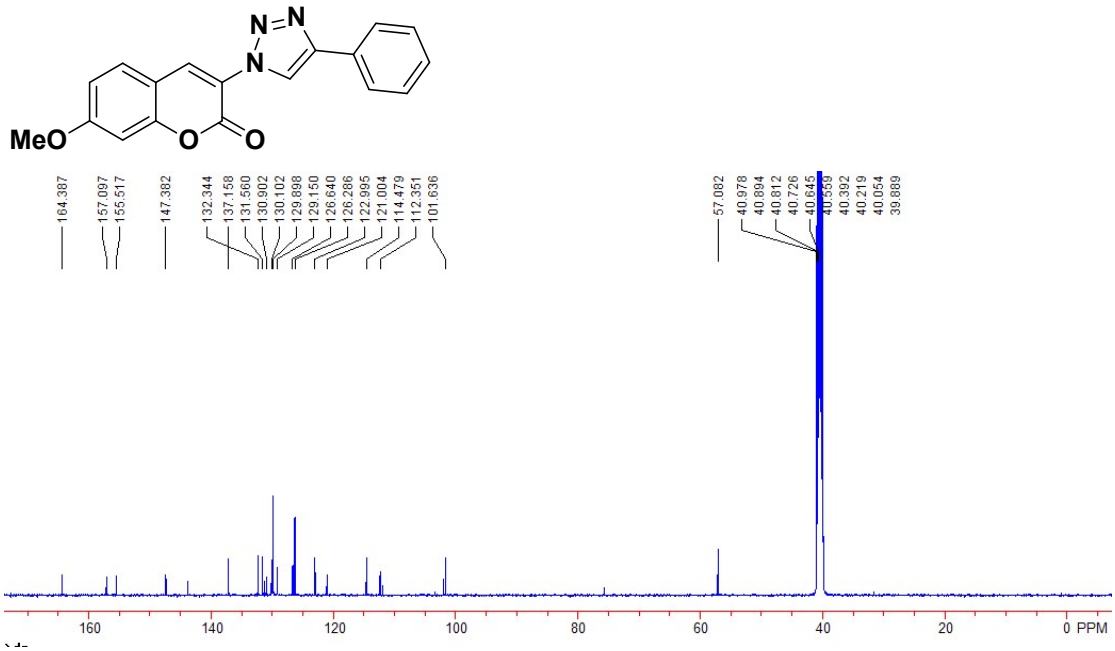




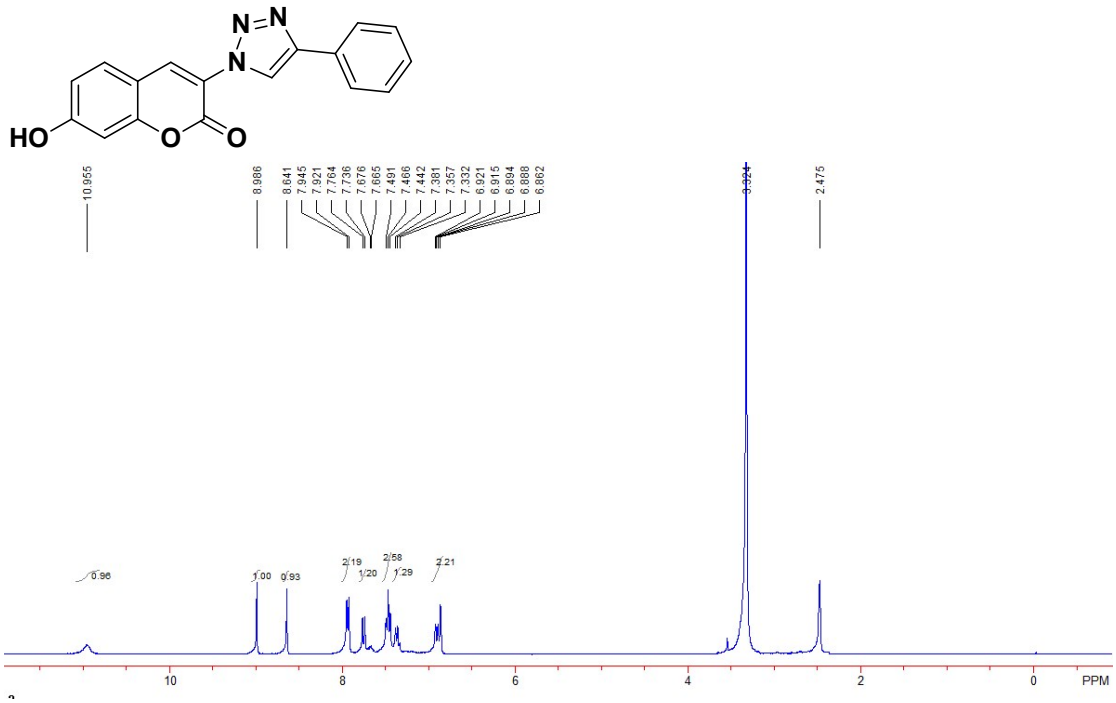


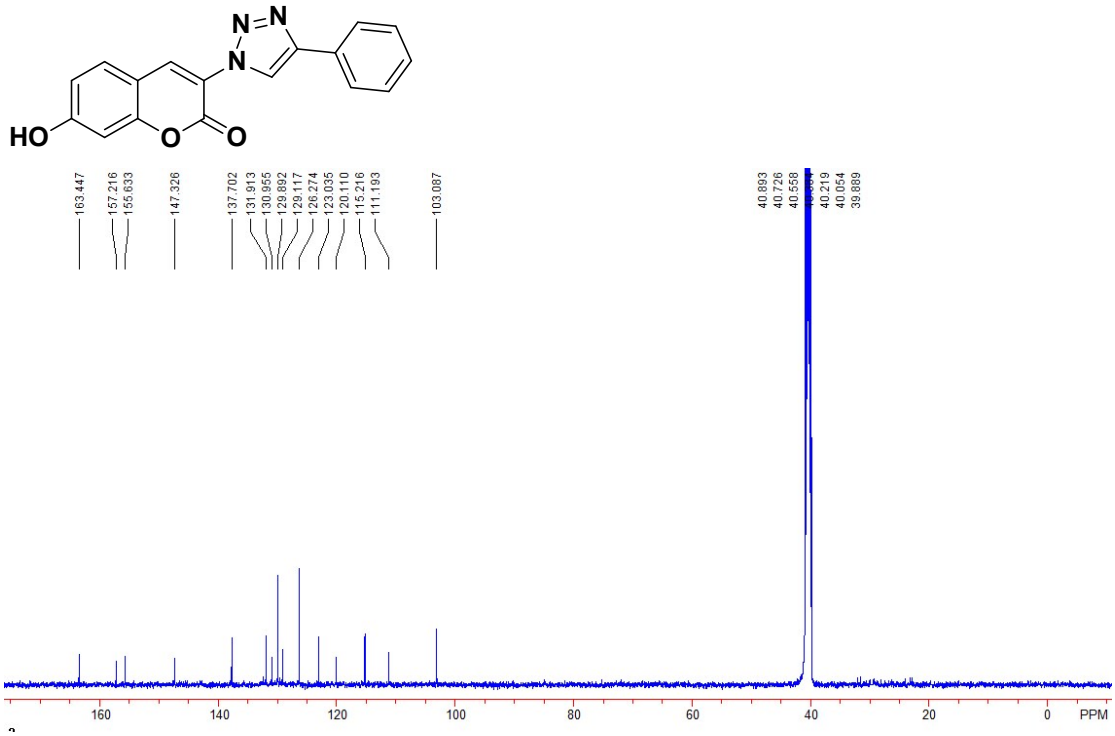
^{1}H and ^{13}C NMR spectra of compound 4i





^{1}H and ^{13}C NMR spectra of compound 4j





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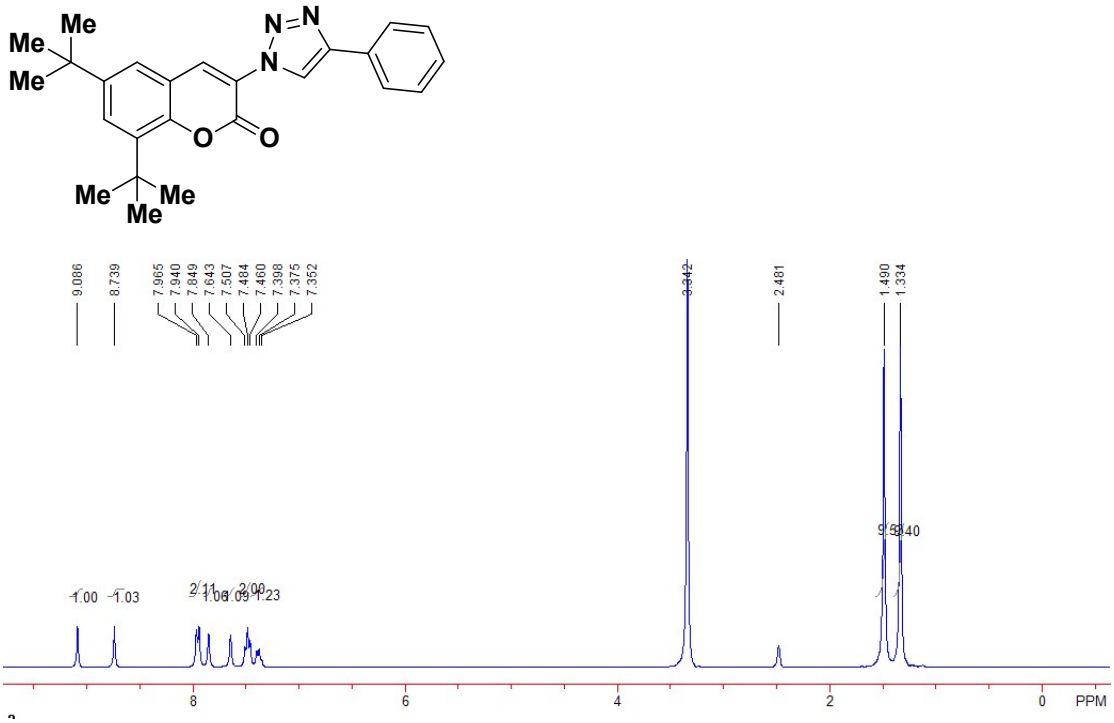

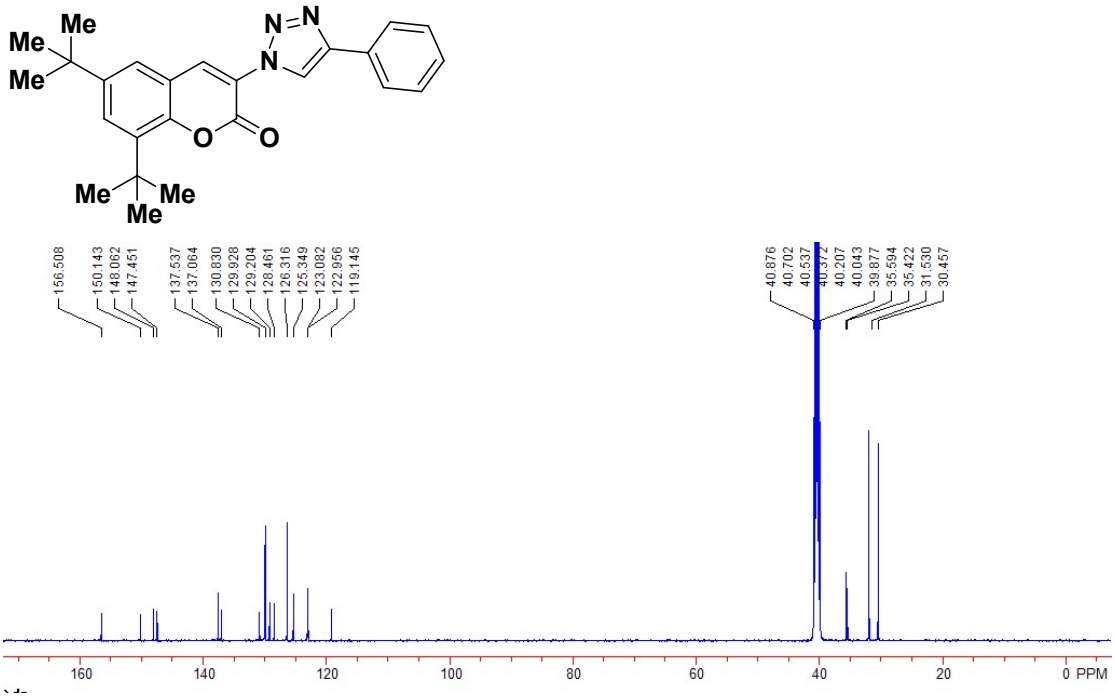

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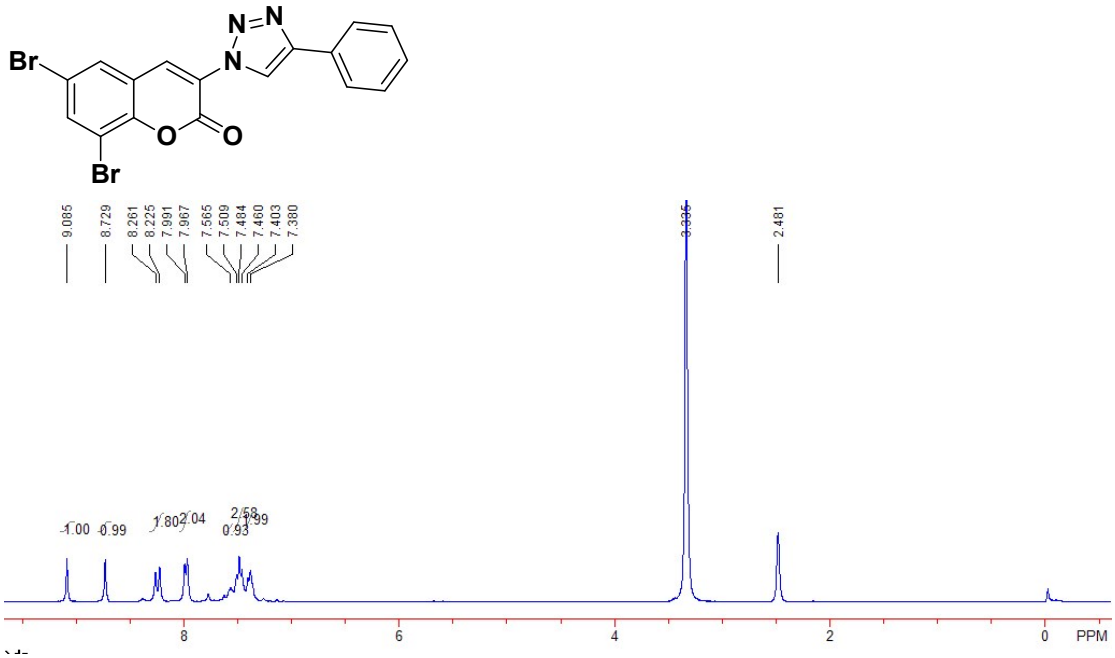
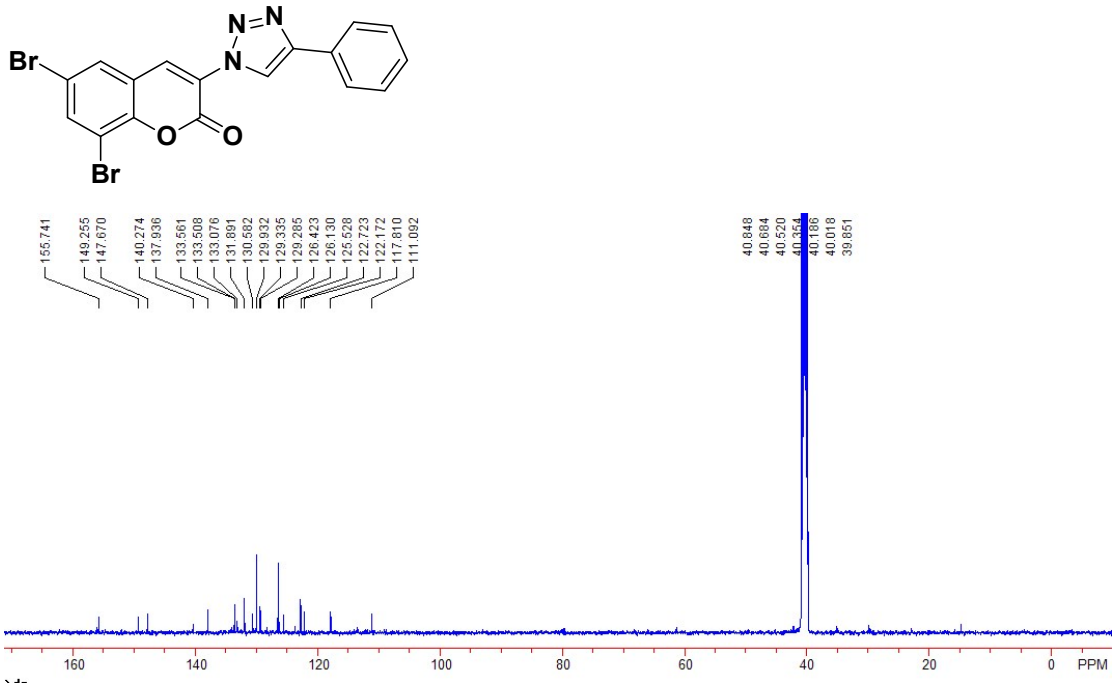
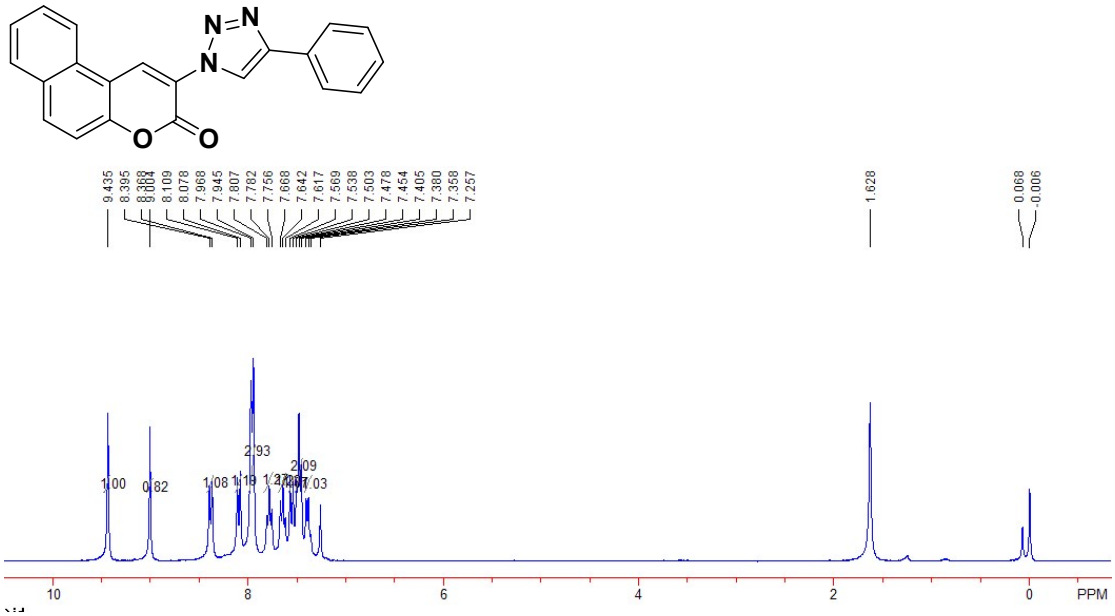
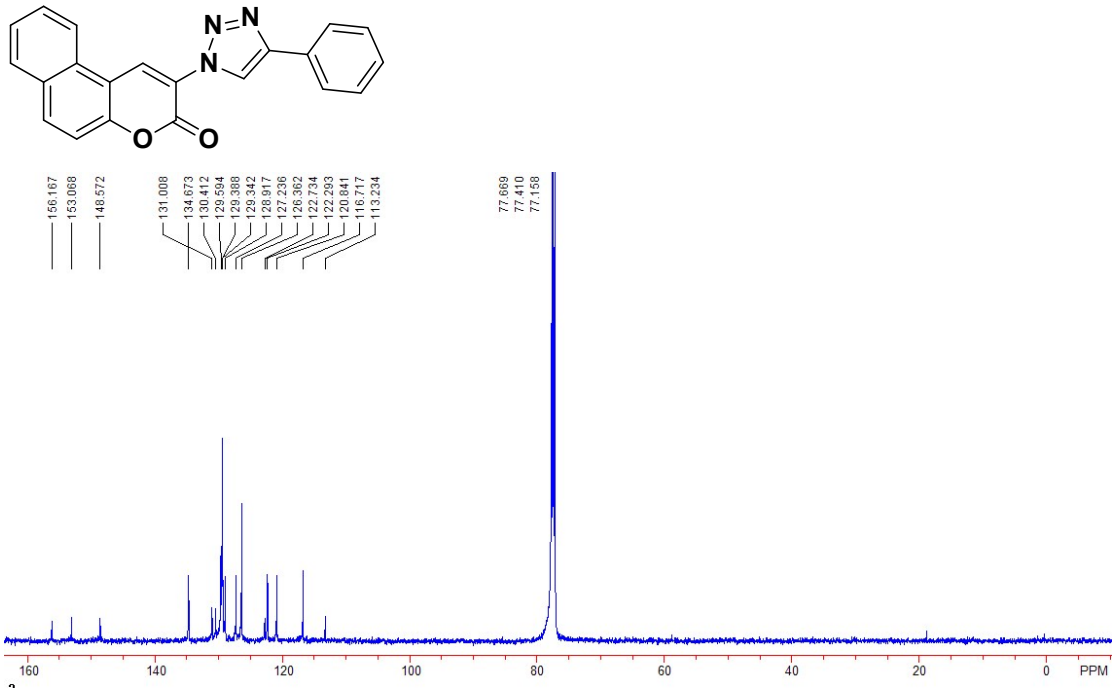


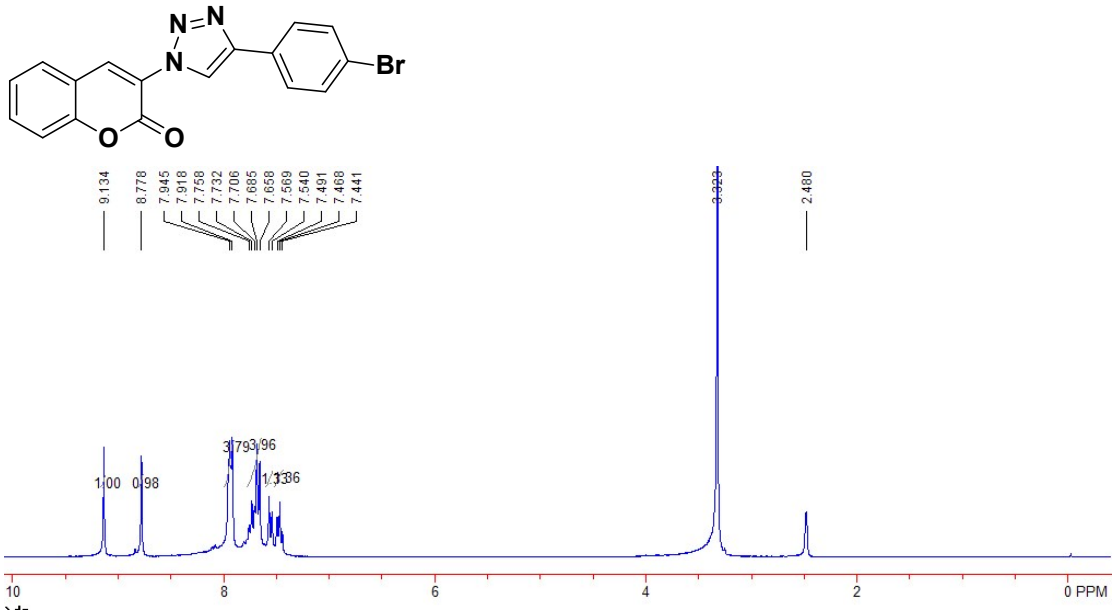


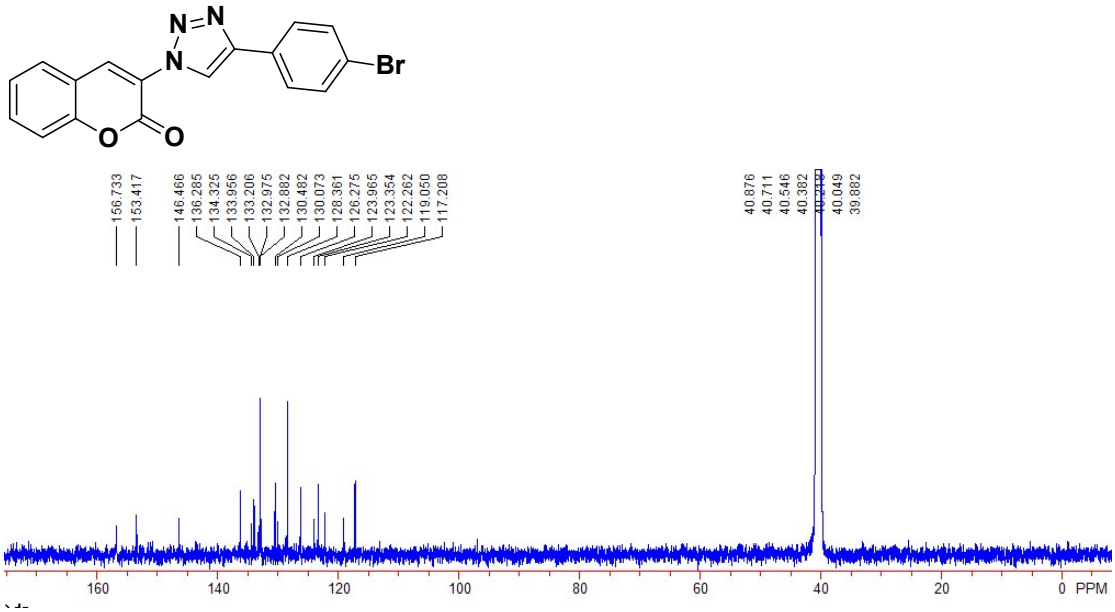
^{1}H and ^{13}C NMR spectra of compound 4n



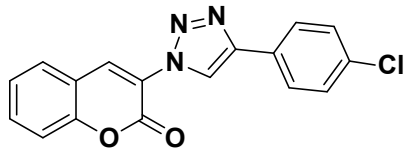


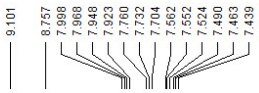
^{1}H and ^{13}C NMR spectra of compound 4o

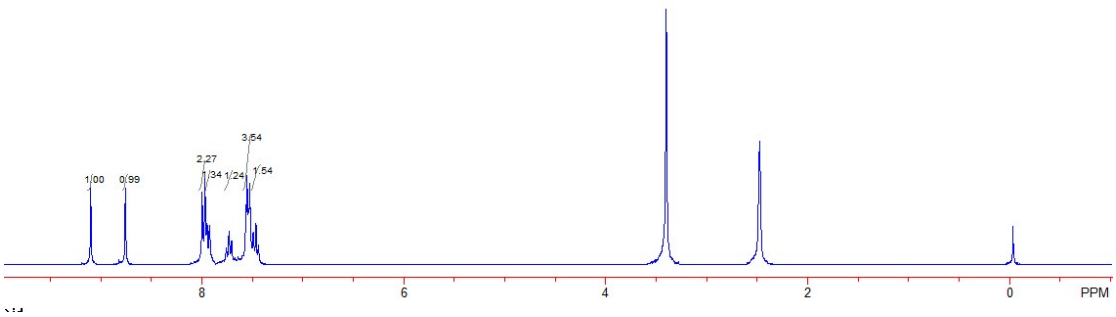


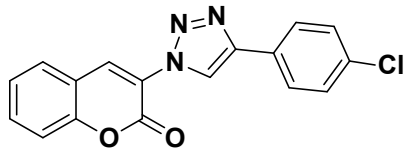


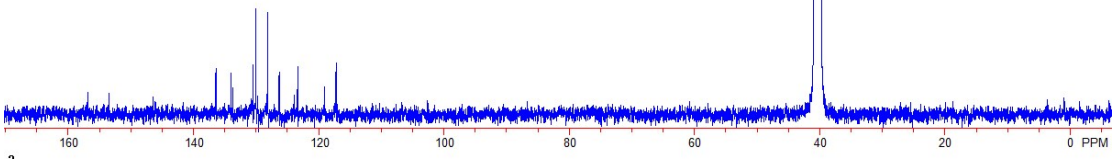
^{1}H and ^{13}C NMR spectra of compound 4p



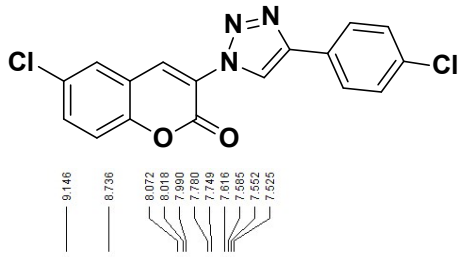


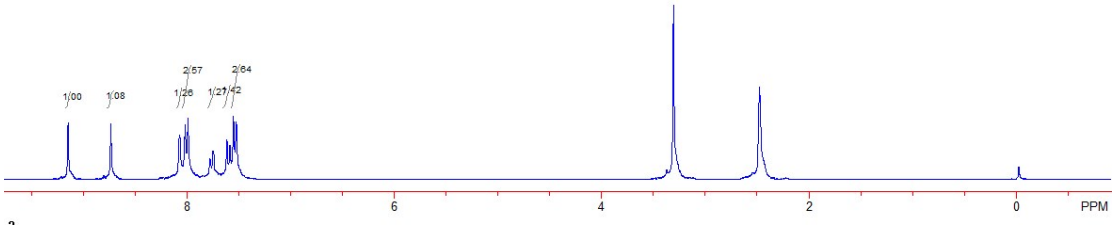


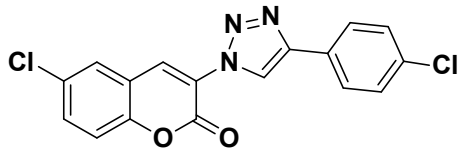


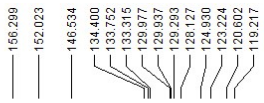


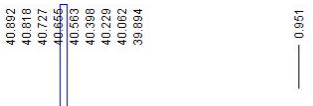
^{1}H and ^{13}C NMR spectra of compound 4q

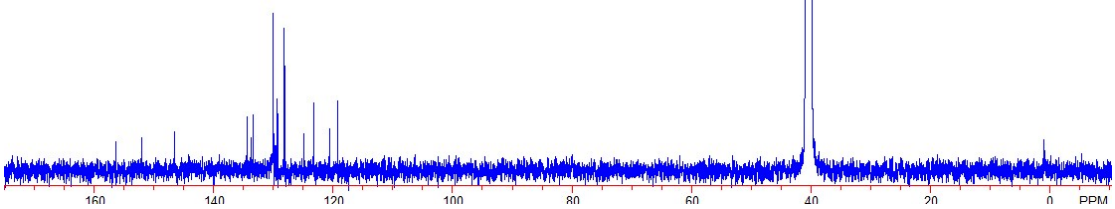




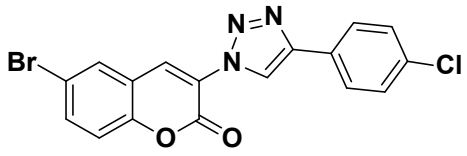


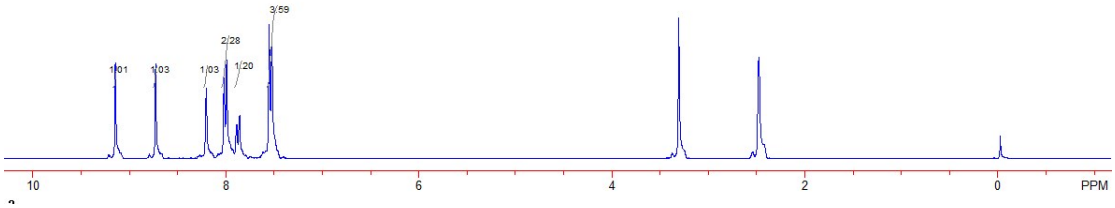


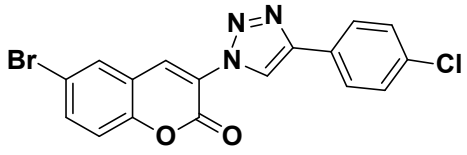


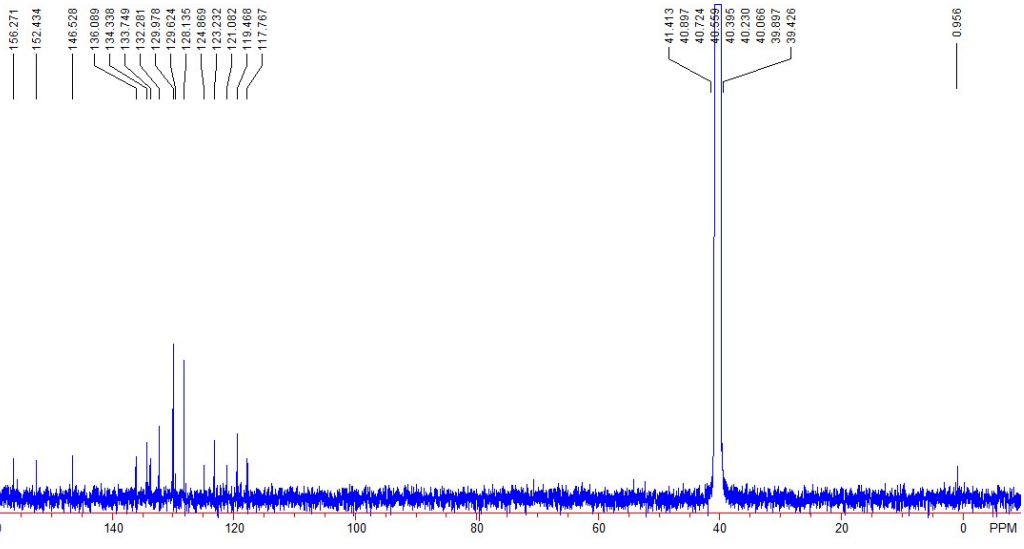


^{1}H and ^{13}C NMR spectra of compound 4r

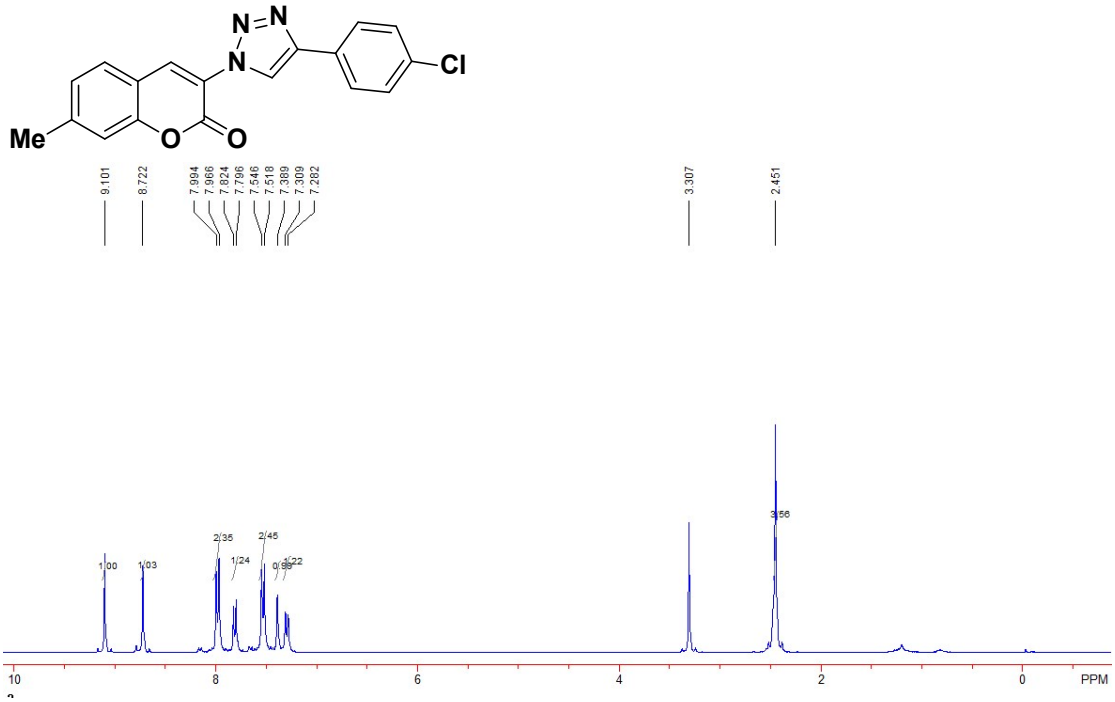


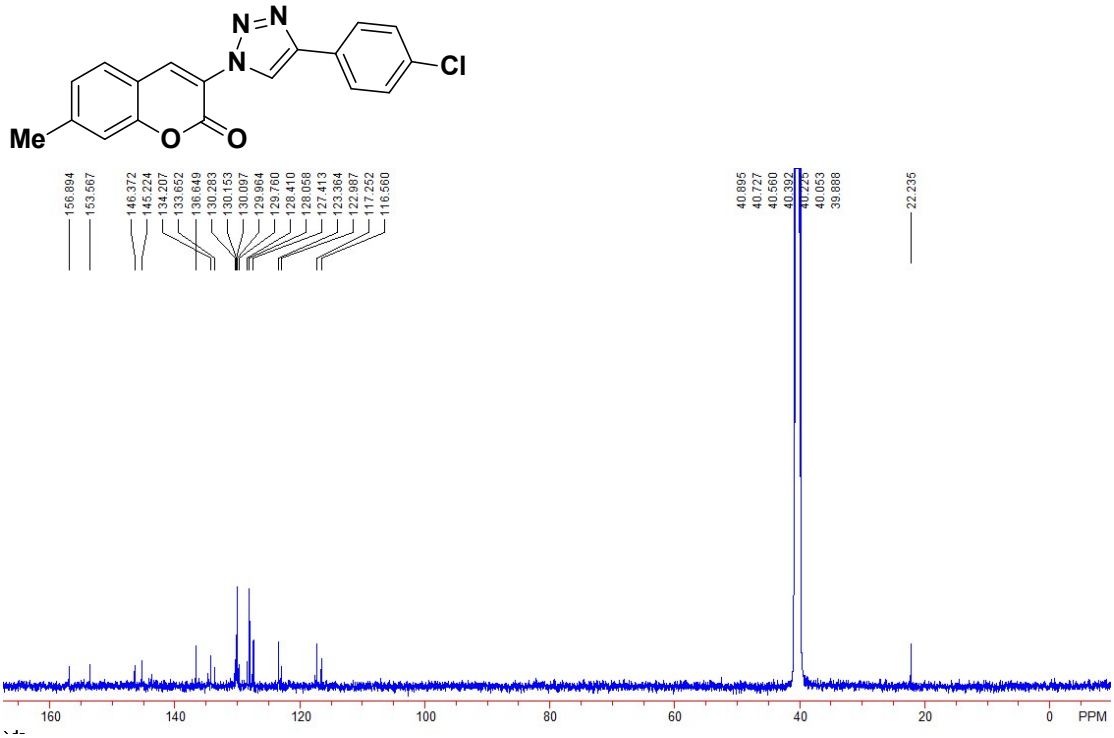






^{1}H and ^{13}C NMR spectra of compound 4s





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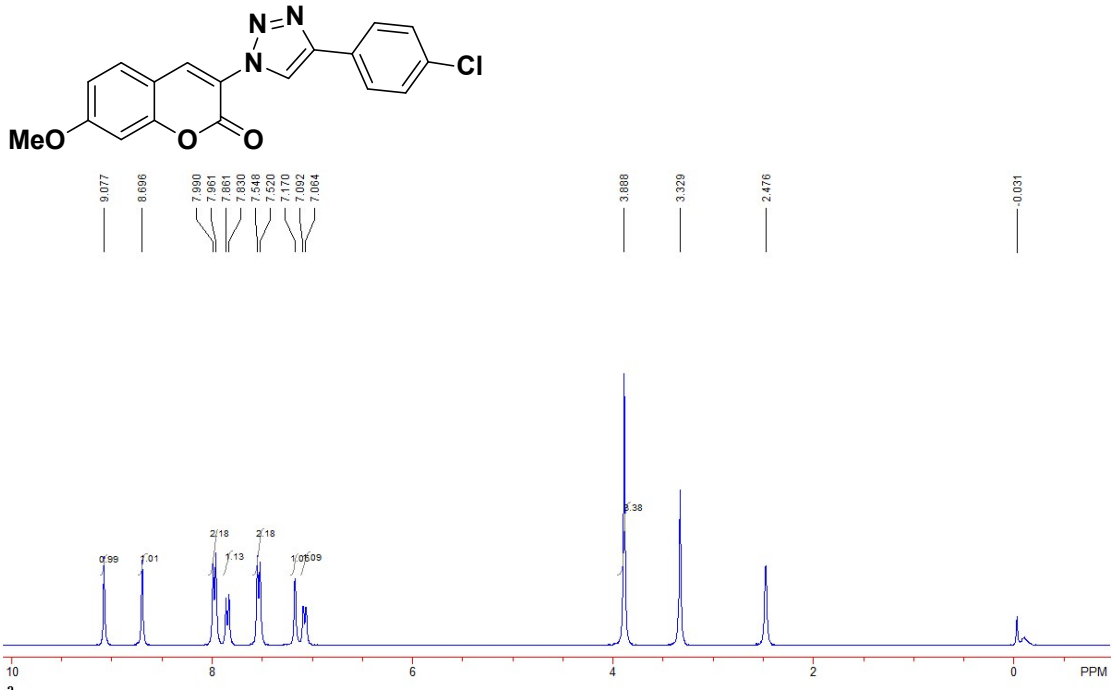

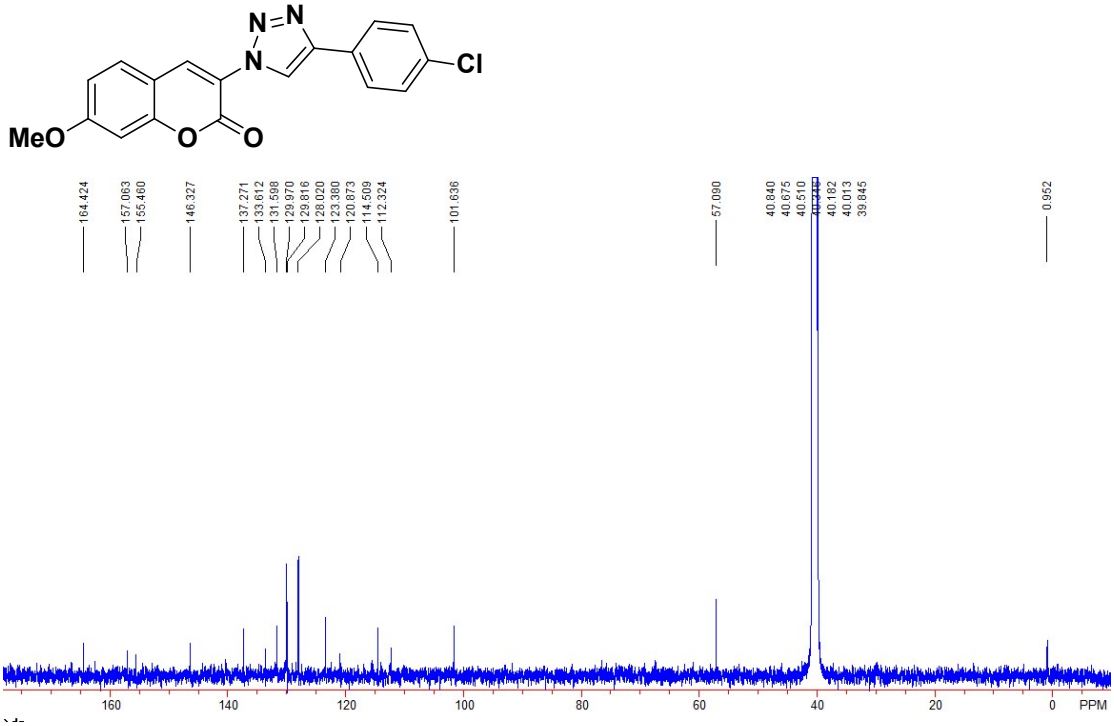

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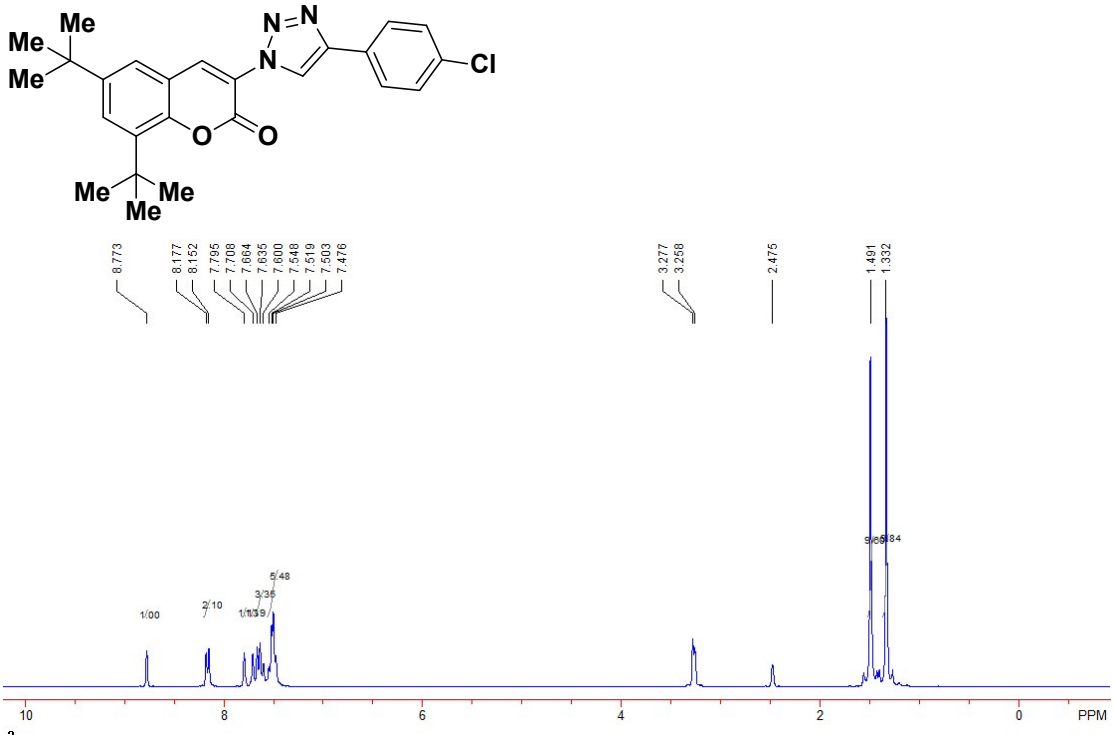
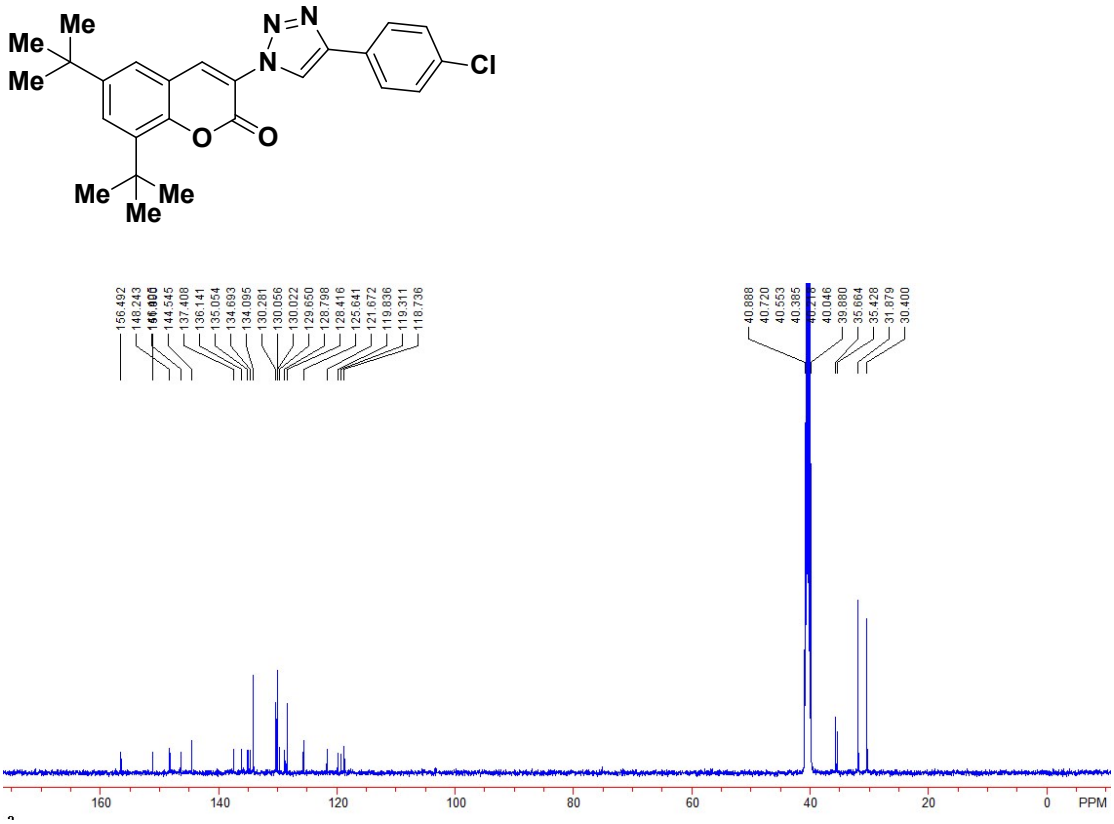
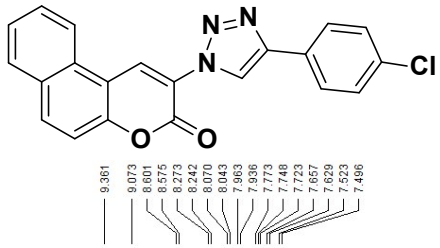
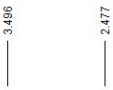
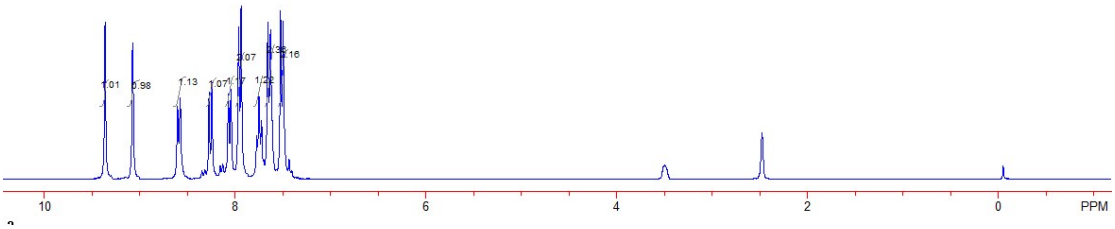


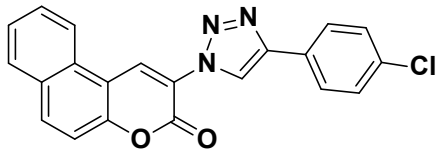


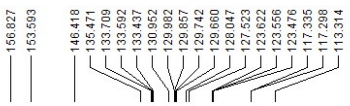
^{1}H and ^{13}C NMR spectra of compound 4v

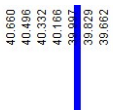


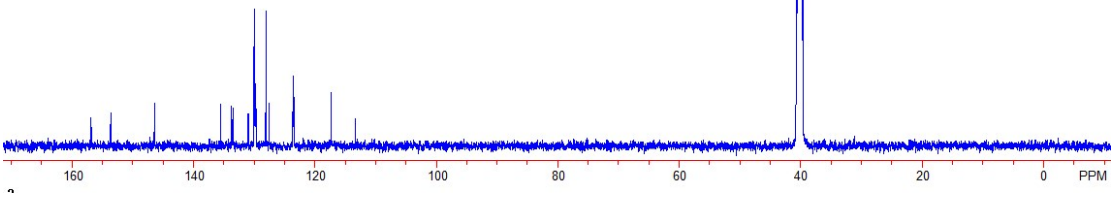




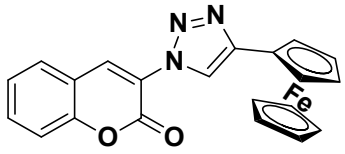


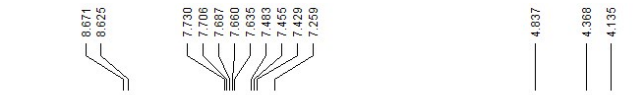


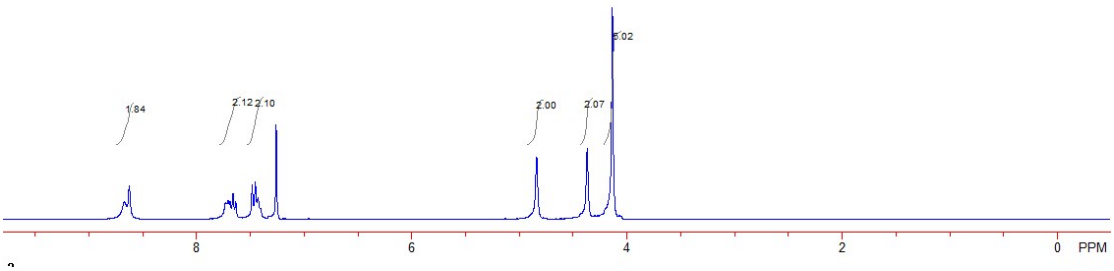


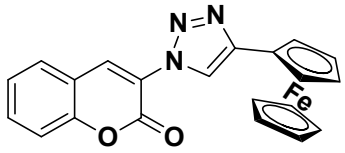


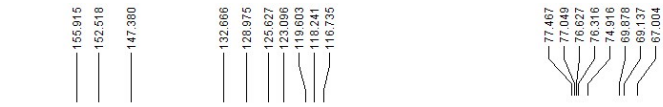
^{1}H and ^{13}C NMR spectra of compound 4w

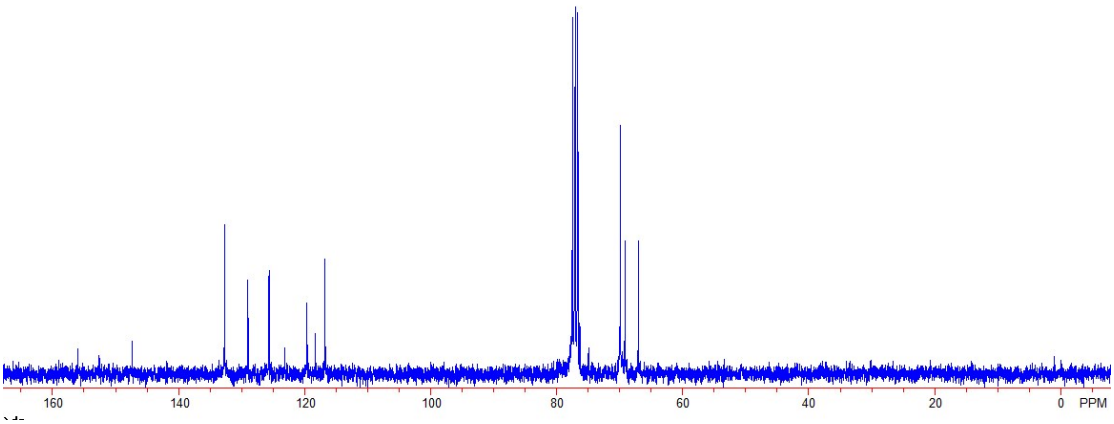




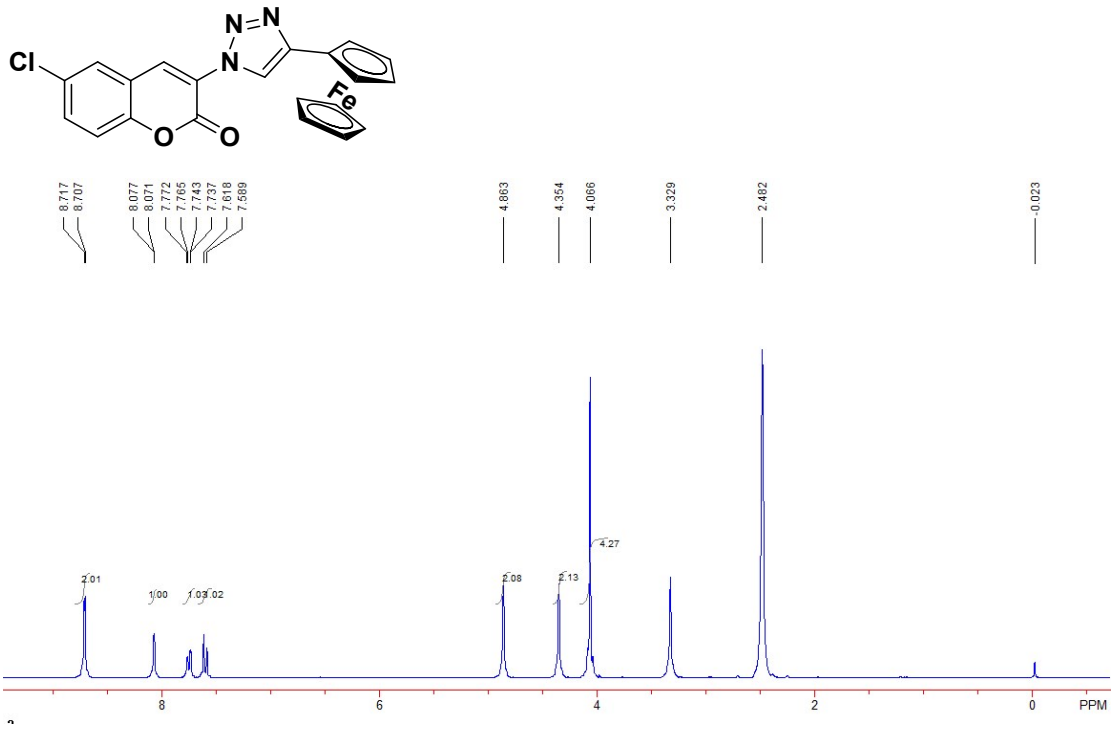


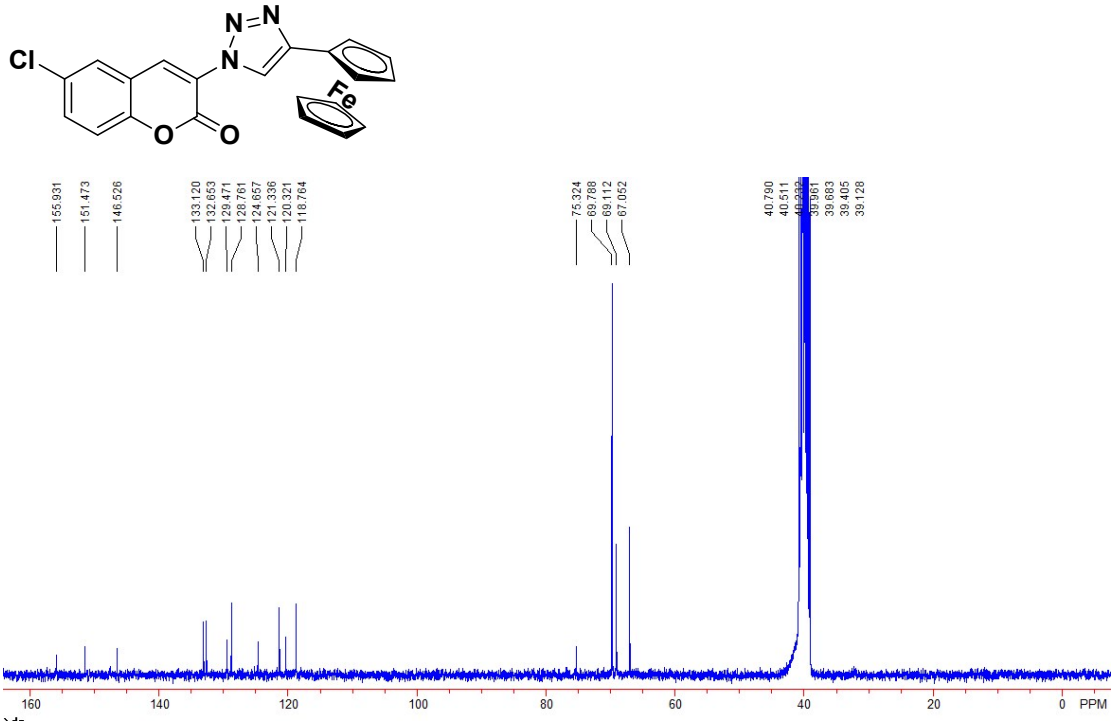




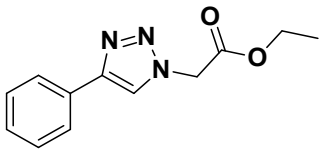


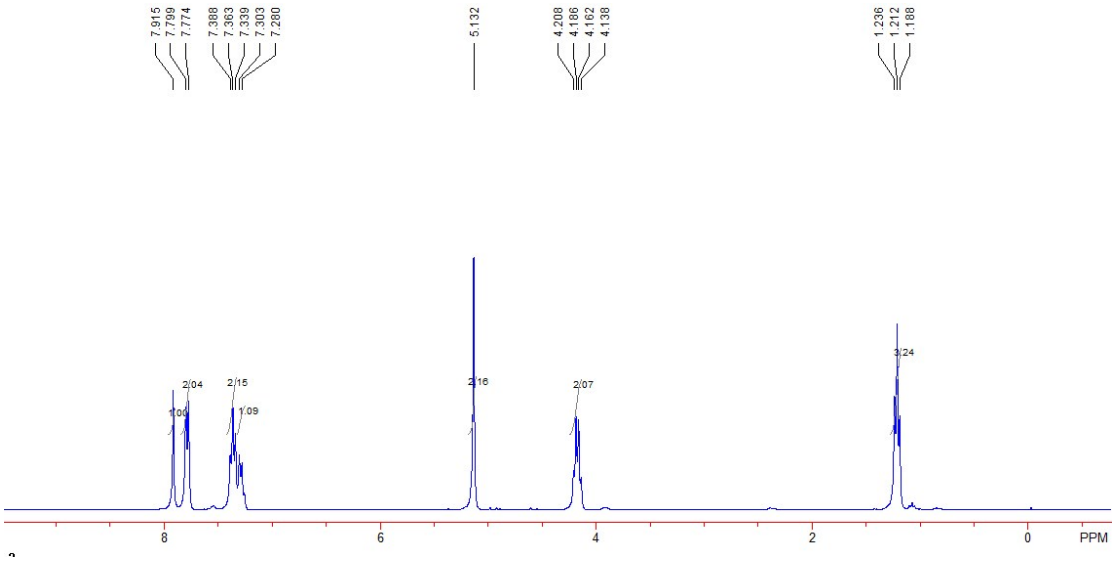
^{1}H and ^{13}C NMR spectra of compound 4x

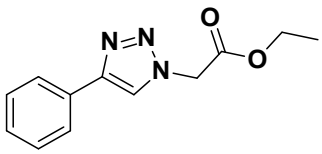


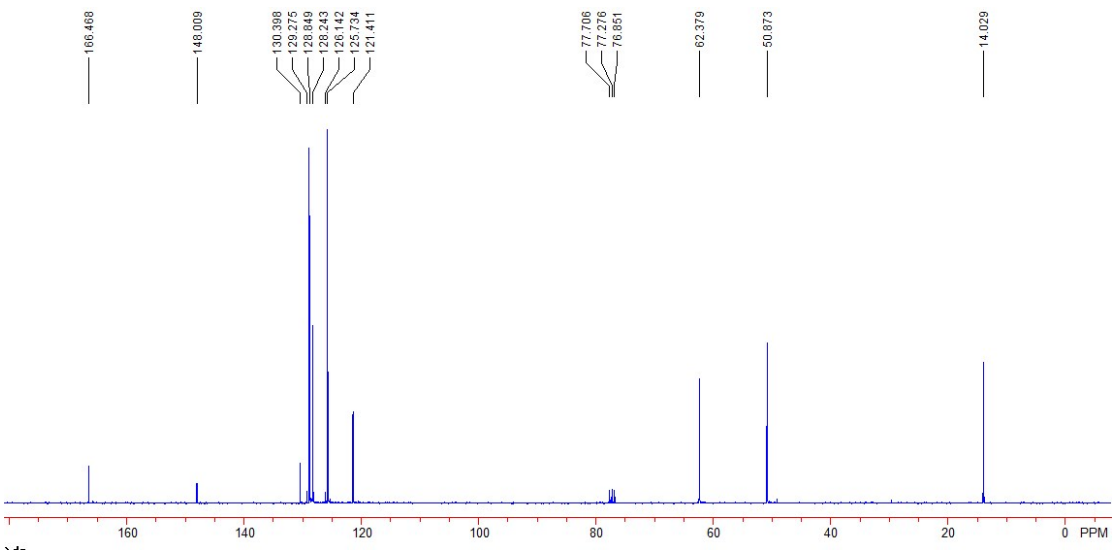


^{1}H and ^{13}C NMR spectra of compound 5a

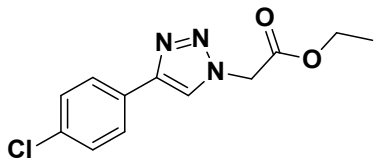


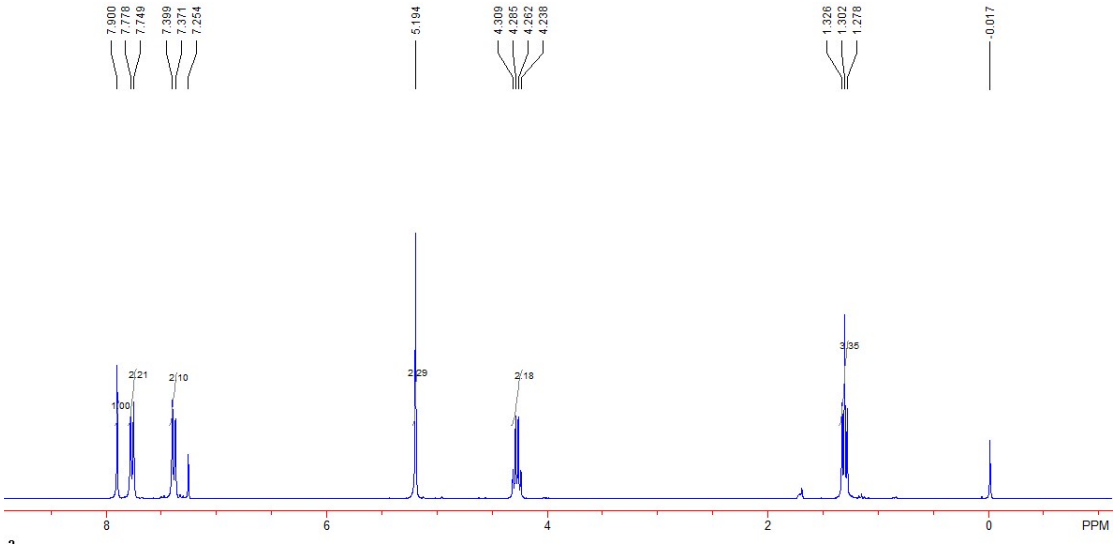


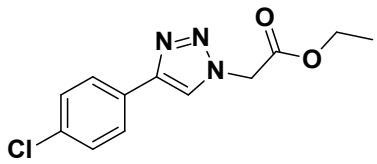


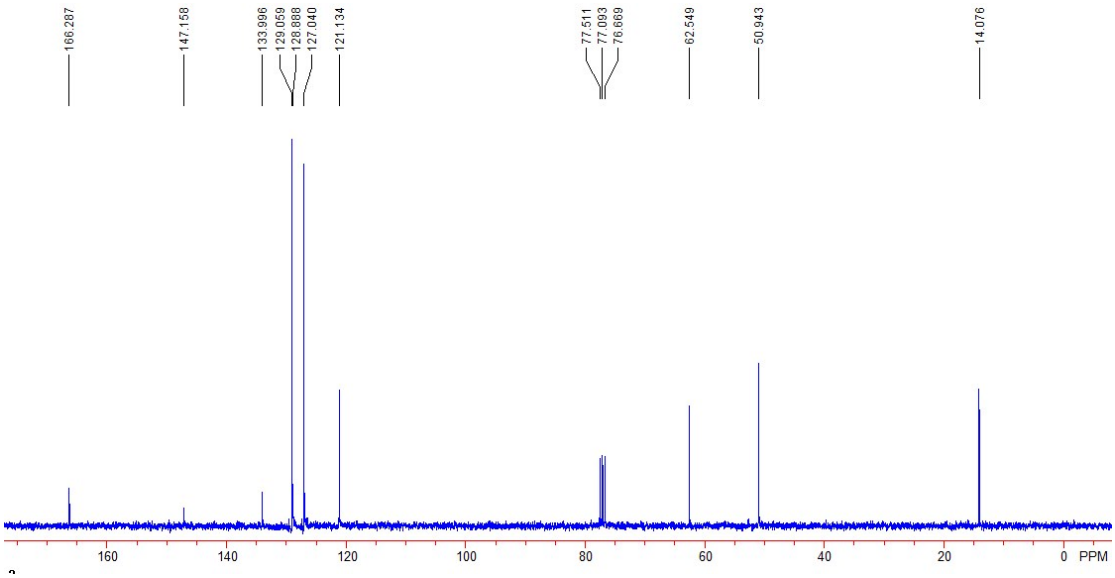


^{1}H and ^{13}C NMR spectra of compound 5c



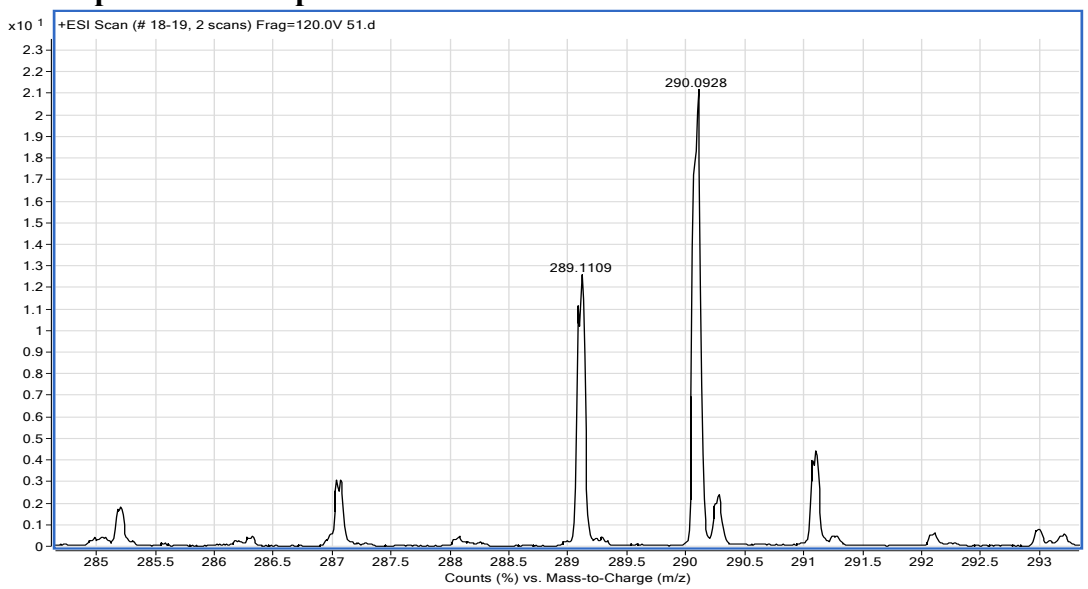




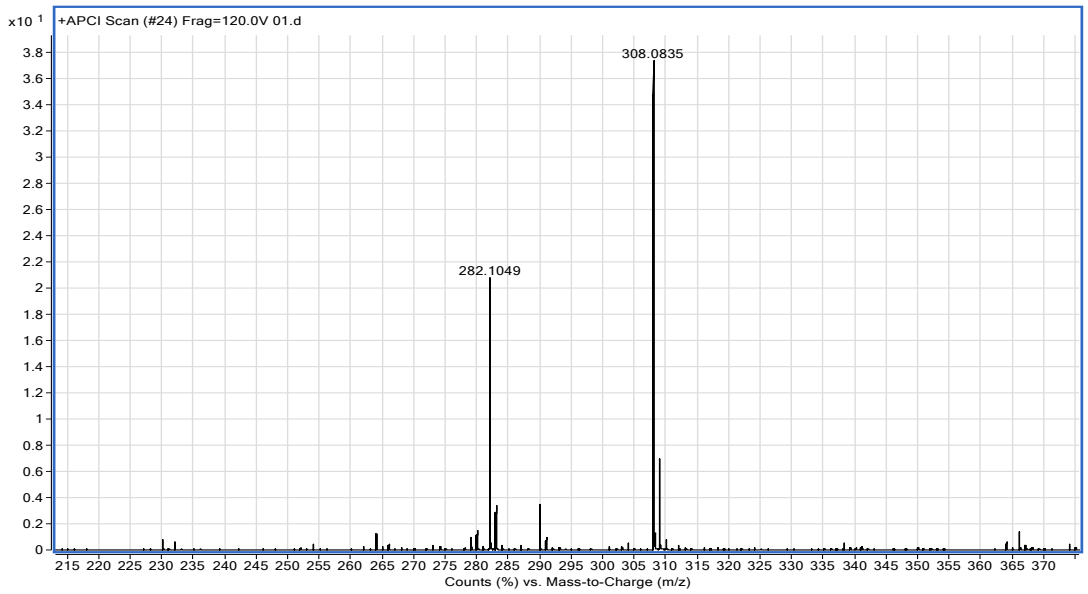


HRMS spectra for all compounds

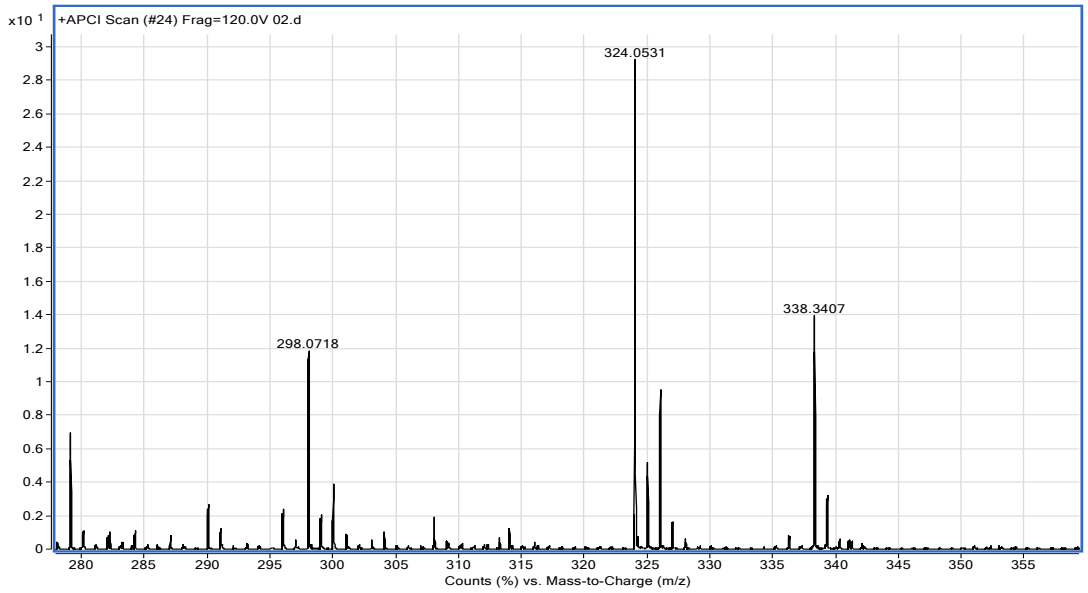
HRMS spectra for compound 4a



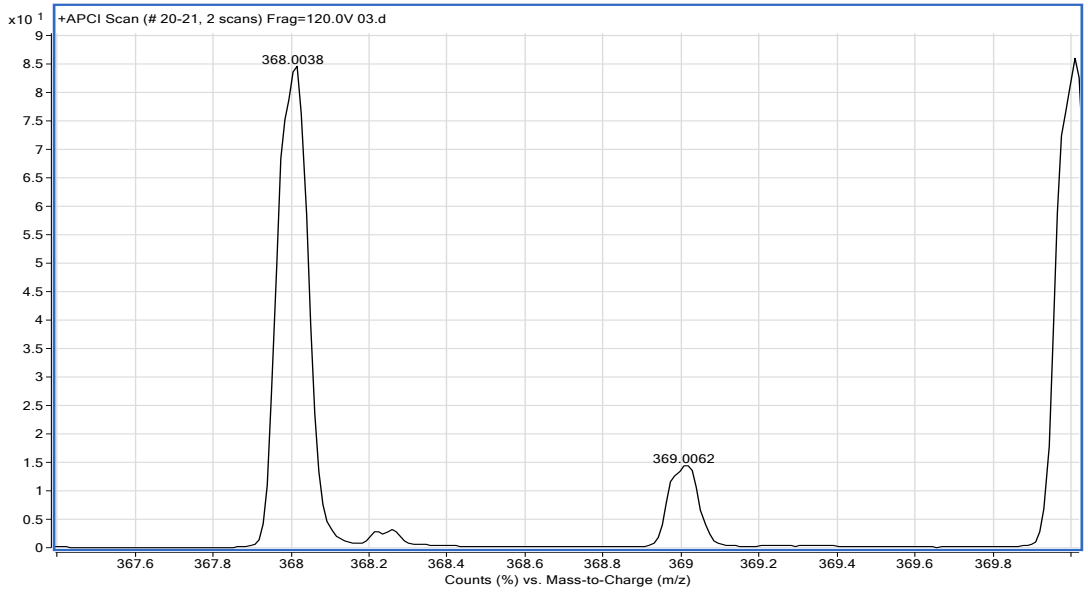
HRMS spectra for compound 4b



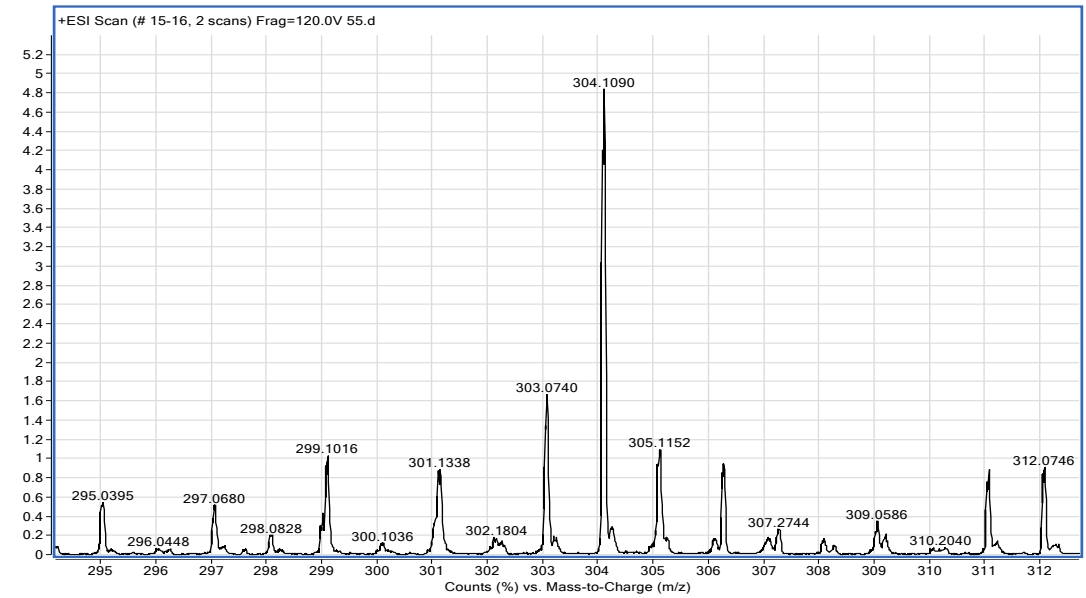
HRMS spectra for compound 4c



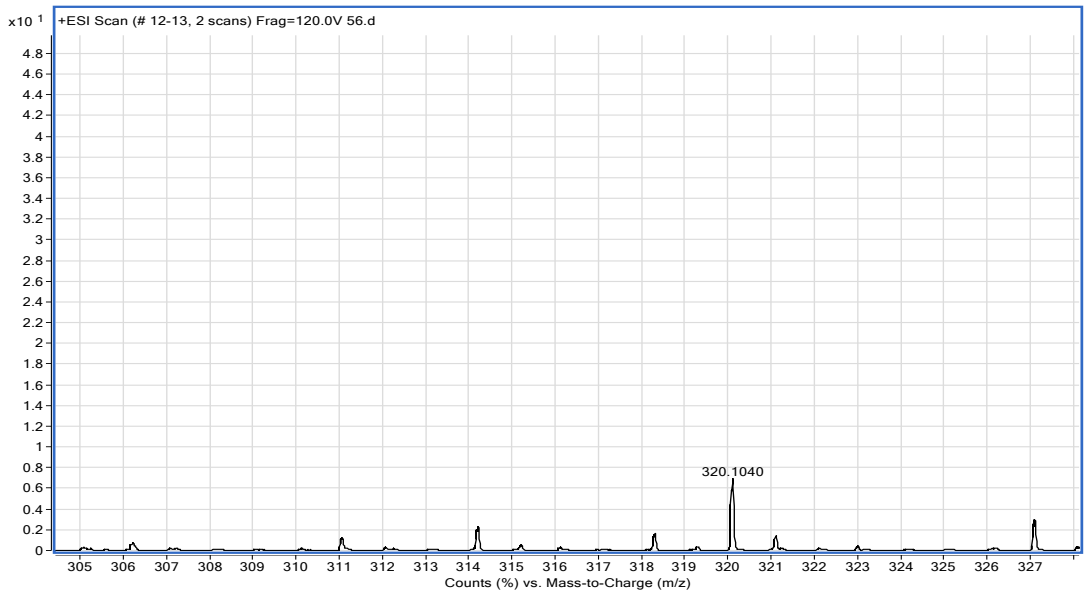
HRMS spectra for compound 4d



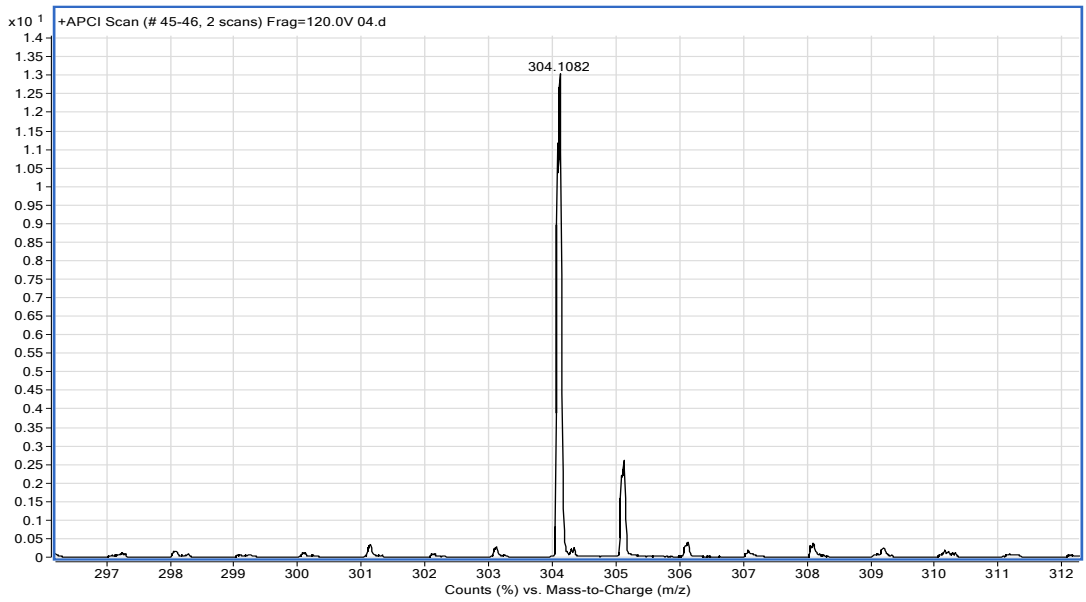
HRMS spectra for compound 4f



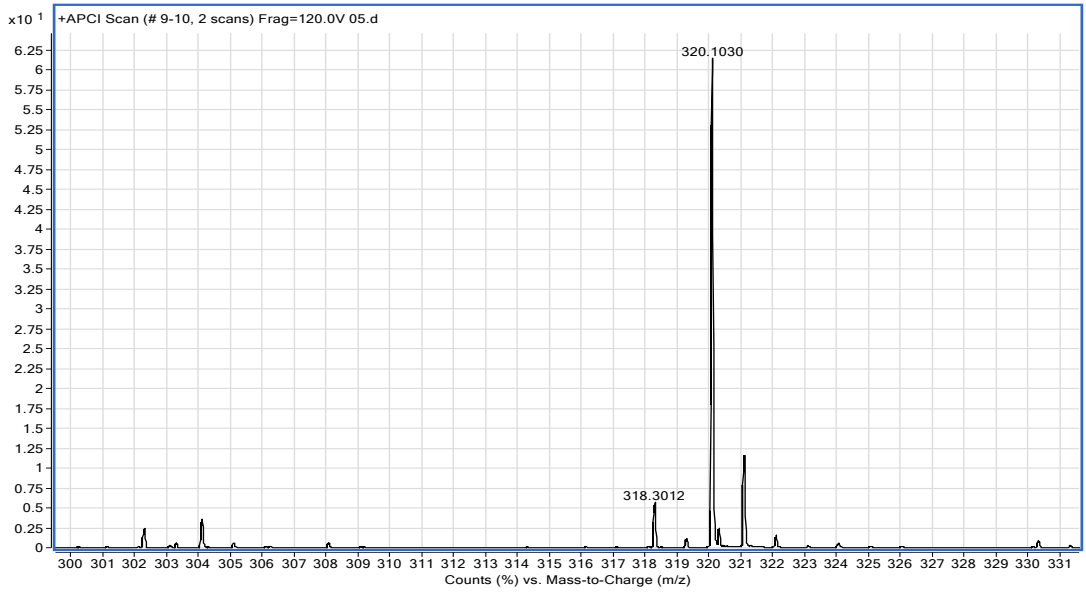
HRMS spectra for compound 4g



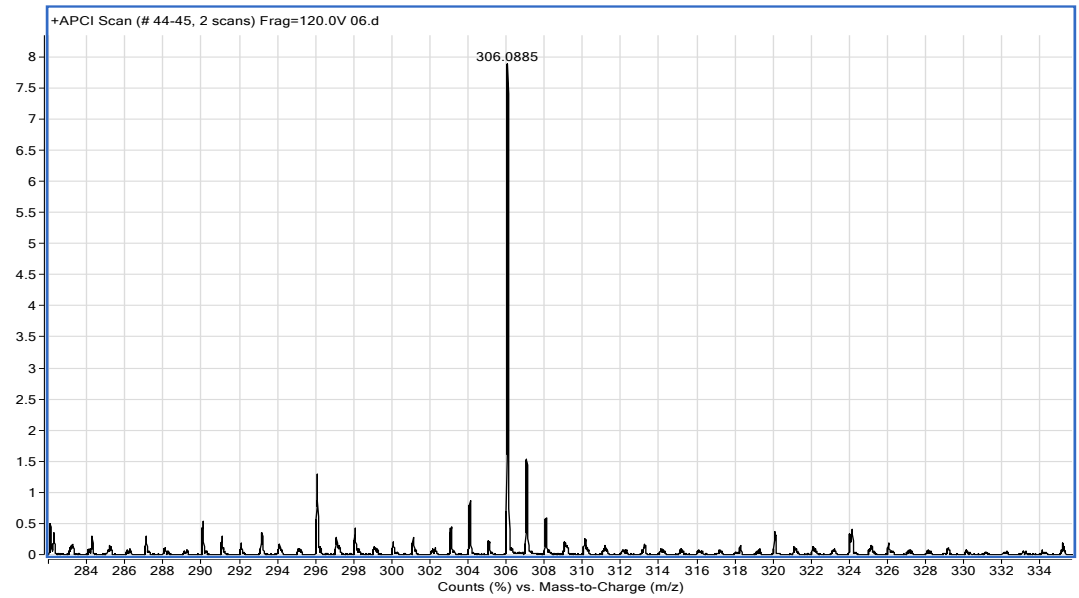
HRMS spectra for compound 4h



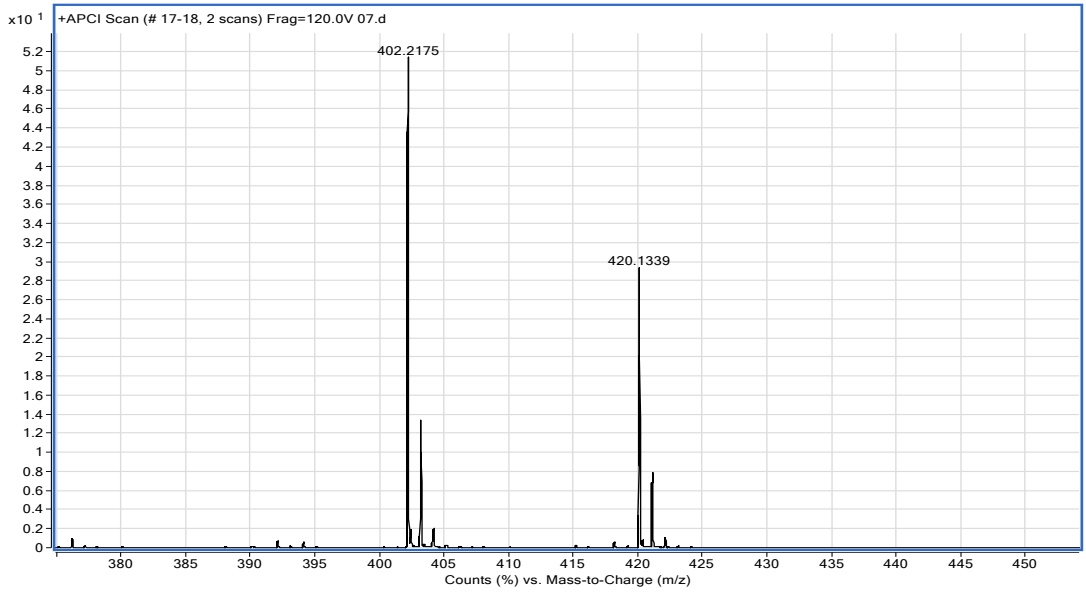
HRMS spectra for compound 4i



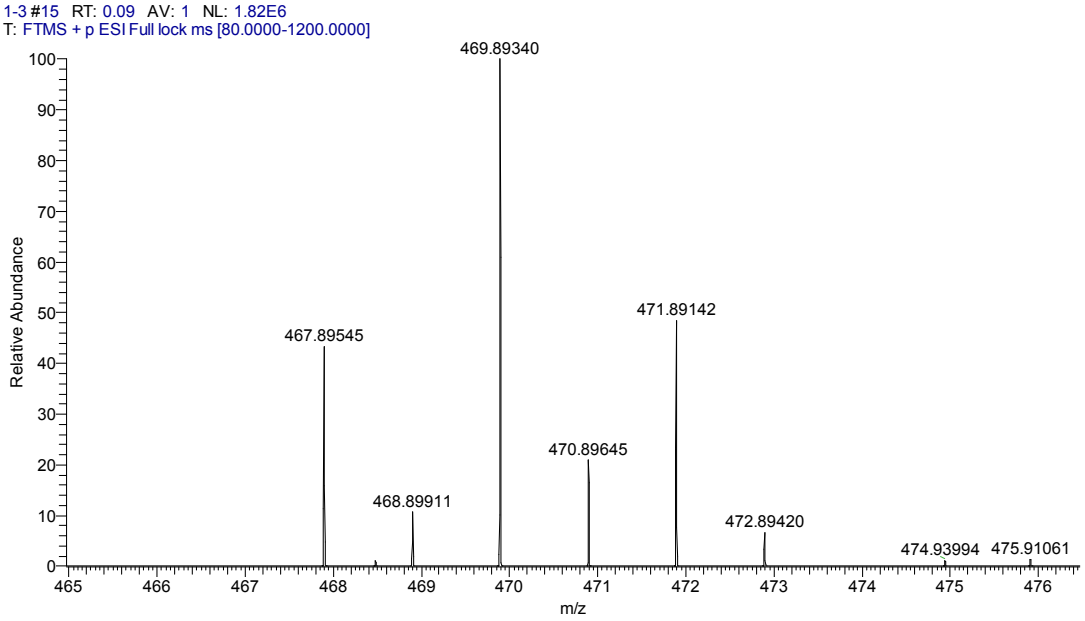
HRMS spectra for compound 4j



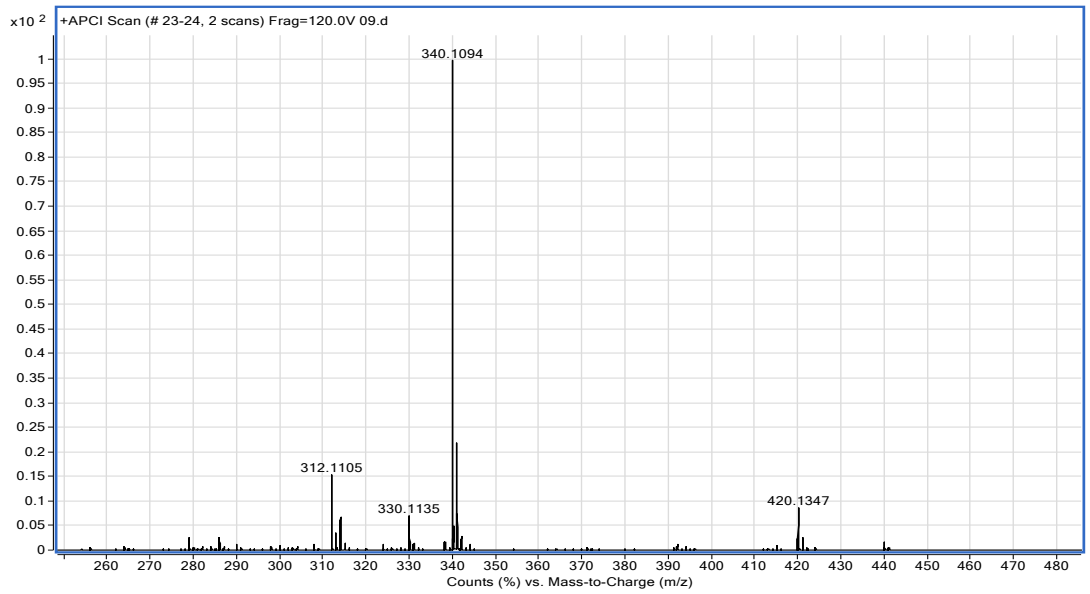
HRMS spectra for compound 4l



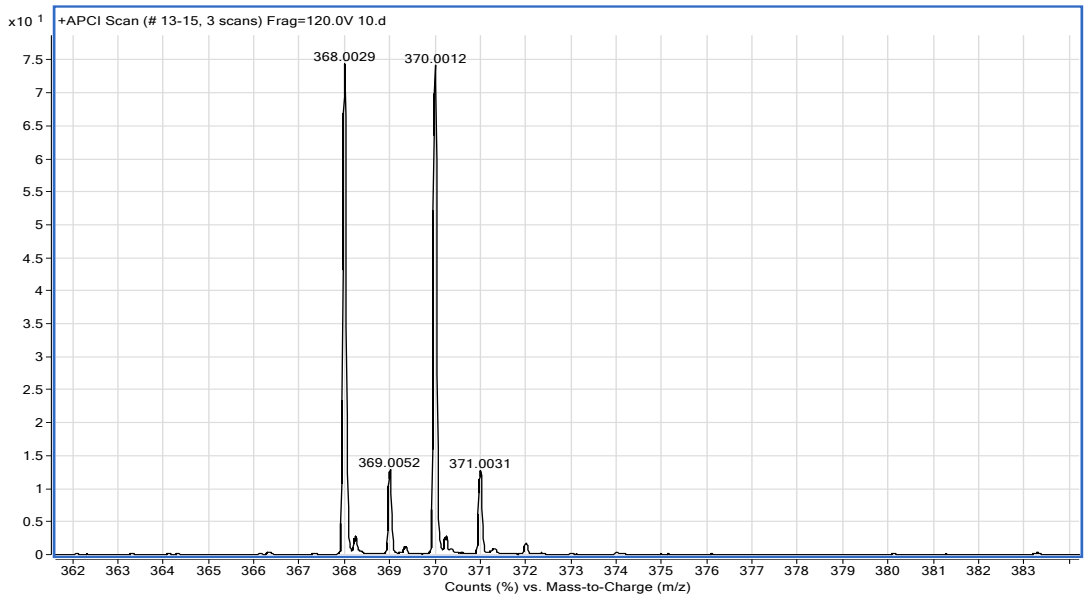
HRMS spectra for compound 4m



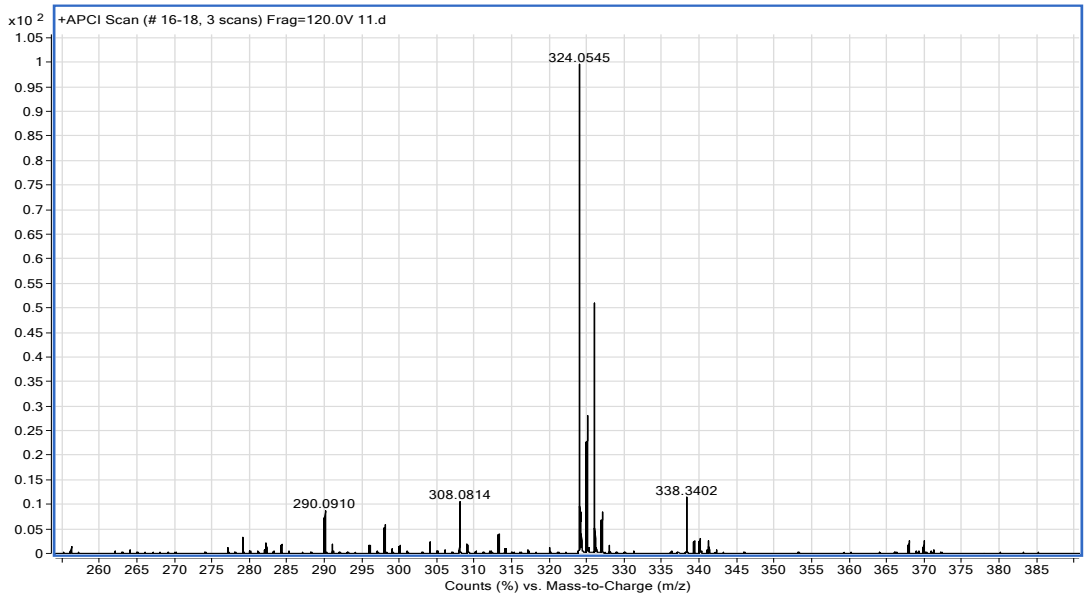
HRMS spectra for compound 4n



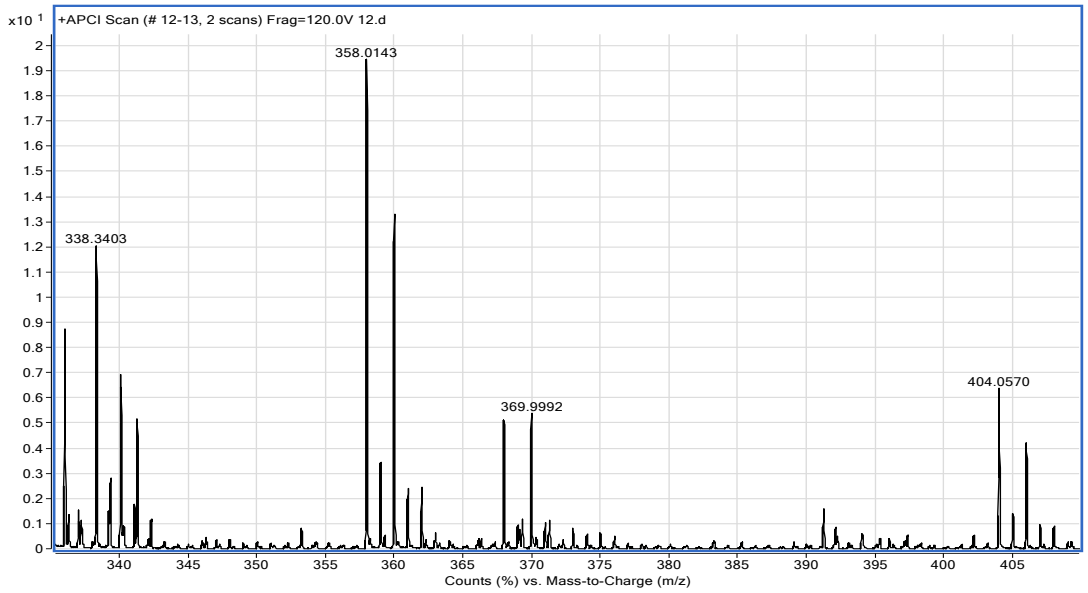
HRMS spectra for compound 4o



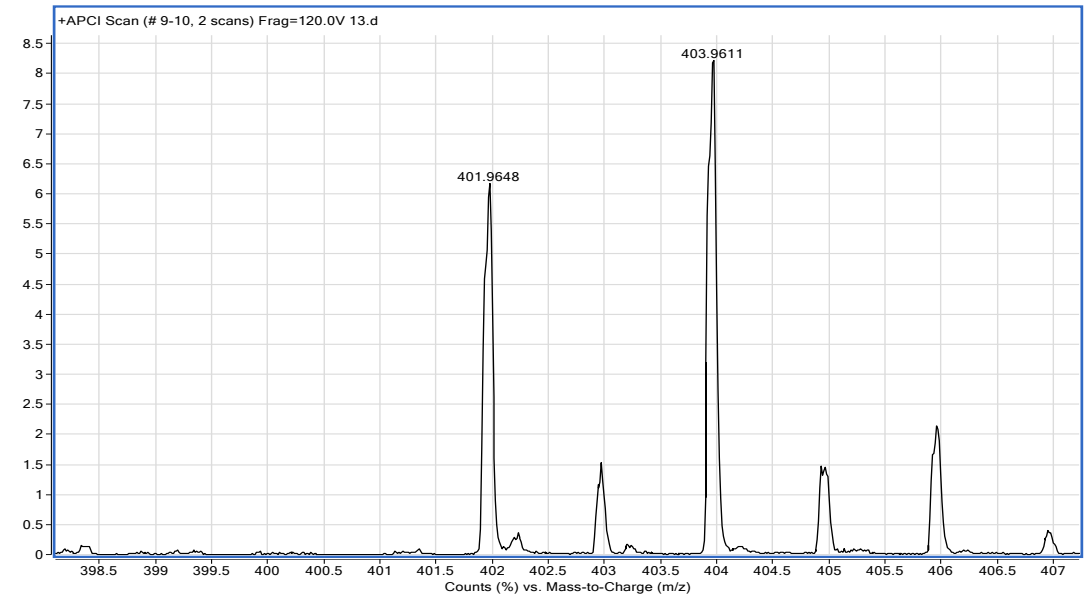
HRMS spectra for compound 4p



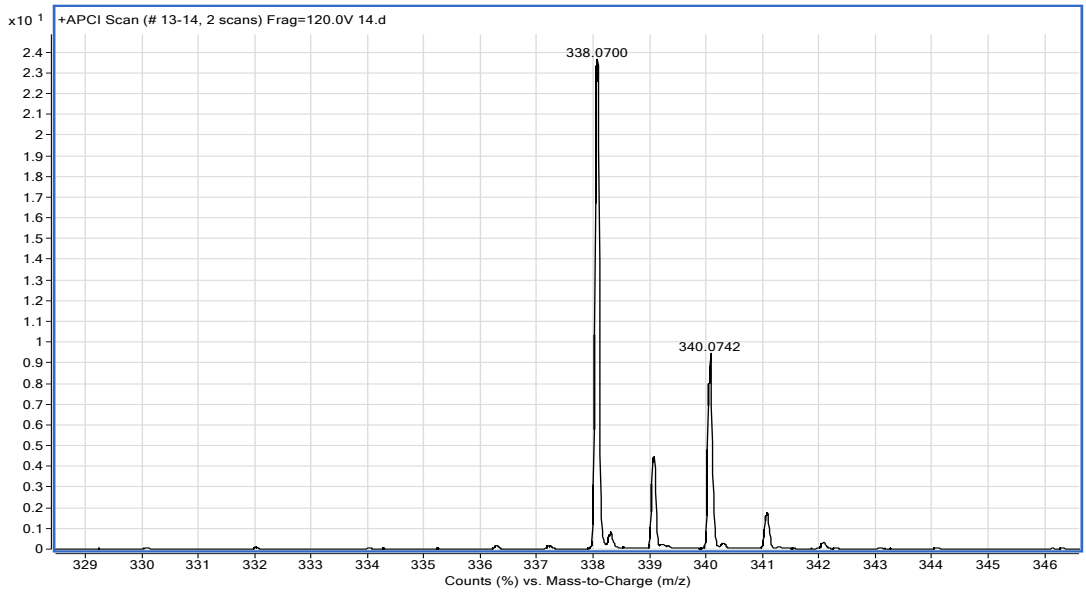
HRMS spectra for compound 4q



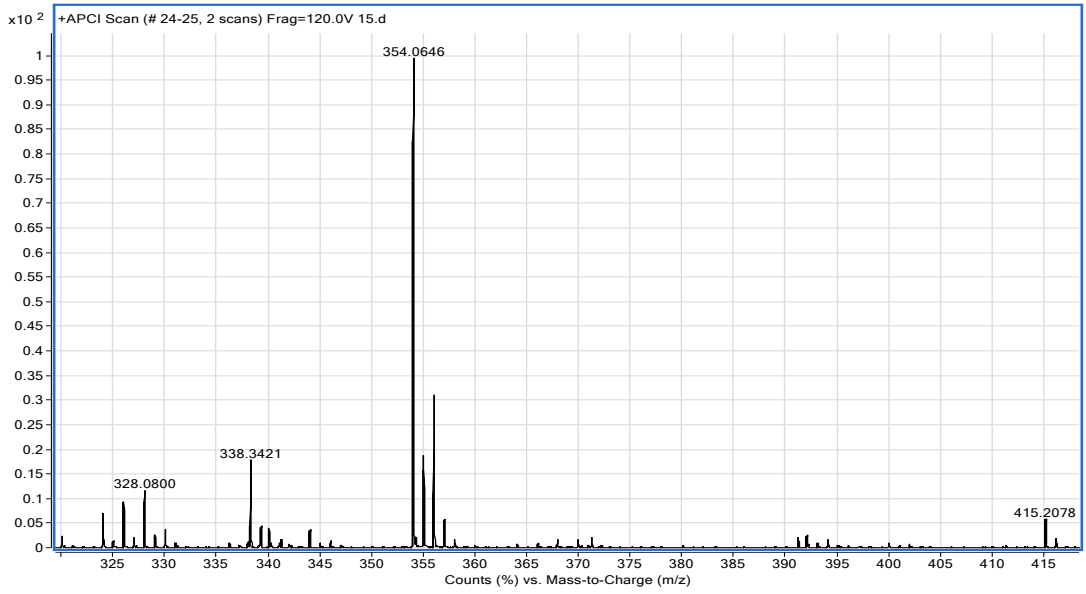
HRMS spectra for compound 4r



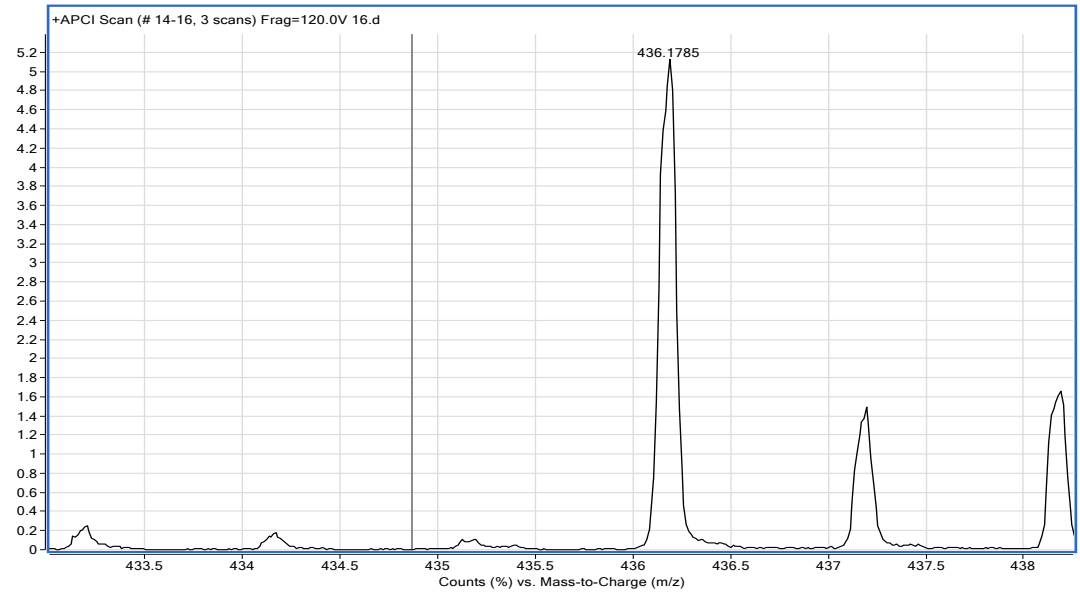
HRMS spectra for compound 4s



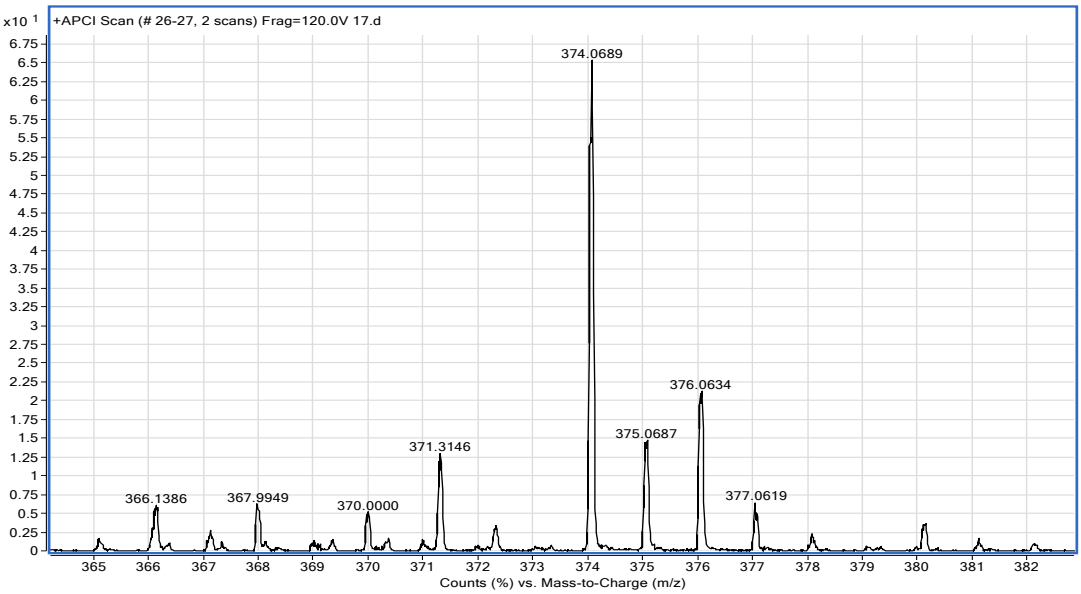
HRMS spectra for compound 4t



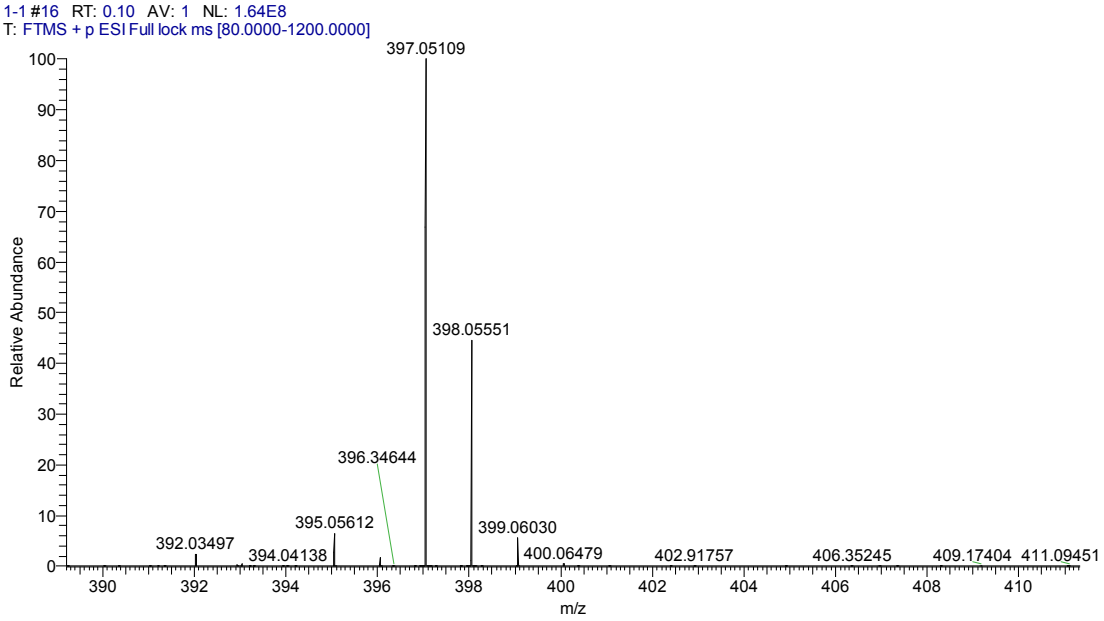
HRMS spectra for compound 4u



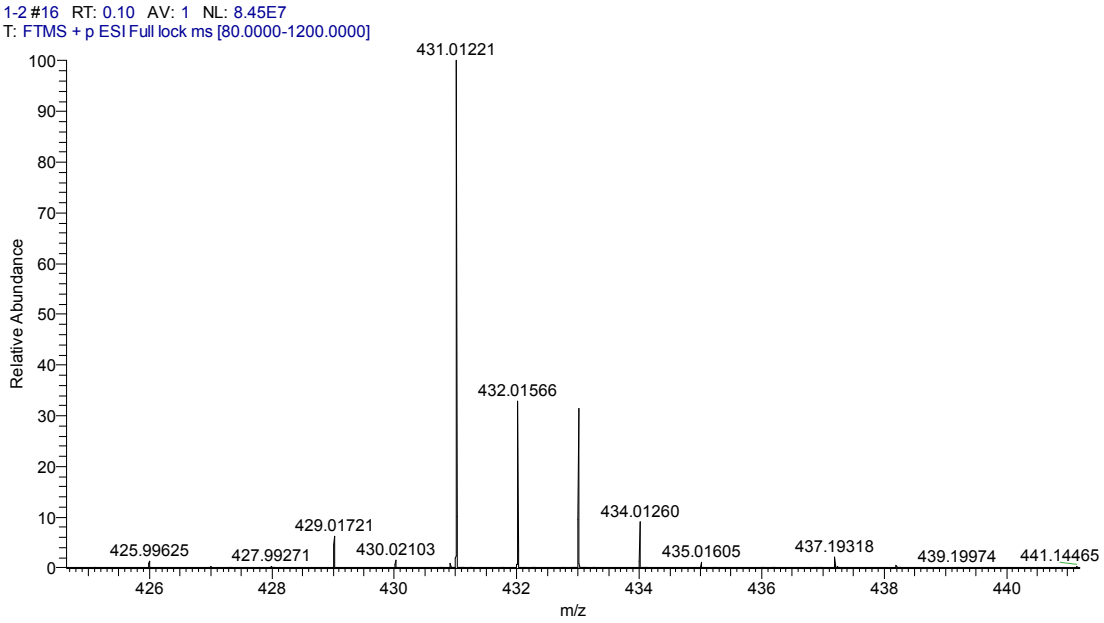
HRMS spectra for compound 4v



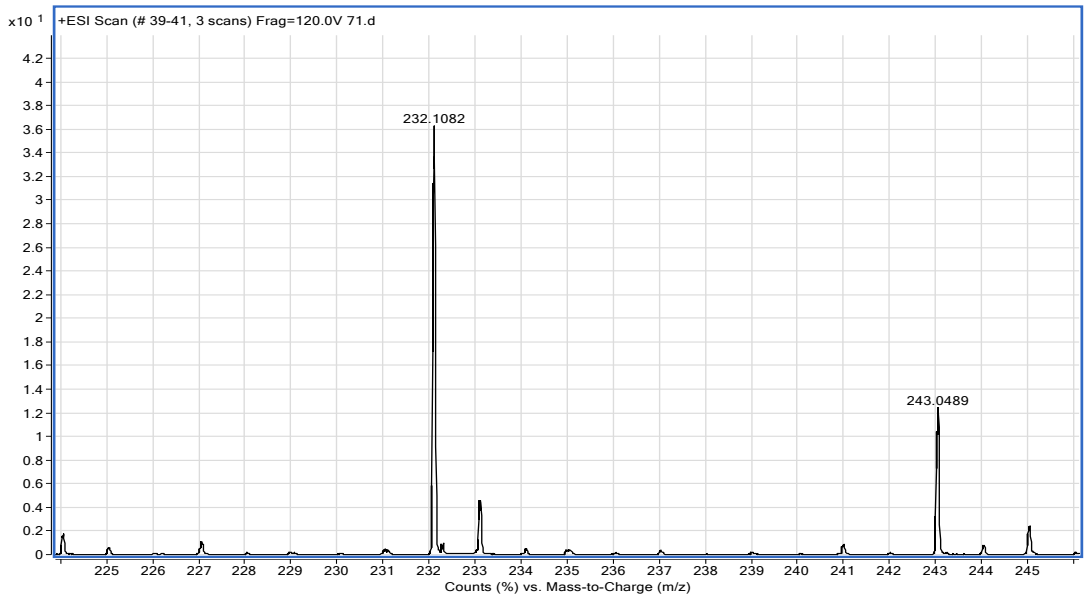
HRMS spectra for compound 4w



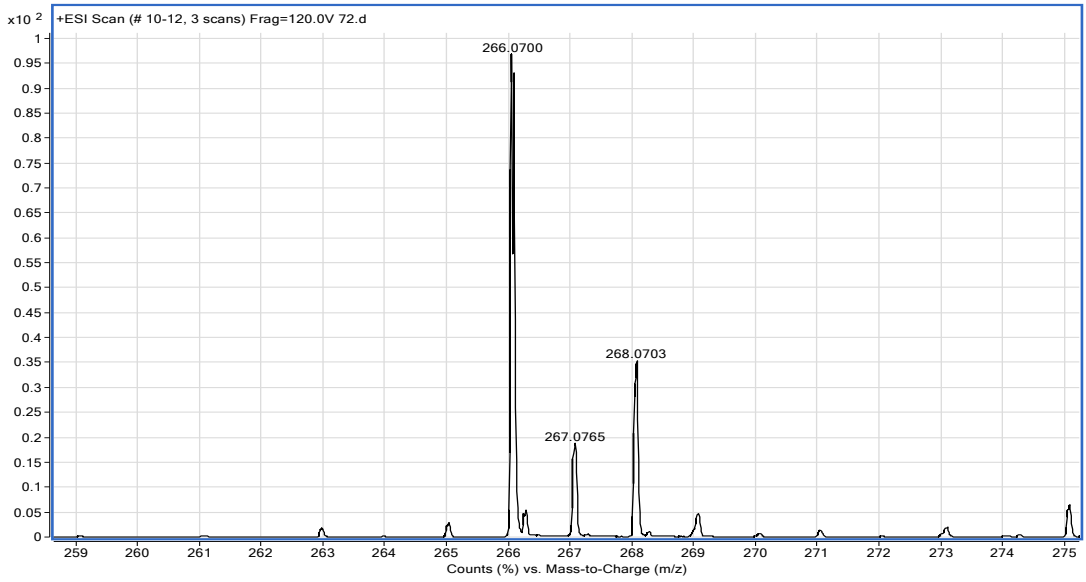
HRMS spectra for compound 4x



HRMS spectra for compound 5a



HRMS spectra for compound 5c



X-ray data of compound 4c.

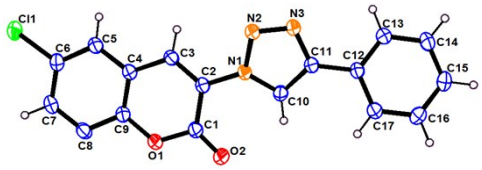


Figure S1. ORTEP of compound **4c**.

Table S1. Crystal data and structure refinement for 141117a_0m.

Identification code	141117a_0m
CCDC number	1998453
Empirical formula	C17 H10 Cl N3 O2
Formula weight	323.73
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 6.0960(7) Å alpha = 85.0800(10) deg.
	b = 7.6004(9) Å beta = 87.5620(10) deg.
	c = 15.3686(18) Å gamma = 78.9580(10) deg.
Volume	696.05(14) $Å^3$
Z, Calculated density	2, 1.545 Mg/m^3
Absorption coefficient	0.288 mm^{-1}
F(000)	332
Crystal size	0.16 x 0.15 x 0.12 mm
Theta range for data collection	2.66 to 25.02 deg.
Limiting indices	-6<=h<=7, -9<=k<=9, -18<=l<=18
Reflections collected / unique	4982 / 2436 [R(int) = 0.0174]
Completeness to theta = 25.02	99.1 %
Absorption correction	None
Max. and min. transmission	0.9662 and 0.9553
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2436 / 0 / 208
Goodness-of-fit on F^2	1.026
Final R indices [I>2sigma(I)]	R1 = 0.0350, wR2 = 0.0976
R indices (all data)	R1 = 0.0394, wR2 = 0.1023
Largest diff. peak and hole	0.125 and -0.250 $e.Å^{-3}$

Table S2. Bond lengths [Å] and angles [deg] for 141117a_0m.

C(1)-O(2)	1.196(2)
C(1)-O(1)	1.368(2)
C(1)-C(2)	1.465(2)
C(2)-C(3)	1.342(2)
C(2)-N(1)	1.423(2)
C(3)-C(4)	1.437(2)
C(3)-H(3)	0.9300

C(4)-C(9)	1.389(2)
C(4)-C(5)	1.397(2)
C(5)-C(6)	1.378(2)
C(5)-H(5)	0.9300
C(6)-C(7)	1.386(2)
C(6)-Cl(1)	1.7388(17)
C(7)-C(8)	1.369(2)
C(7)-H(7)	0.9300
C(8)-C(9)	1.383(2)
C(8)-H(8)	0.9300
C(9)-O(1)	1.3723(19)
C(10)-N(1)	1.353(2)
C(10)-C(11)	1.359(2)
C(10)-H(10)	0.9300
C(11)-N(3)	1.366(2)
C(11)-C(12)	1.469(2)
C(12)-C(13)	1.387(2)
C(12)-C(17)	1.391(2)
C(13)-C(14)	1.385(2)
C(13)-H(13)	0.9300
C(14)-C(15)	1.372(3)
C(14)-H(14)	0.9300
C(15)-C(16)	1.372(3)
C(15)-H(15)	0.9300
C(16)-C(17)	1.380(2)
C(16)-H(16)	0.9300
C(17)-H(17)	0.9300
N(1)-N(2)	1.3574(19)
N(2)-N(3)	1.303(2)
O(2)-C(1)-O(1)	117.36(15)
O(2)-C(1)-C(2)	126.91(15)
O(1)-C(1)-C(2)	115.73(14)
C(3)-C(2)-N(1)	121.41(14)
C(3)-C(2)-C(1)	121.92(14)
N(1)-C(2)-C(1)	116.67(13)
C(2)-C(3)-C(4)	120.10(15)
C(2)-C(3)-H(3)	120.0
C(4)-C(3)-H(3)	120.0
C(9)-C(4)-C(5)	118.45(14)
C(9)-C(4)-C(3)	117.92(14)
C(5)-C(4)-C(3)	123.63(15)
C(6)-C(5)-C(4)	119.02(16)
C(6)-C(5)-H(5)	120.5

C(4)-C(5)-H(5)	120.5
C(5)-C(6)-C(7)	121.60(16)
C(5)-C(6)-Cl(1)	120.57(14)
C(7)-C(6)-Cl(1)	117.83(13)
C(8)-C(7)-C(6)	119.88(15)
C(8)-C(7)-H(7)	120.1
C(6)-C(7)-H(7)	120.1
C(7)-C(8)-C(9)	118.88(16)
C(7)-C(8)-H(8)	120.6
C(9)-C(8)-H(8)	120.6
O(1)-C(9)-C(8)	116.85(14)
O(1)-C(9)-C(4)	121.03(14)
C(8)-C(9)-C(4)	122.12(15)
N(1)-C(10)-C(1)	105.27(14)
N(1)-C(10)-H(10)	127.4
C(11)-C(10)-H(10)	127.4
C(10)-C(11)-N(3)	108.09(14)
C(10)-C(11)-C(12)	129.68(15)
N(3)-C(11)-C(12)	122.19(14)
C(13)-C(12)-C(17)	118.62(15)
C(13)-C(12)-C(11)	120.87(14)
C(17)-C(12)-C(11)	120.50(14)
C(14)-C(13)-C(12)	120.31(16)
C(14)-C(13)-H(13)	119.8
C(12)-C(13)-H(13)	119.8
C(15)-C(14)-C(13)	120.45(17)
C(15)-C(14)-H(14)	119.8
C(13)-C(14)-H(14)	119.8
C(16)-C(15)-C(14)	119.73(16)
C(16)-C(15)-H(15)	120.1
C(14)-C(15)-H(15)	120.1
C(15)-C(16)-C(17)	120.49(17)
C(15)-C(16)-H(16)	119.8
C(17)-C(16)-H(16)	119.8
C(16)-C(17)-C(12)	120.40(16)
C(16)-C(17)-H(17)	119.8
C(12)-C(17)-H(17)	119.8
C(10)-N(1)-N(2)	110.18(13)
C(10)-N(1)-C(2)	131.13(13)
N(2)-N(1)-C(2)	118.69(12)
N(3)-N(2)-N(1)	107.05(13)
N(2)-N(3)-C(11)	109.41(13)
C(1)-O(1)-C(9)	123.22(13)