Supporting information

Design, Synthesis and Anticancer Activity Studies of Novel Pyrazolo[1,5-a]pyrimidine-Nitrogen Mustard Derivatives

Zhao Mingxia [1], Zhang Dongxia [2], Chang Jin [3], Zhao Zhiju [4], Qi Chuanmin [5,*], Jiang Junbing [1,*]

([1] Department of Mining Engineering, Shanxi Institute of Technology, Yangquan 045000; [2]Xingtang General Hospital, Xingtang, 050600; [3]College of Biomedical Engineering, Taiyuan University of Technology, [4]College of Chemical Engineering and Biotechnology, Xingtai University, Xingtai 054001; [5]Key Laboratory of Radiopharmaceuticals, Ministry of Education, College of Chemistry, Beijing Normal University, Beijing 100875)

Contents:

1. Table S1: Details of data collection and structure refinement for compounds 7m and 9b.

compounds	**7m**	**9b**
Formula	$C_{18}H_{17}N_6Cl$	$C_{18}H_{17}N_6Cl_3$
Mr	352.83	423.73
CCDC	1014303	1014302
Temperature (K)	296(2)	296(2)
Wavelength (Å)	0.71073	0.71073
Crystal system	Monoclinic	Triclinic
Space group	P2(1)/c	P-1
a/Å	10.014(2)	8.427(3)
b/Å	14.029(3)	8.754(3)
c/Å	12.205(3)	15.384(5)
α/°	90	78.074(6)
β/°	101.978(4)	74.564(5)
γ/°	90	70.411(5)
V/Å^3	1677.3(6)	1022.0(6)
Z	4	2
*D*c/ g cm^{-3}	1.397	1.377
μ /mm^{-1}	0.242	0.464
F(000)	736.0	436.0
Crystal size (mm)	0.28×0.22×0.16	0.28×0.26×0.18
θ range /deg.	2.08-27.48	1.38-27.64
reflns collected /unique	3828/2959	4699/3088
GOF on F^2	1.072	1.073
R_{int}	0.0332	0.0254
R_1[a)], wR_2[b)] [$I > 2\sigma(I)$]	0.0559, 0.1575	0.0938, 0.2895
R_1, wR_2 (all data)	0.0737, 0.1693	0.1269, 0.3220

Largest diff. peak, hole /e·Å^{-3}	0.357, -0.575	3.086, -0.536

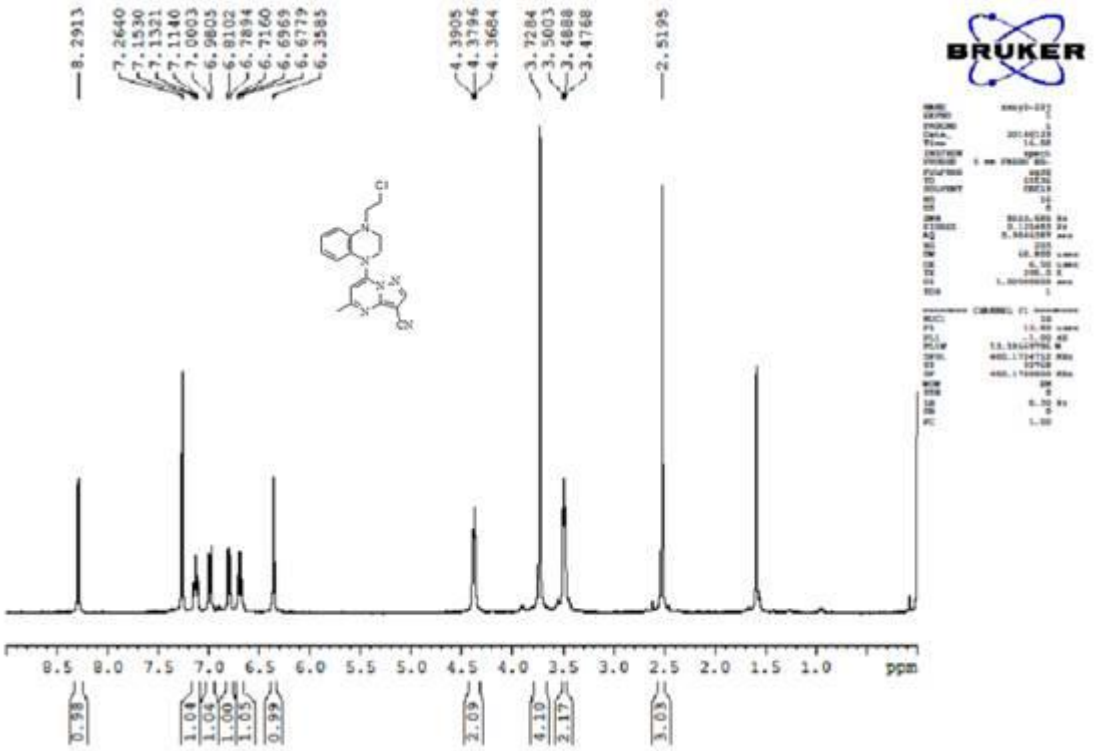
a) $R_1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$. b) $wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$.

2. Table S2: Selected bond lengths (Å) and bond angles (°) for compounds 7m and 9b.

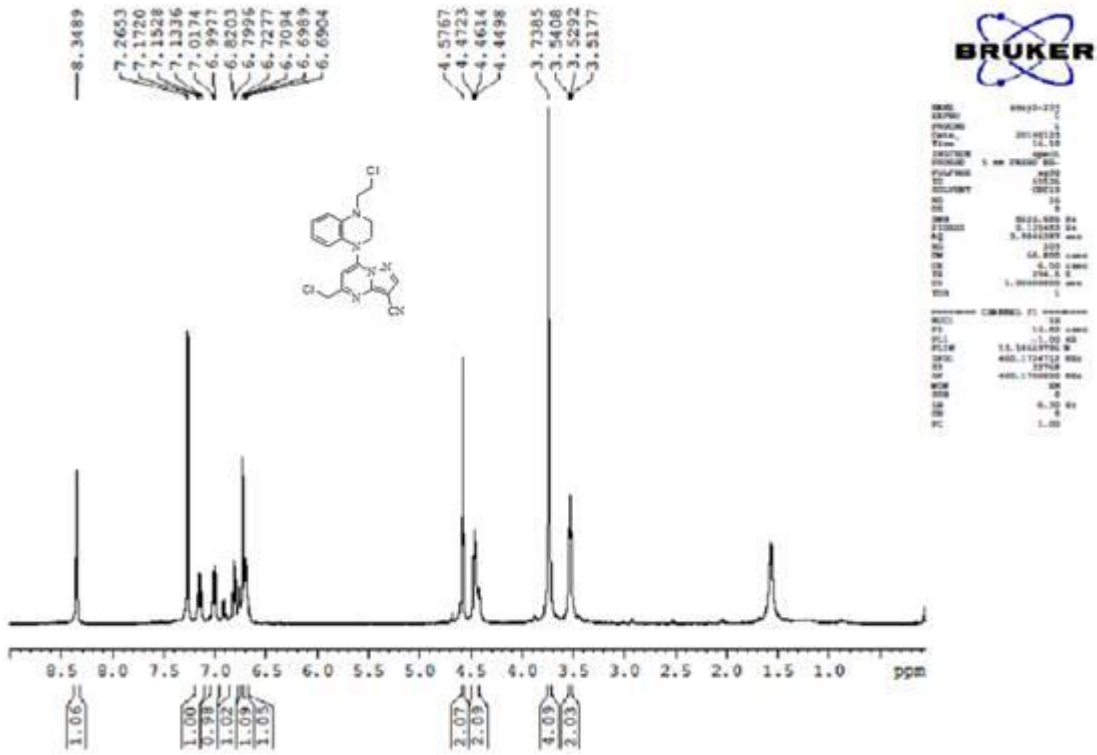
Bond Length [Å]		Bond Angles [°]	
Compound **7m**			
Cl1−C18	1.773(3)	C9−N1−C16	112.67(19)
N1−C9	1.435(3)	C3−N2−C4	115.2(2)
N1−C16	1.483(3)	N4−N3−C4	112.74(19)
N2−C3	1.338(3)	C1−N3−C4	121.27(19)
N2−C4	1.348(3)	C6−N4−N3	103.5(2)
N3−N4	1.383(3)	C14−N6−C15	119.7(2)
N3−C1	1.386(3)	N3−C1−C2	114.8(2)
N3−C4	1.390(3)	C1−C2−C3	121.0(2)
N4−C6	1.333(3)	N2−C3−C2	123.6(2)
N6−C14	1.382(3)	N2−C4−N3	123.9(2)
N6−C17	1.454(3)	N3−C4−C5	105.0(2)
N6−C15	1.460(3)	C4−C5−C6	105.4(2)
C1−C2	1.387(3)	N4−C6−C5	113.3(2)
C2−C3	1.406(3)	N6−C14−C13	122.6(2)
C3−C8	1.502(3)	N6−C14−C9	120.8(2)
C4−C5	1.400(3)	N6−C15−C16	110.2(2)
C5−C6	1.406(4)	N1−C16−C15	109.1(2)
C15−C16	1.516(4)	N6−C17−C18	114.2(2)
C17−C18	1.511(4)	C17−C18−Cl1	112.0(2)
Compound **9b**			
N1−C6	1.364(5)	C6−N1−C3	122.3(3)
N1−C3	1.371(5)	C6−N1−N2	124.1(3)
N1−N2	1.378(5)	C3−N1−N2	113.5(3)
N2−C1	1.314(6)	C1−N2−N1	103.7(3)
N3−C3	1.337(5)	C3−N3−C4	114.6(3)
N3−C4	1.340(5)	N2−C1−C2	113.5(4)
N6−C12	1.390(6)	C3−C2−C1	104.8(4)
N6−C17	1.444(6)	N3−C3−N1	123.5(4)
N6−C15	1.482(6)	N1−C3−C2	104.6(3)
C1−C2	1.410(6)	N3−C4−C5	124.9(4)
C2−C3	1.411(6)	C5−C4−C8	121.8(4)
C4−C5	1.388(5)	C4−C5−C6	119.4(4)
C5−C6	1.387(6)	N1−C6−C5	115.3(4)
C15−C16	1.506(8)	C4−C8−Cl1	112.4(3)
C17−C18	1.521(8)		

3. [1]H-NMR of target compounds

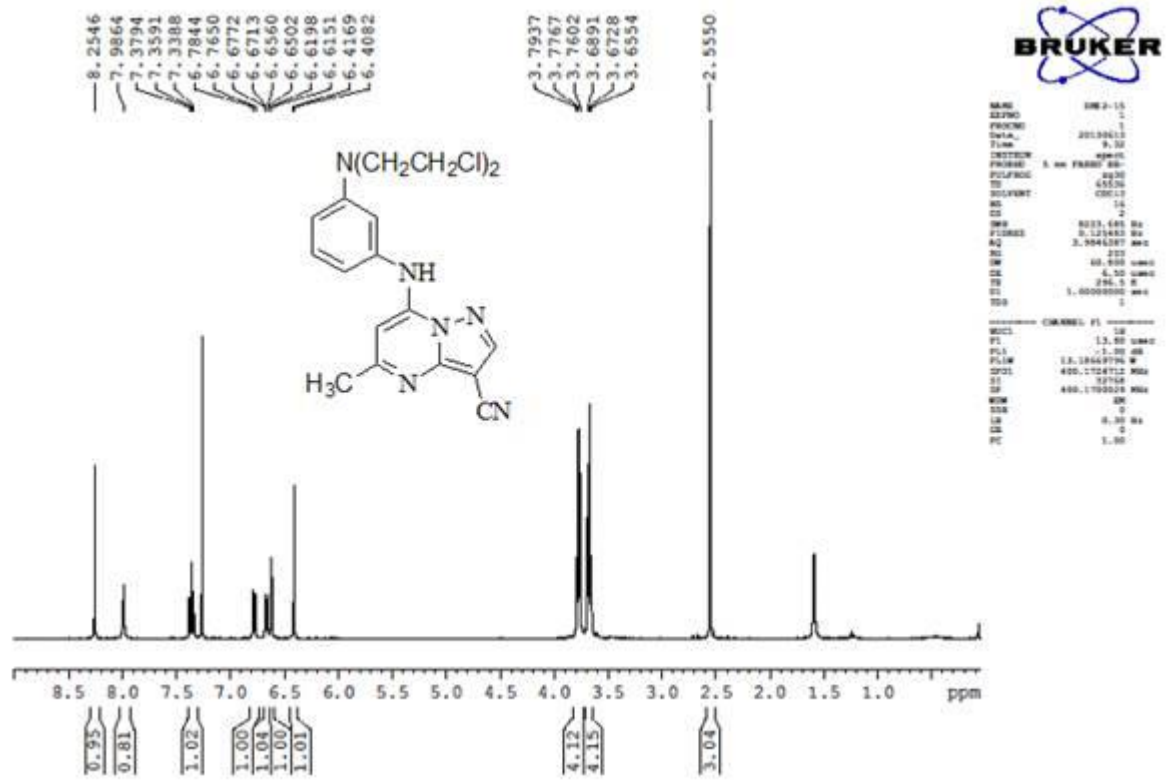
[1]H NMR for compound **7m**



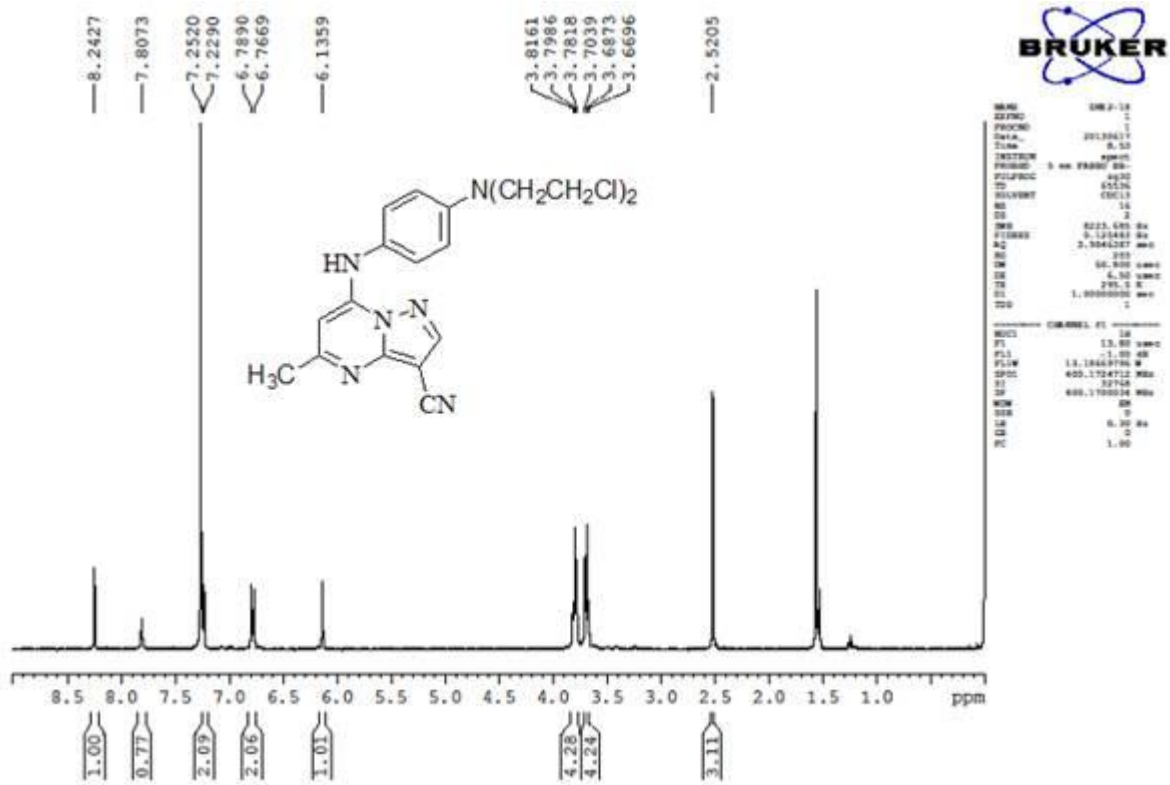
[1]H NMR for compound **7n**



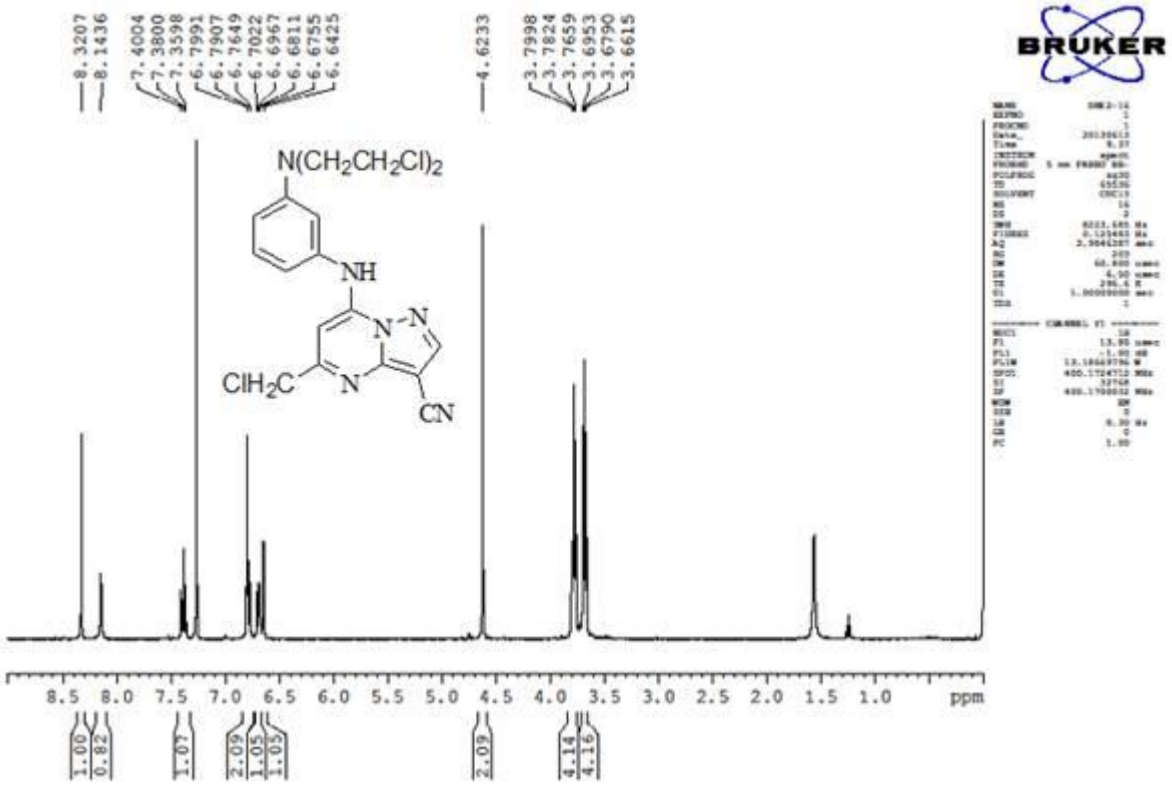
^{1}H NMR for compound **8a**



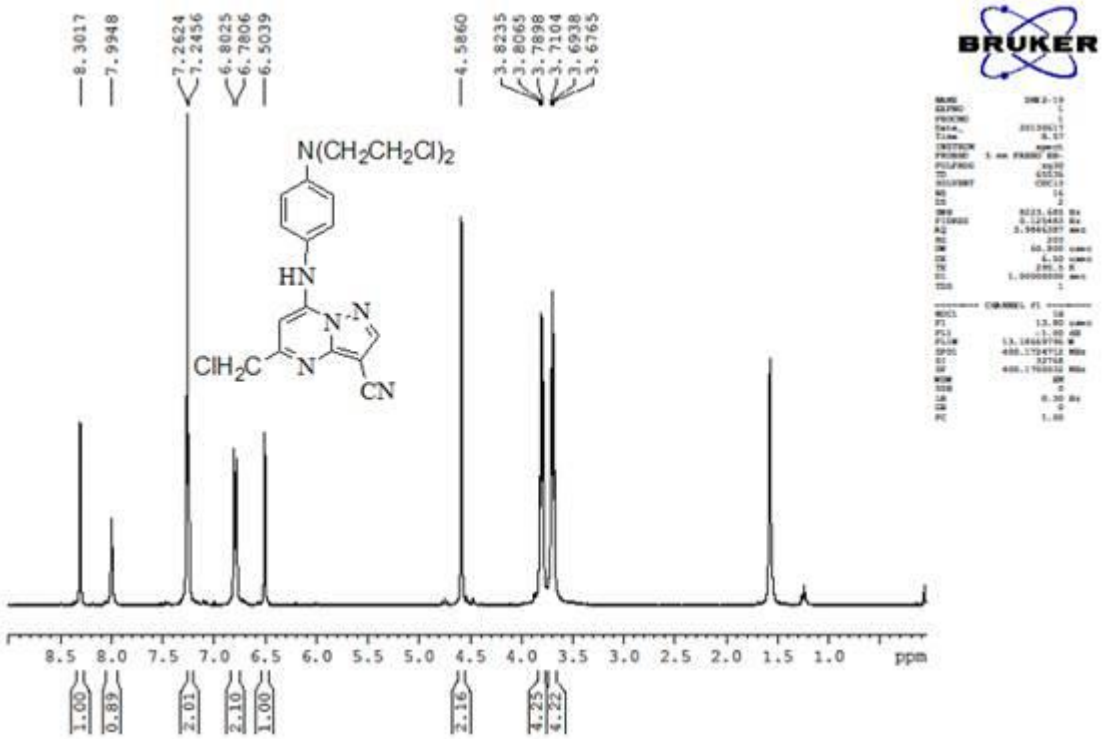
^{1}H NMR for compound **9a**



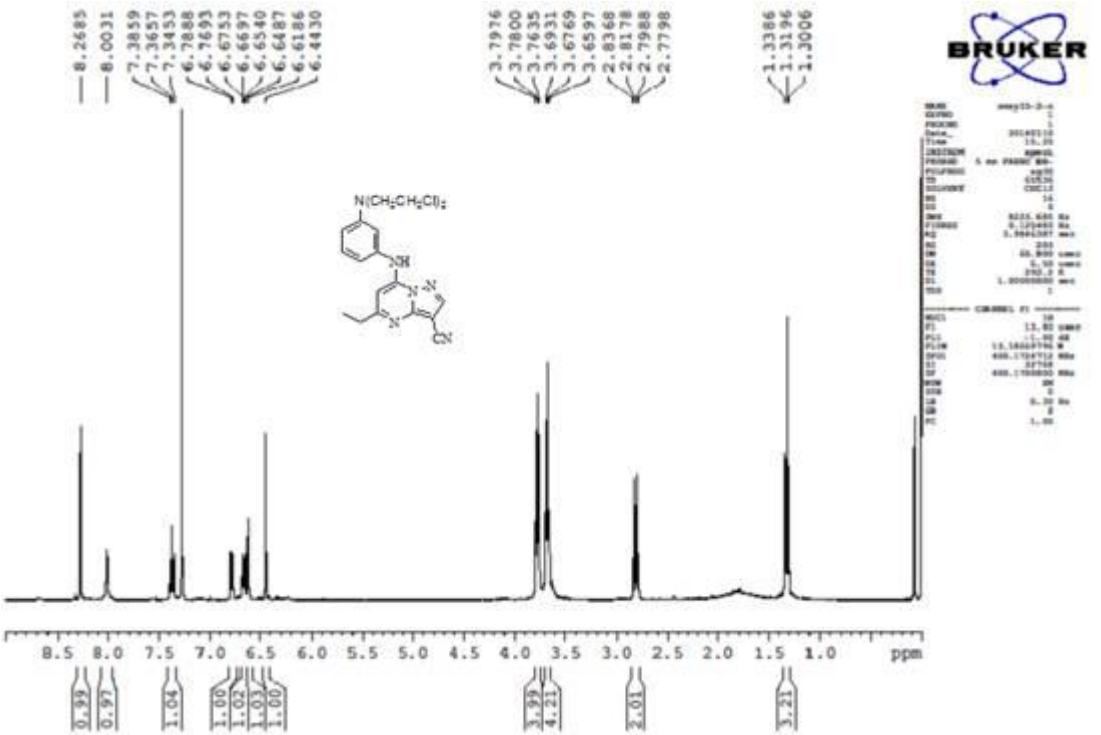
^{1}H NMR for compound **8b**



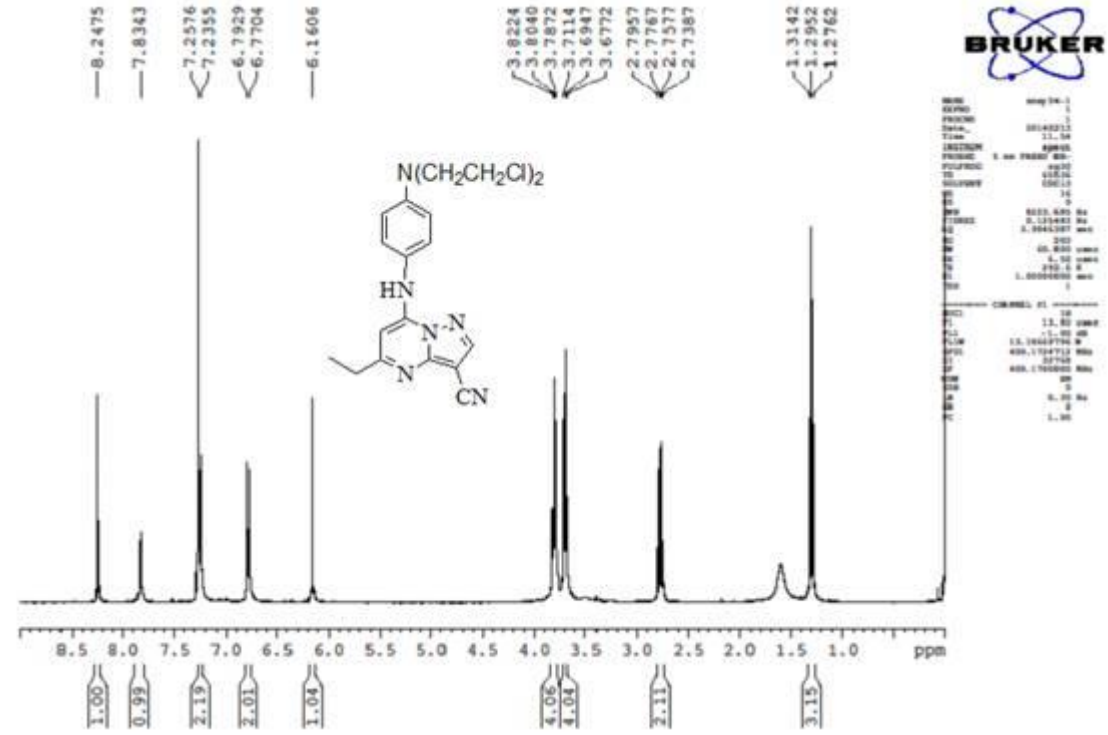
^{1}H NMR for compound **9b**



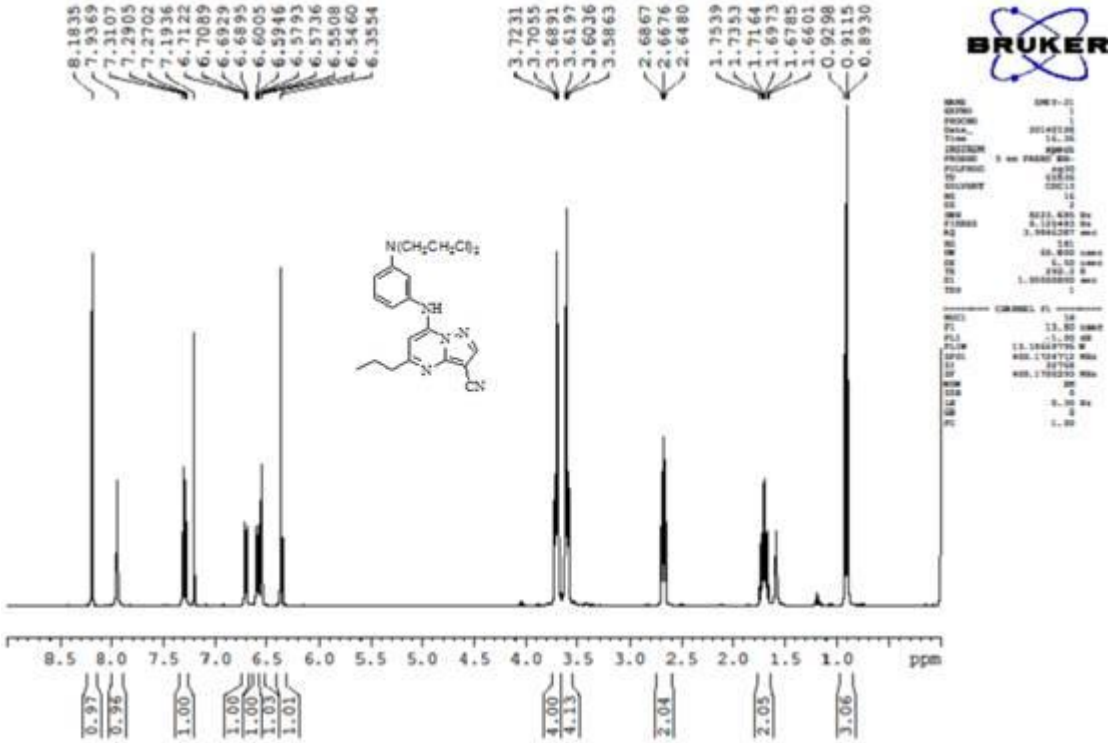
^{1}H NMR for compound **8c**



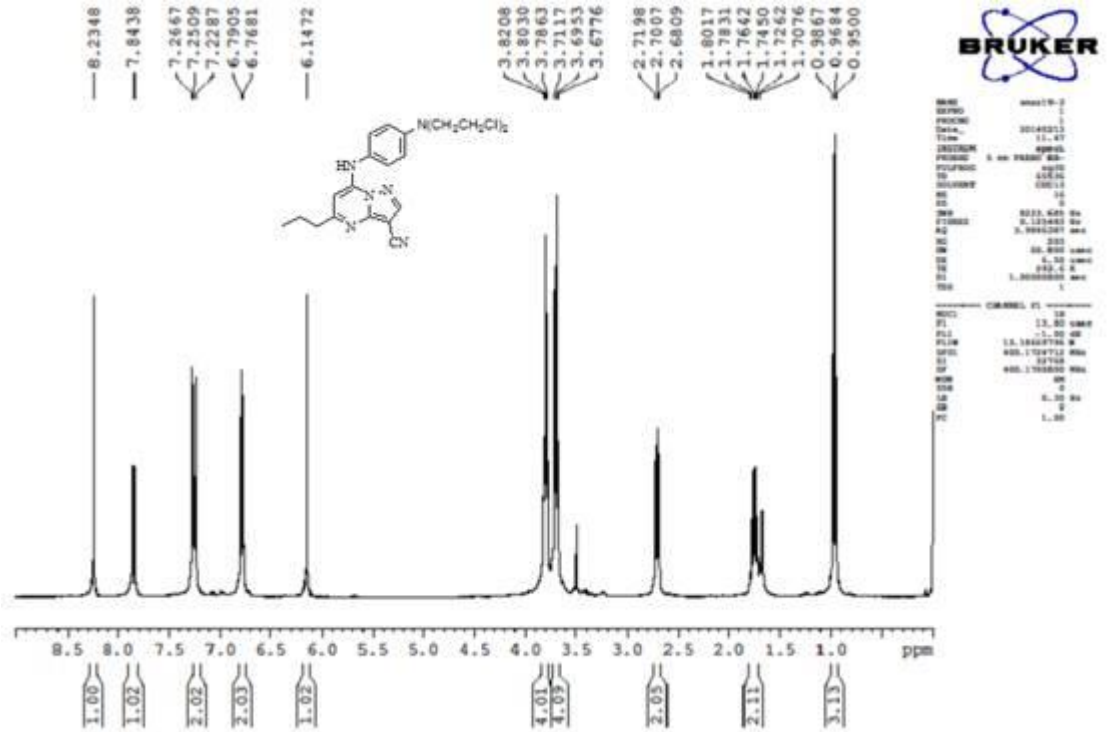
^{1}H NMR for compound **9c**



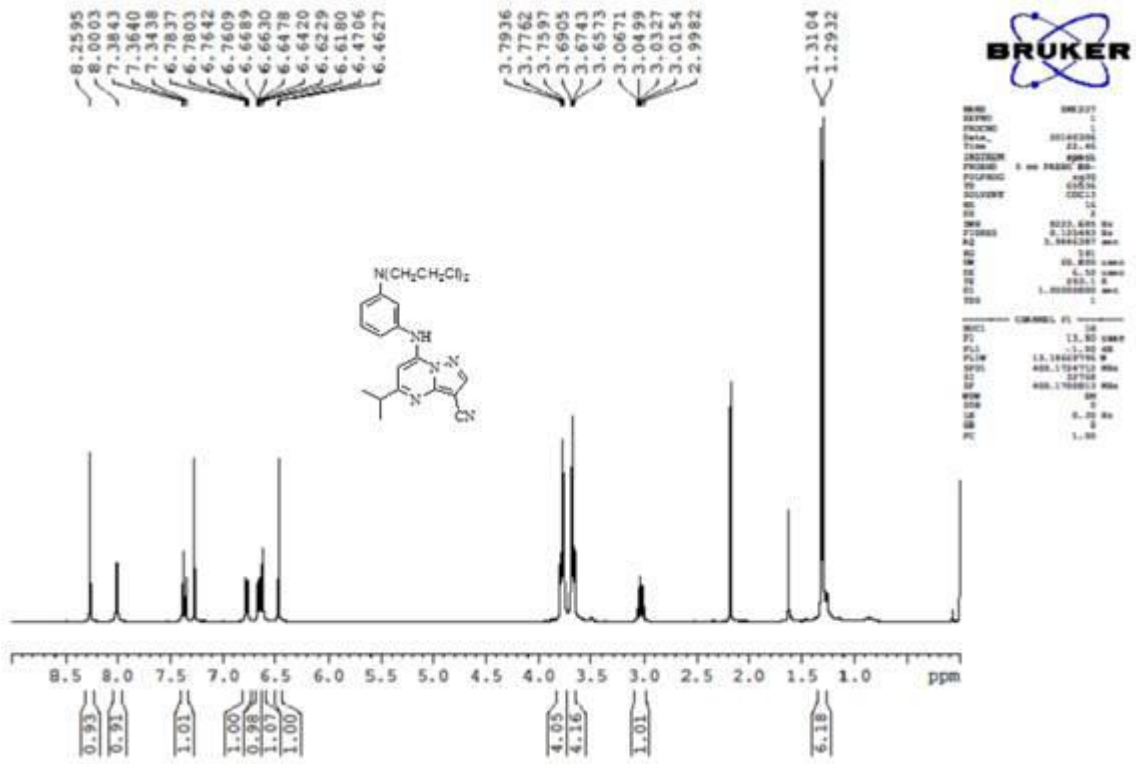
^{1}H NMR for compound **8d**



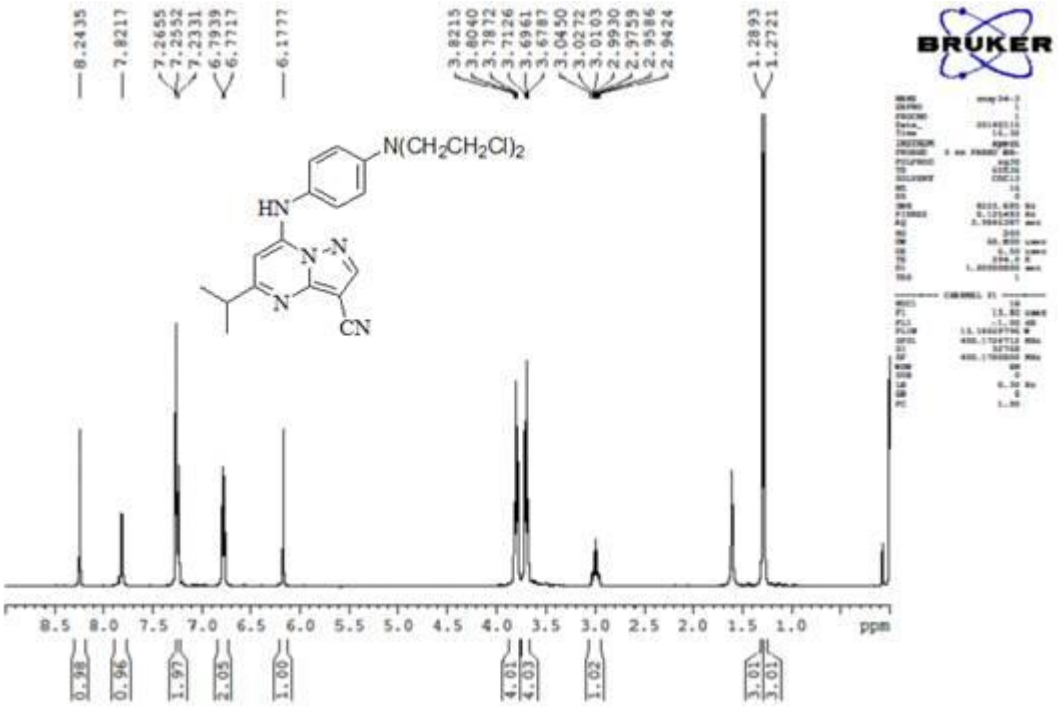
^{1}H NMR for compound **9d**



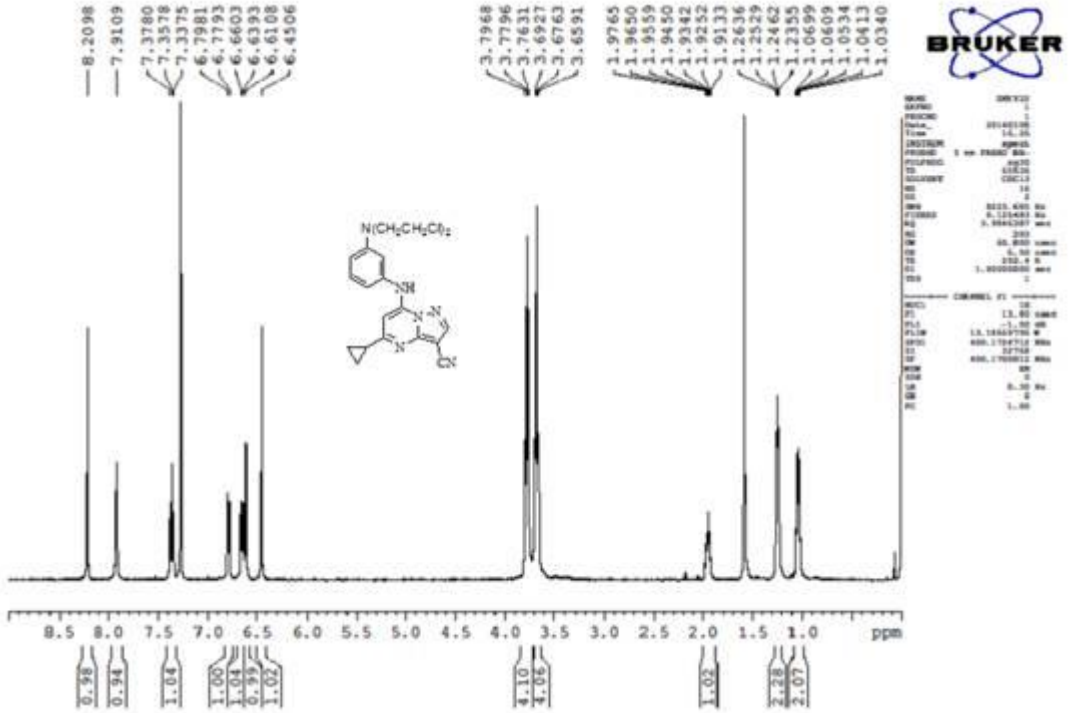
^{1}H NMR for compound **8e**



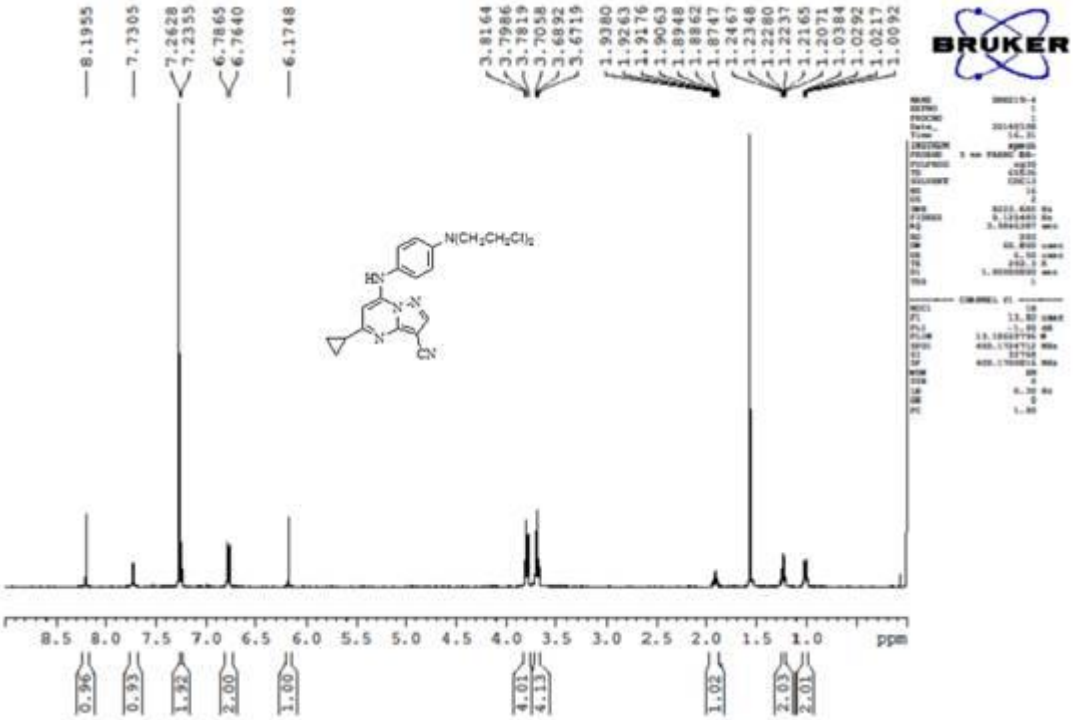
^{1}H NMR for compound **9e**



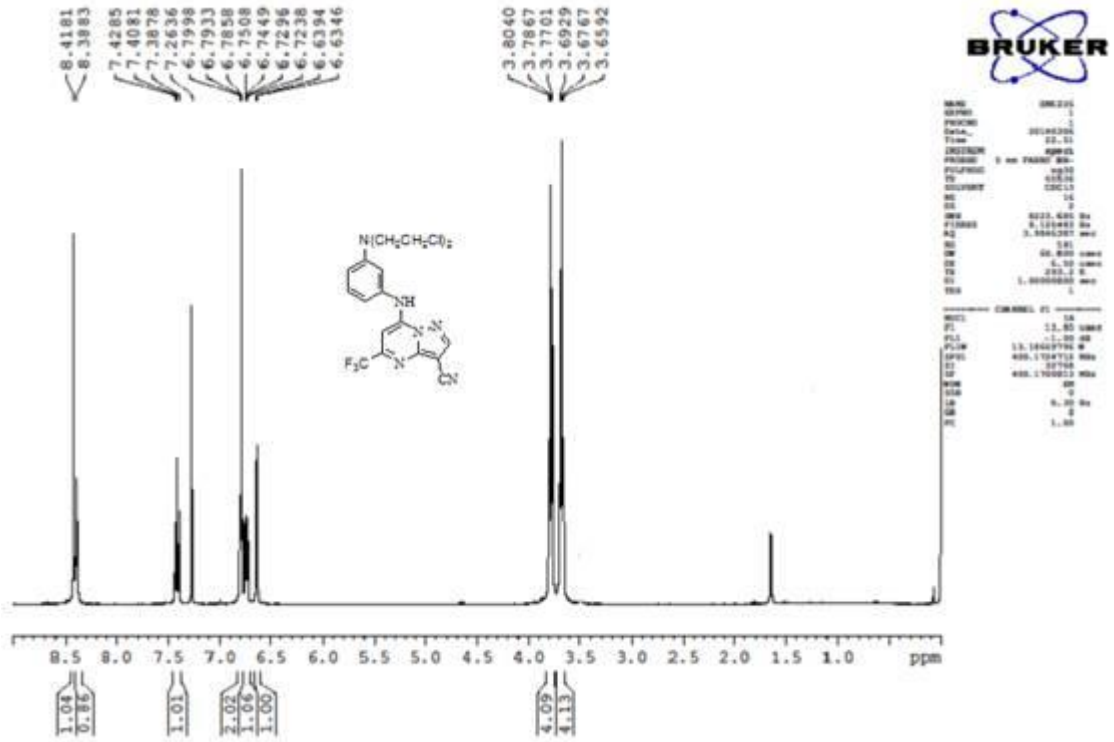
^{1}H NMR for compound **8f**



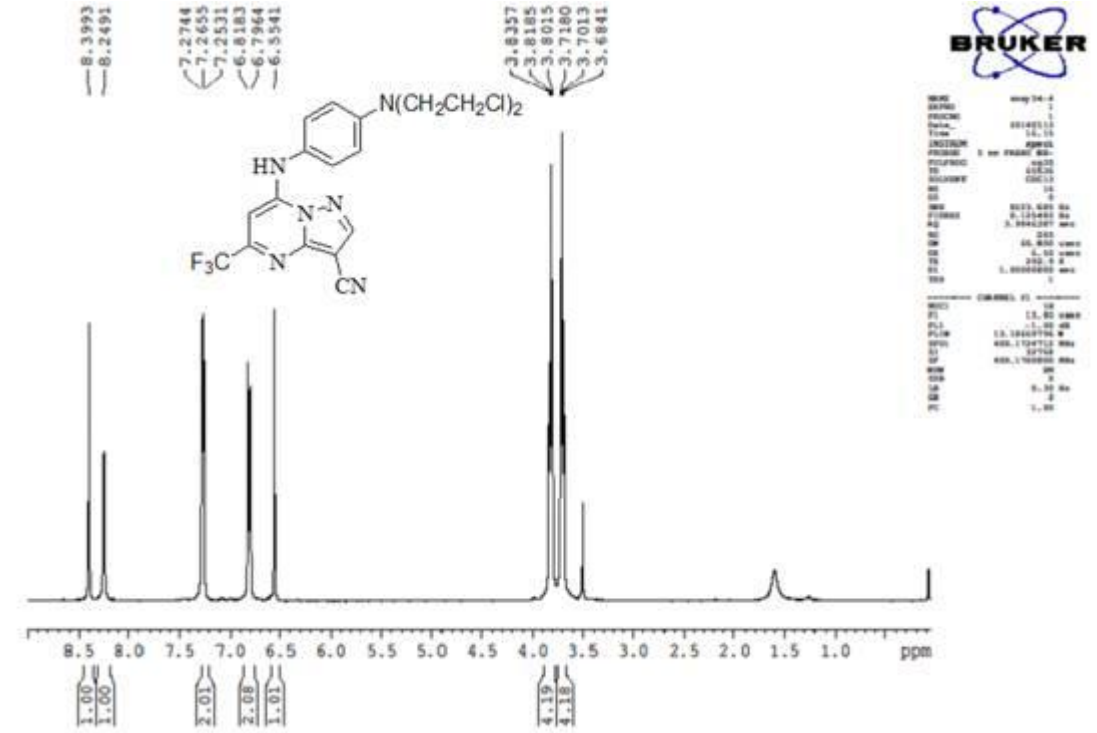
^{1}H NMR for compound **9f**



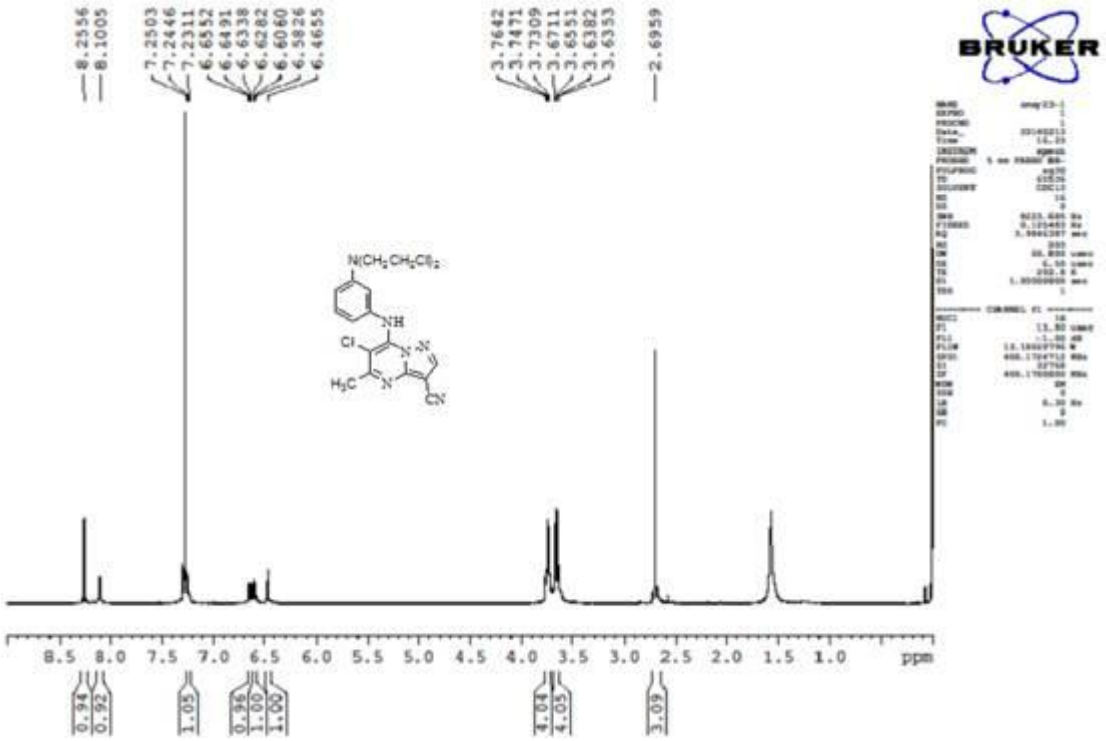
^{1}H NMR for compound **8g**



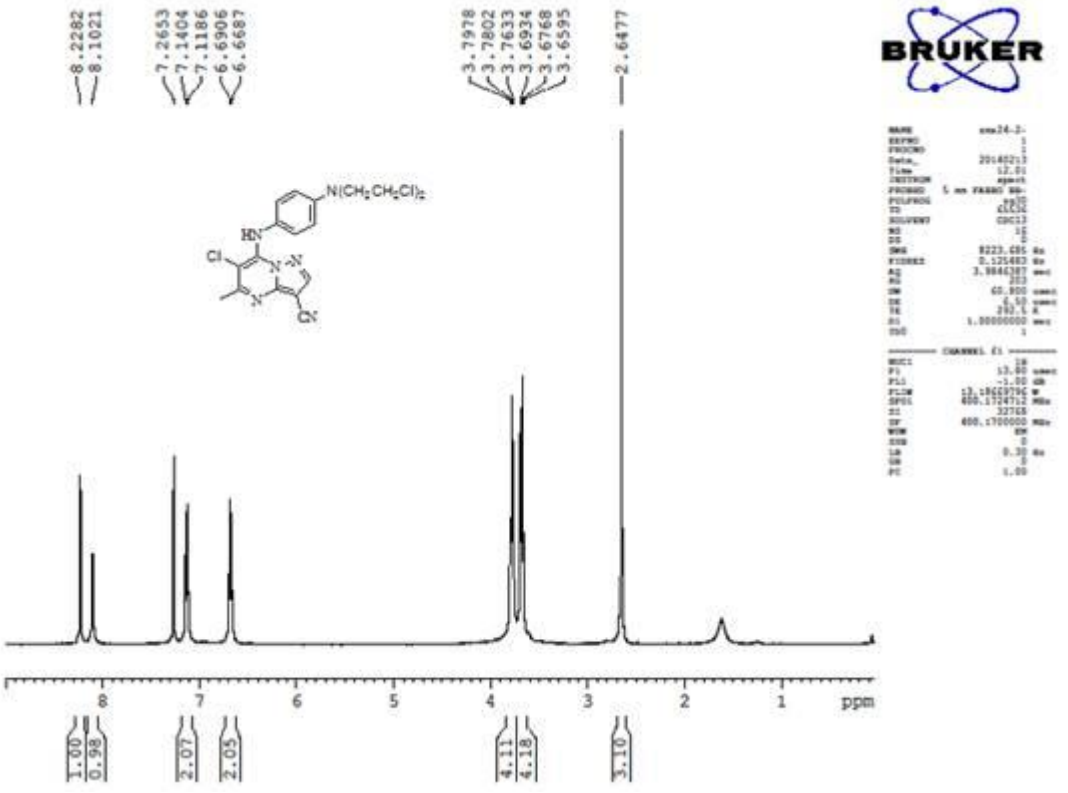
^{1}H NMR for compound **9g**



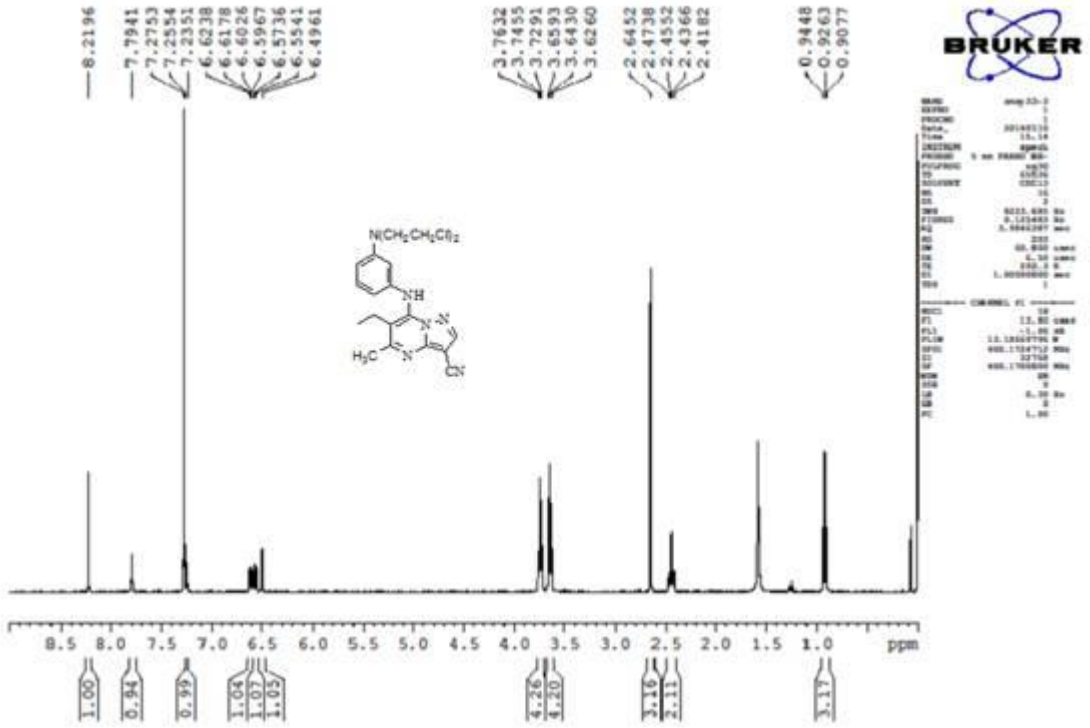
^{1}H NMR for compound **8h**



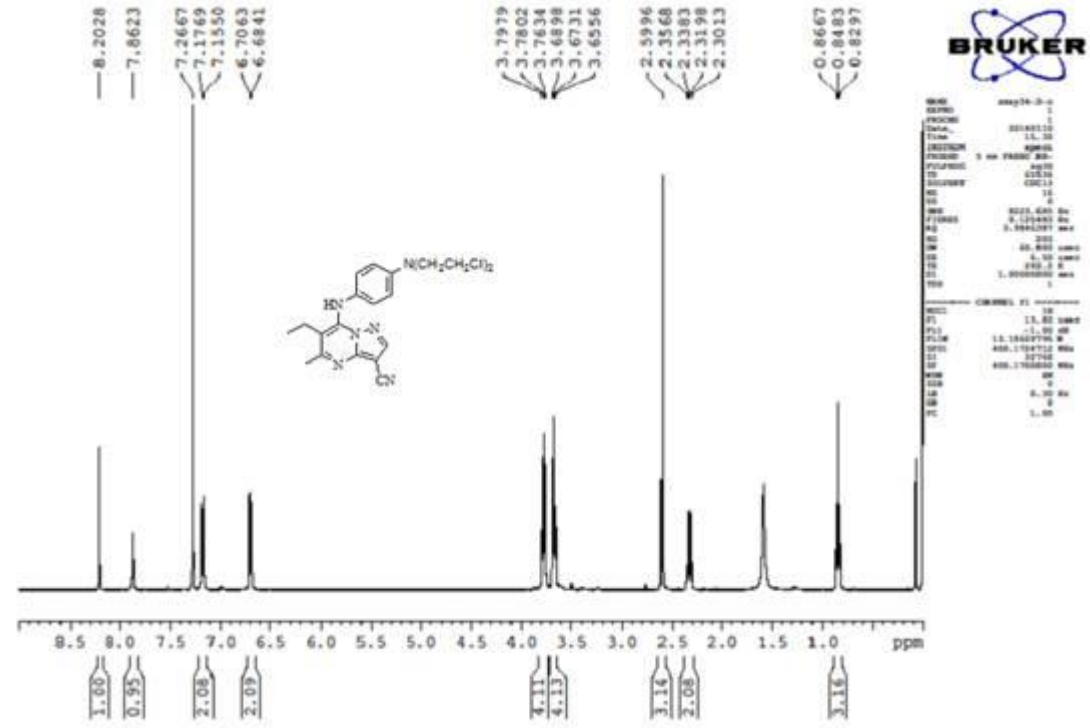
^{1}H NMR for compound **9h**



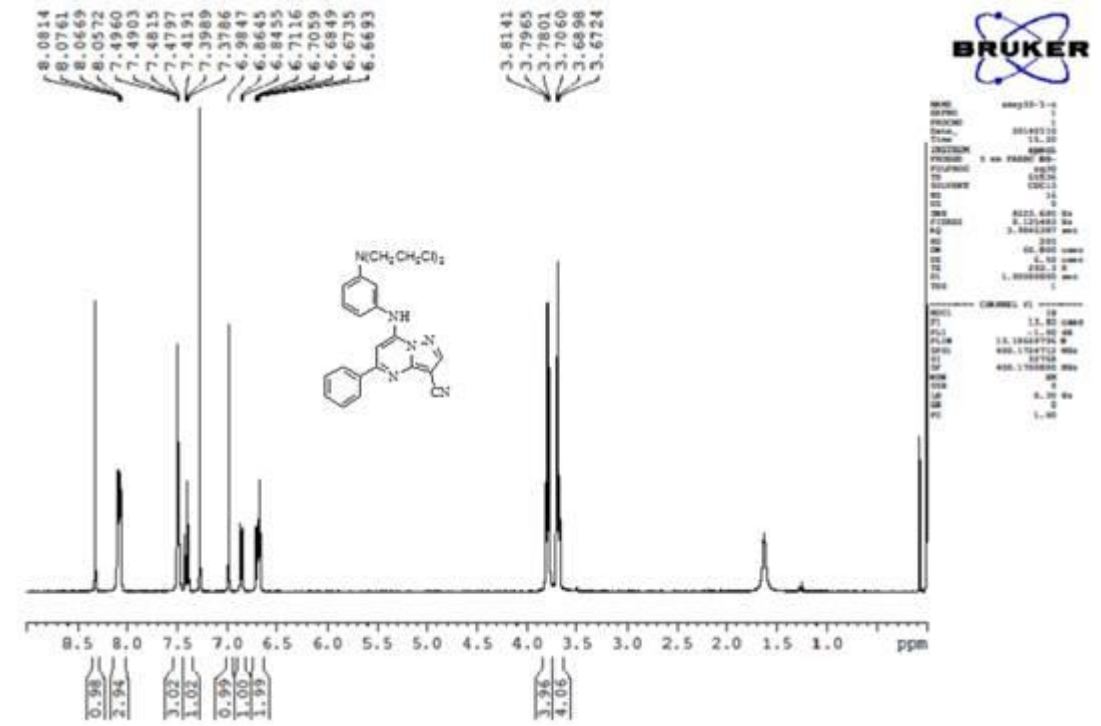
^{1}H NMR for compound **8i**



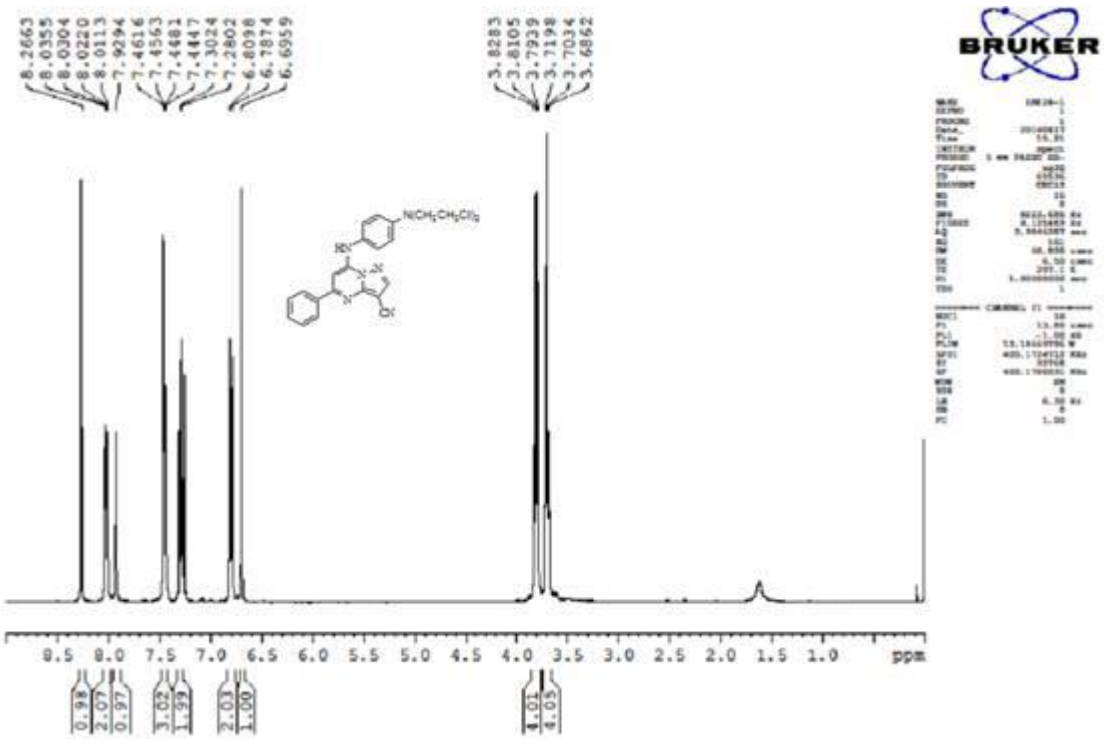
^{1}H NMR for compound **9i**



^{1}H NMR for compound **8j**

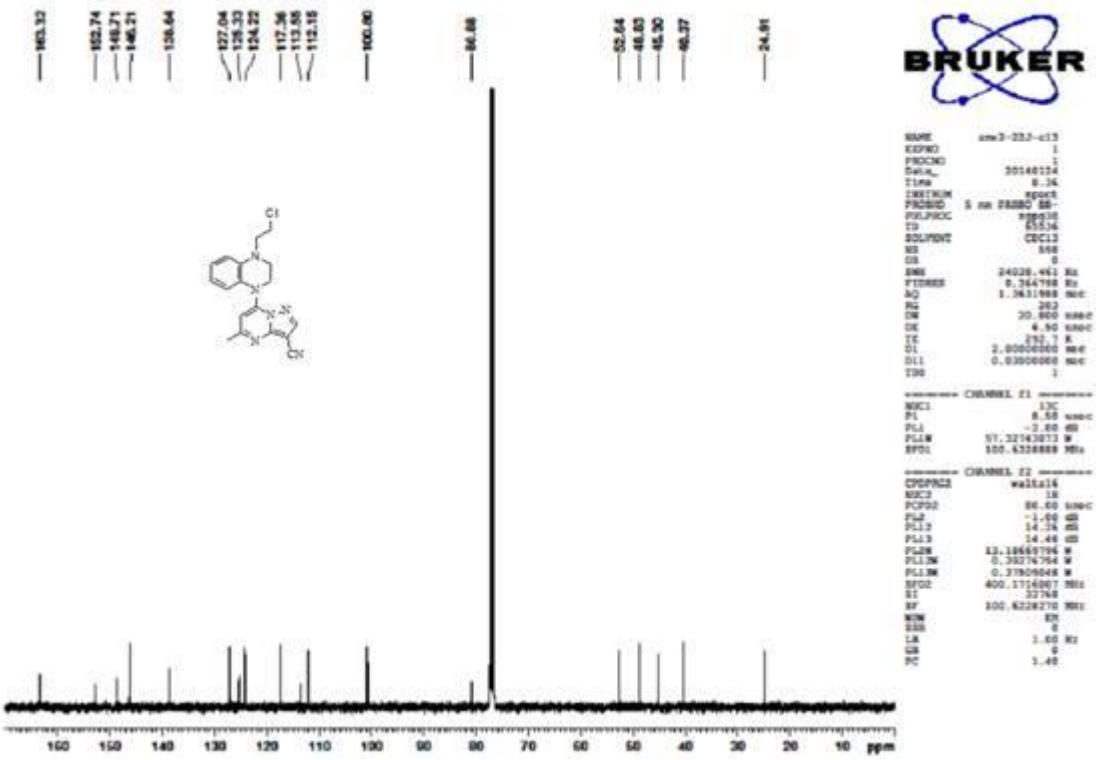


^{1}H NMR for compound **9j**

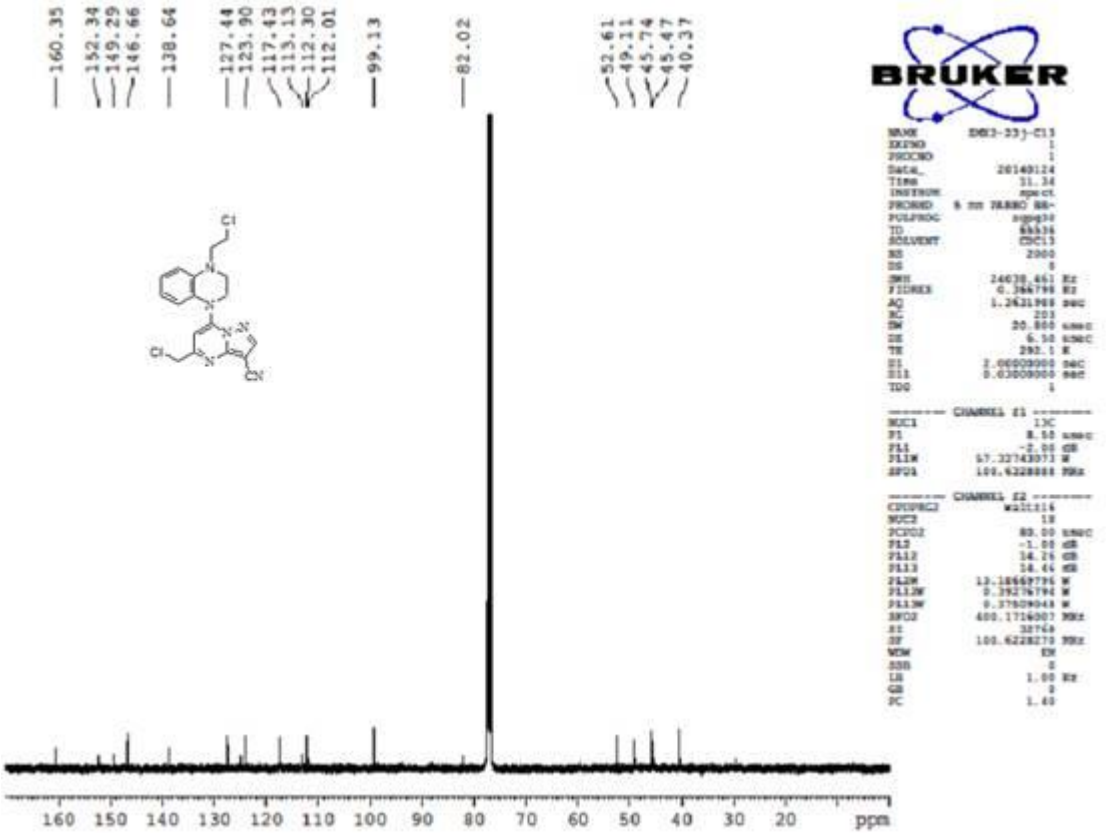


4. ^{13}C-NMR of target compounds

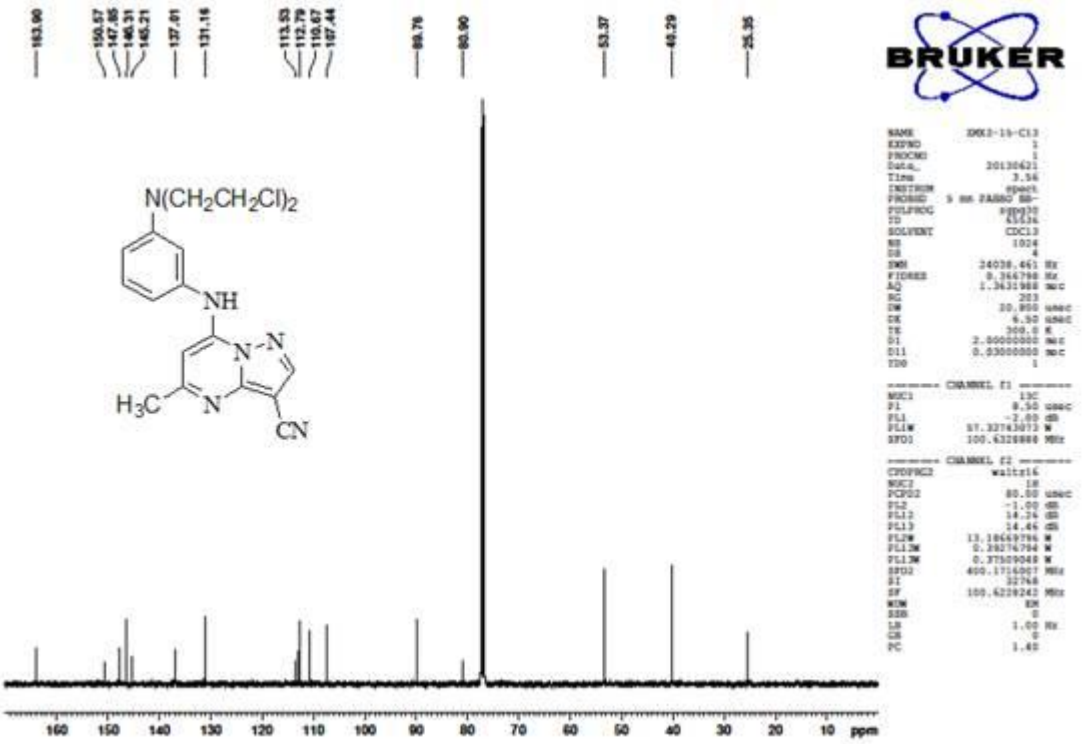
^{13}C NMR for compound **7m**



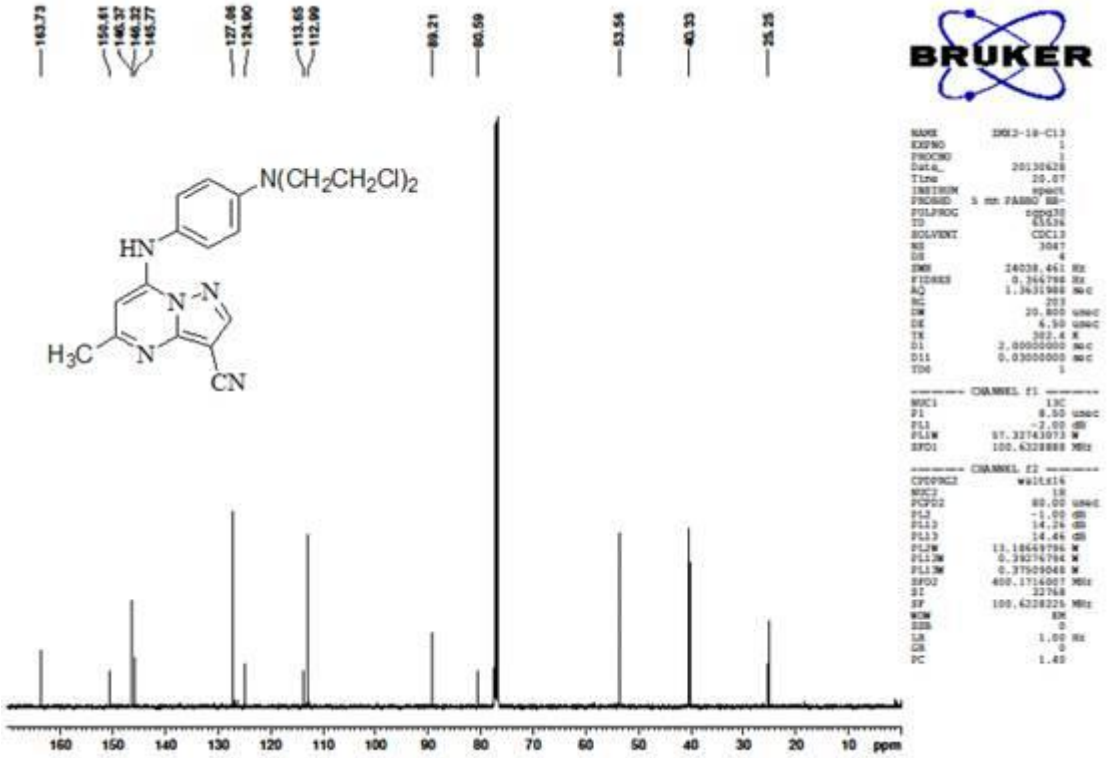
^{13}C NMR for compound **7n**



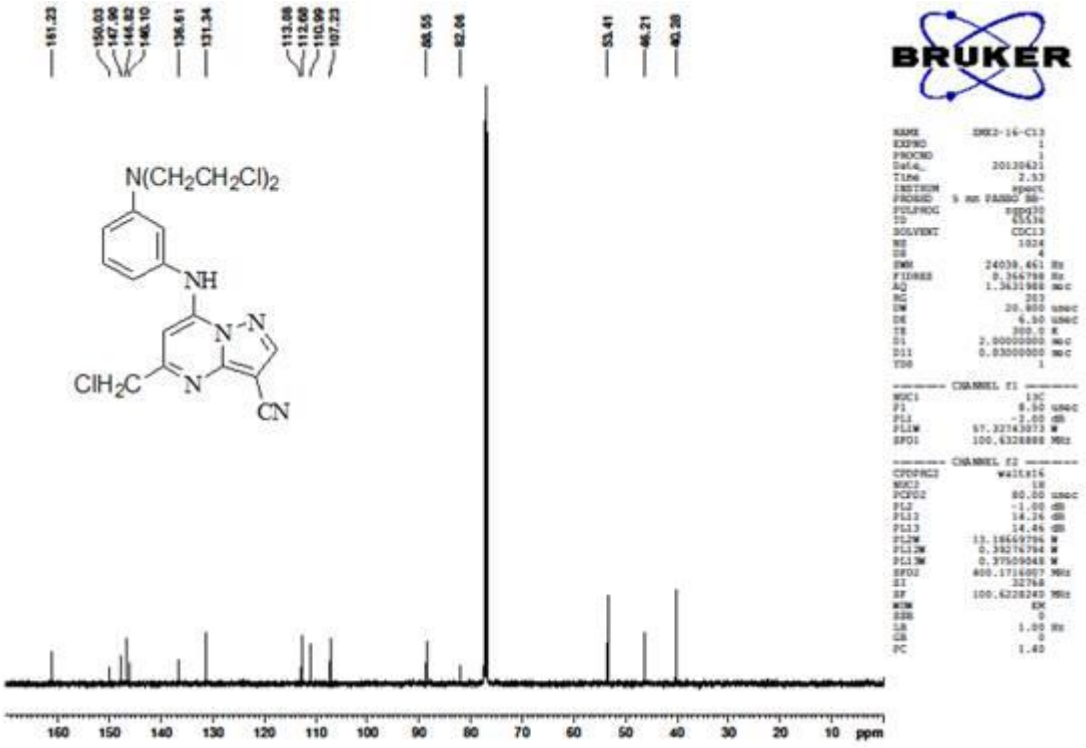
^{13}C NMR for compound **8a**



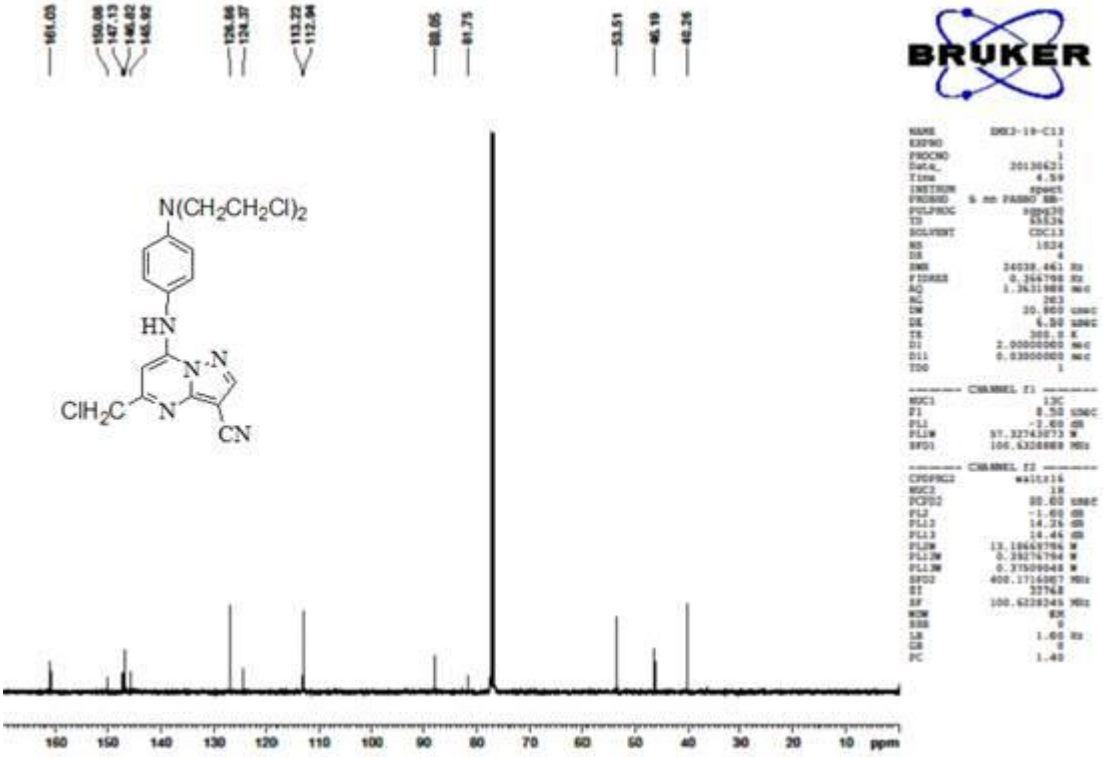
^{13}C NMR for compound **9a**



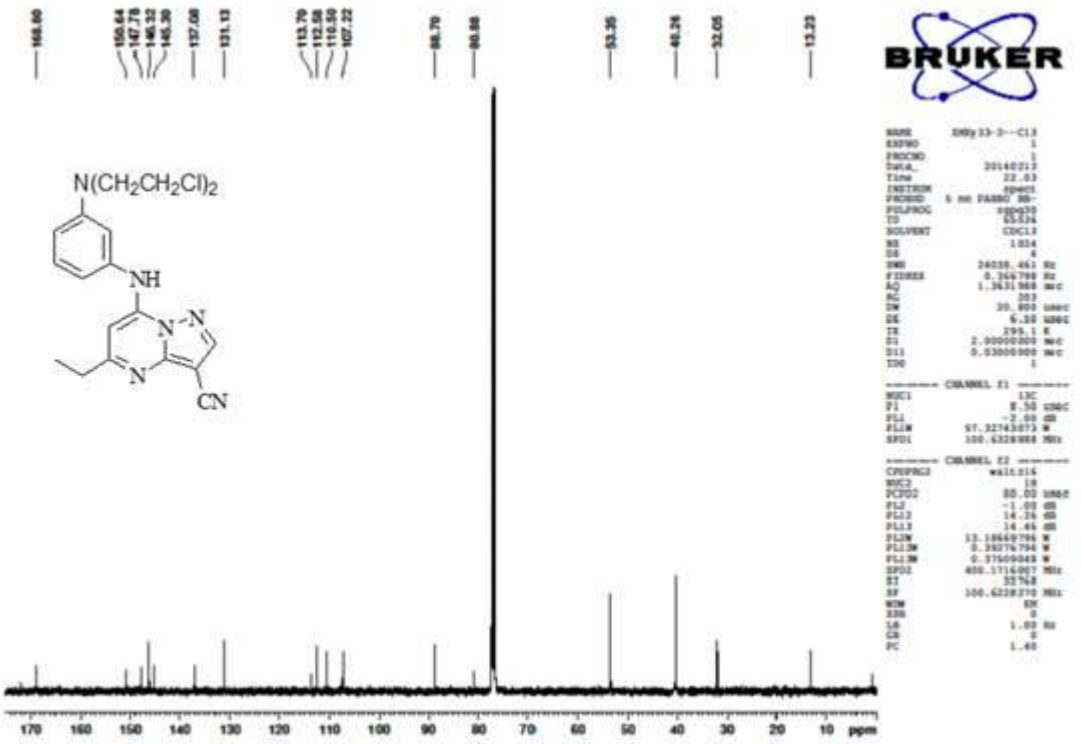
^{13}C NMR for compound **8b**



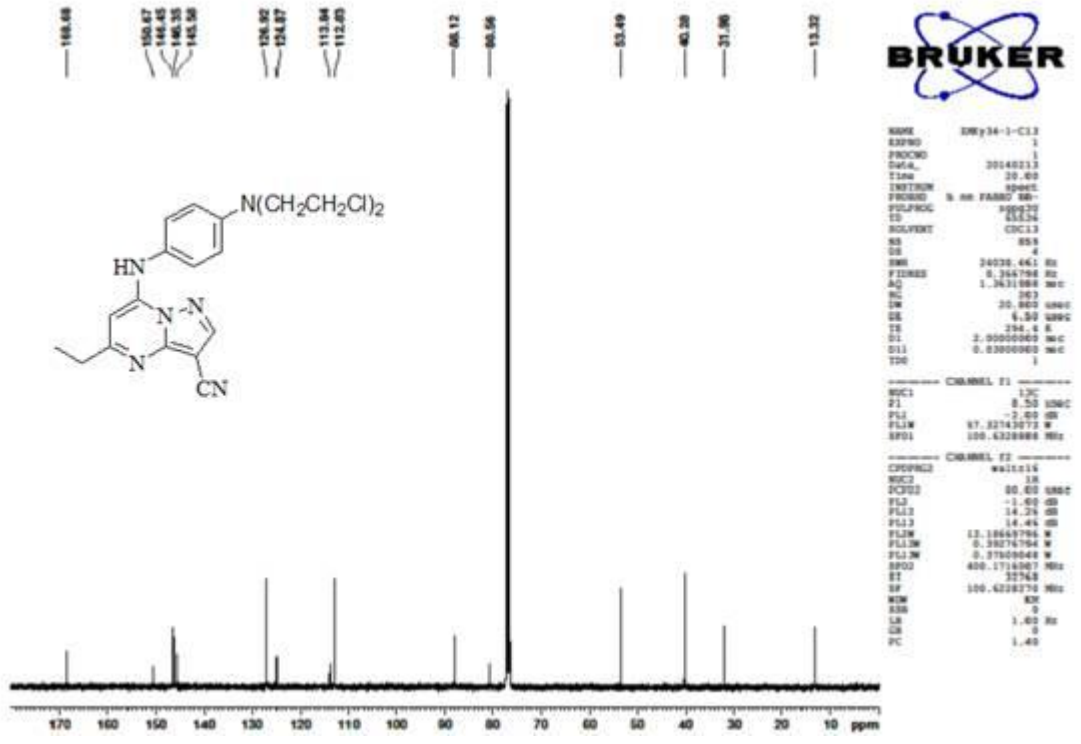
^{13}C NMR for compound **9b**



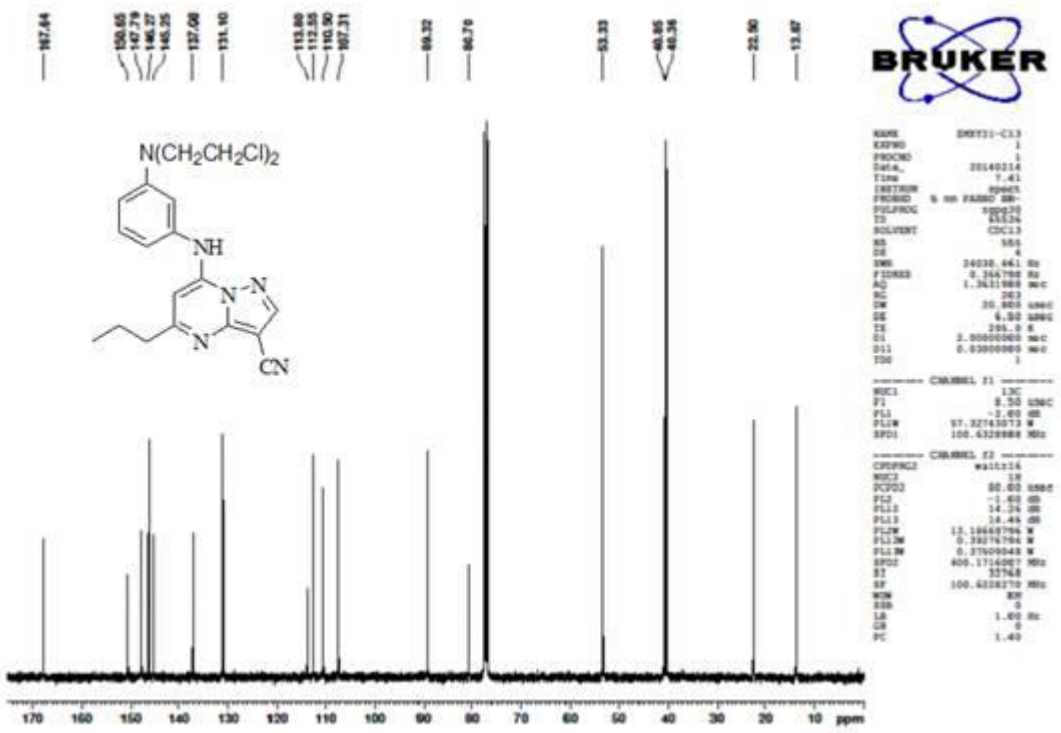
^{13}C NMR for compound **8c**



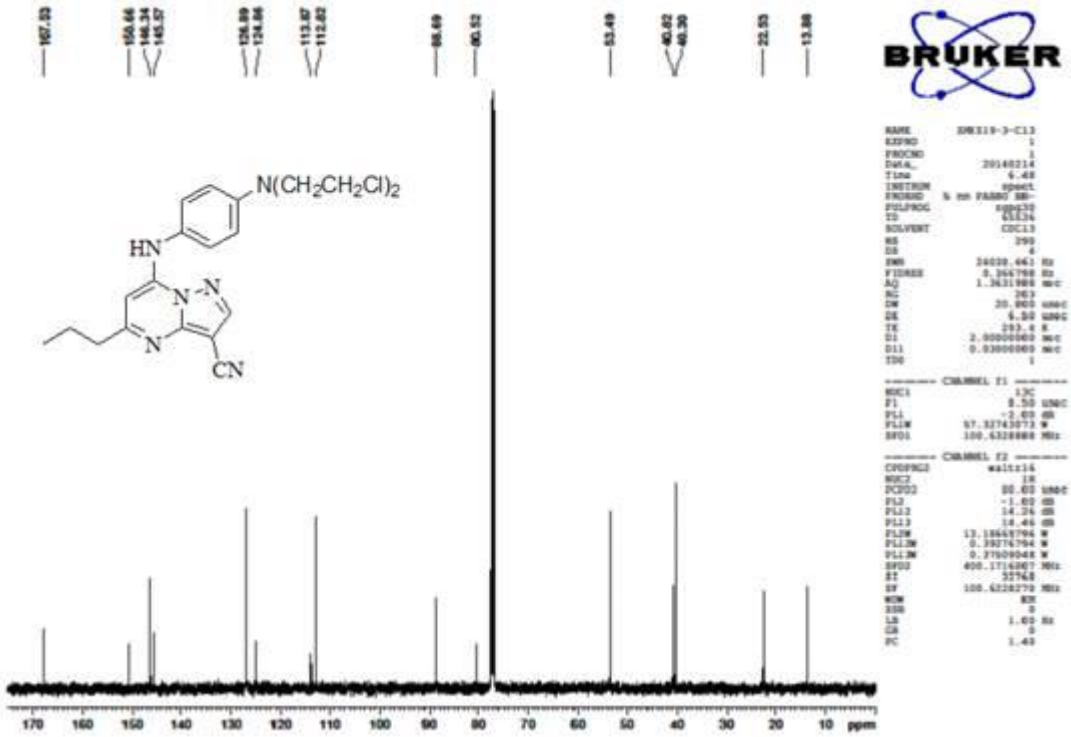
^{13}C NMR for compound **9c**



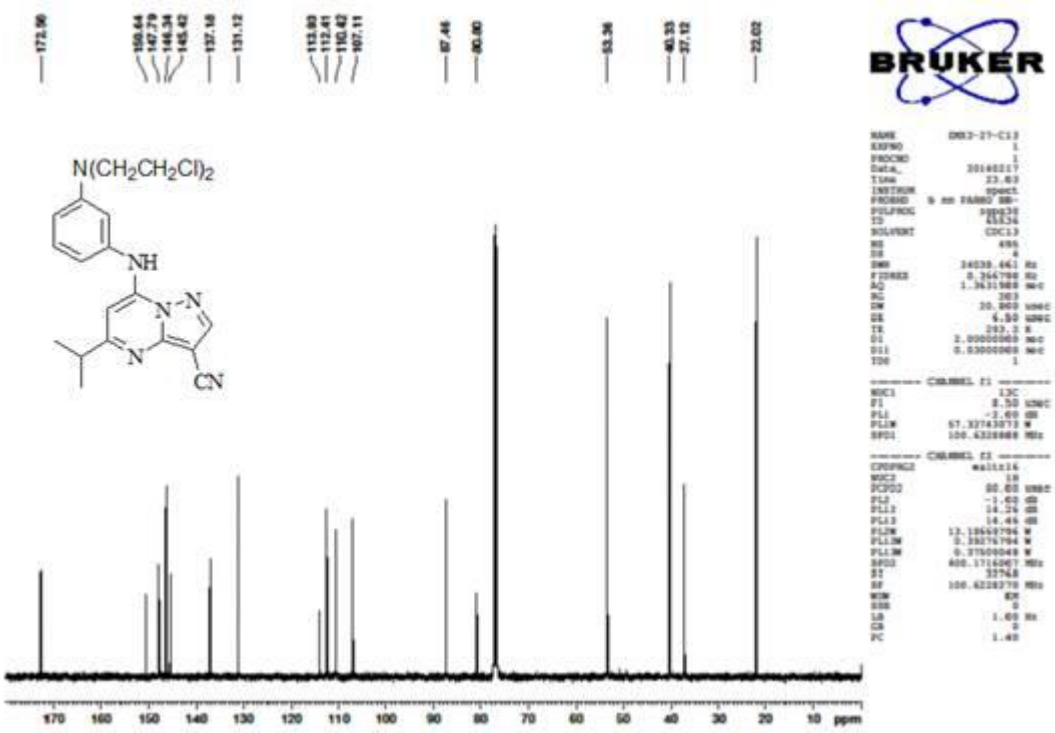
^{13}C NMR for compound **8d**



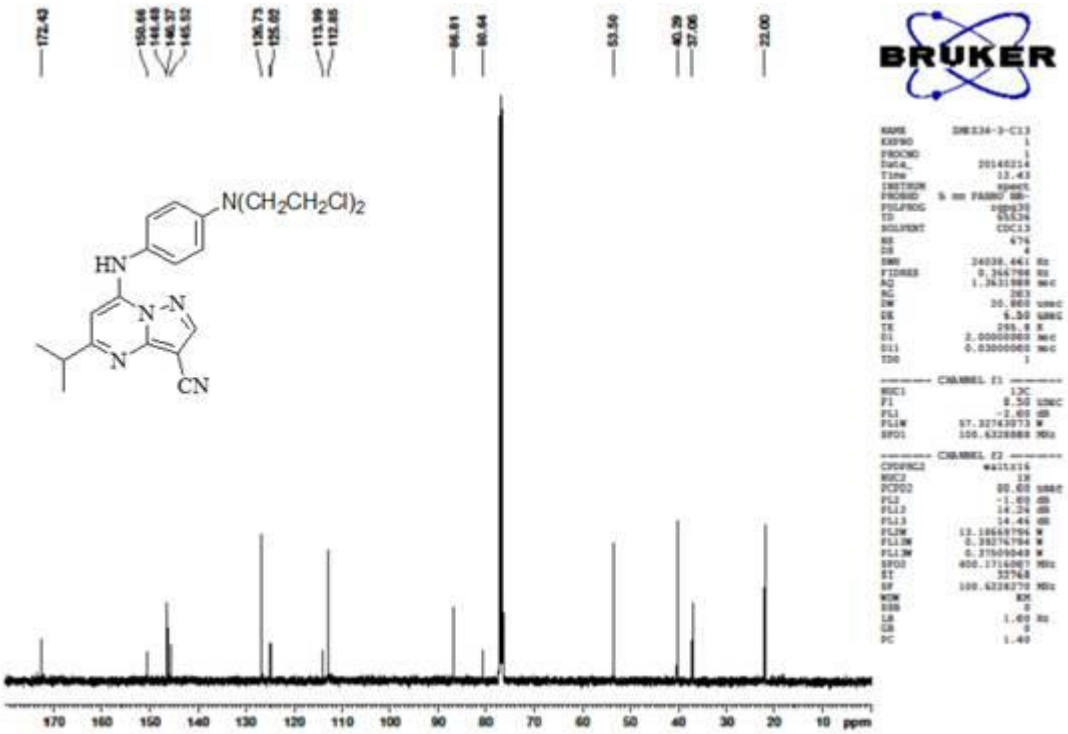
^{13}C NMR for compound **9d**



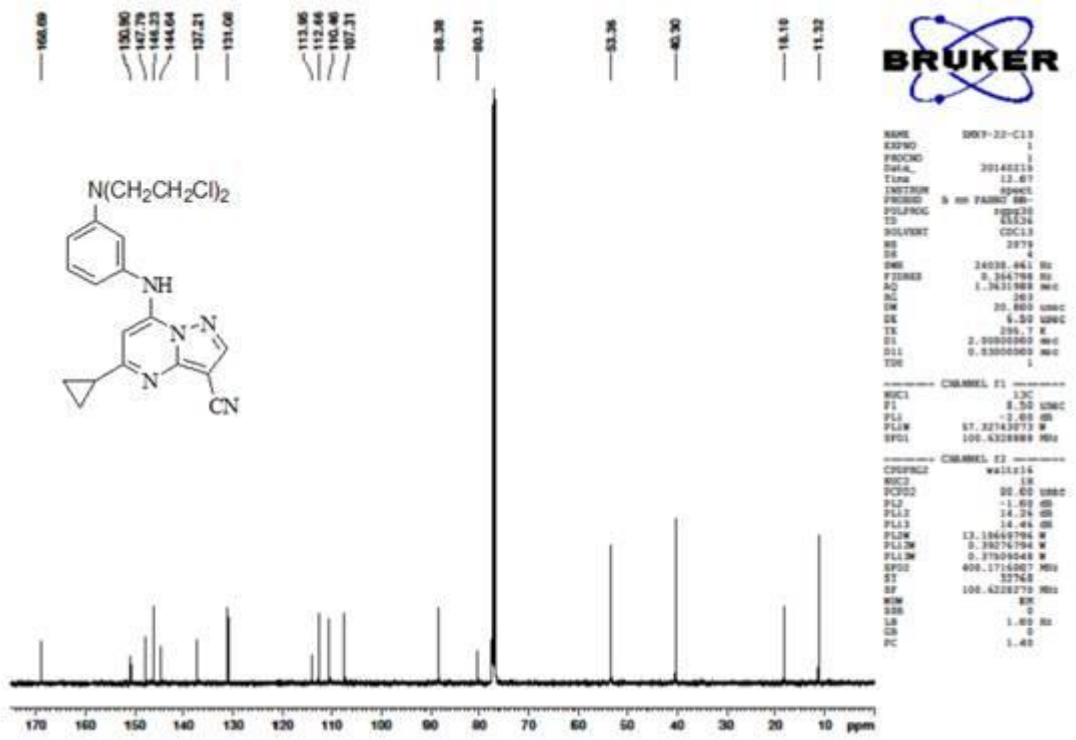
^{13}C NMR for compound **8e**



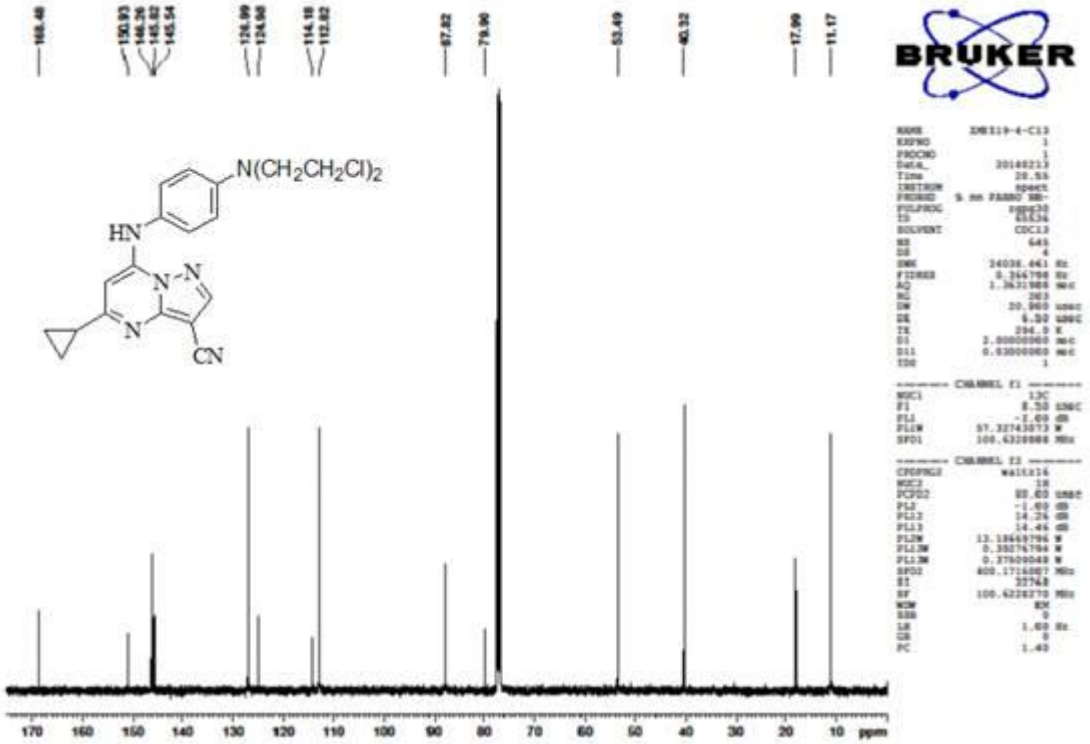
^{13}C NMR for compound **9e**



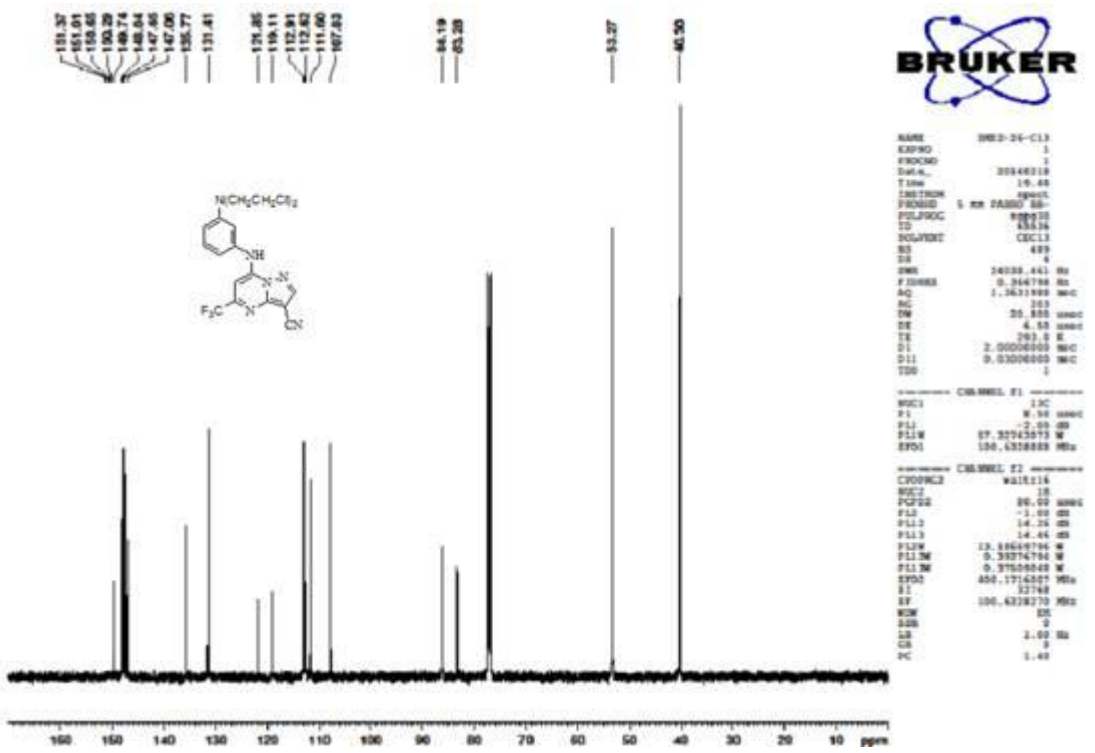
^{13}C NMR for compound **8f**



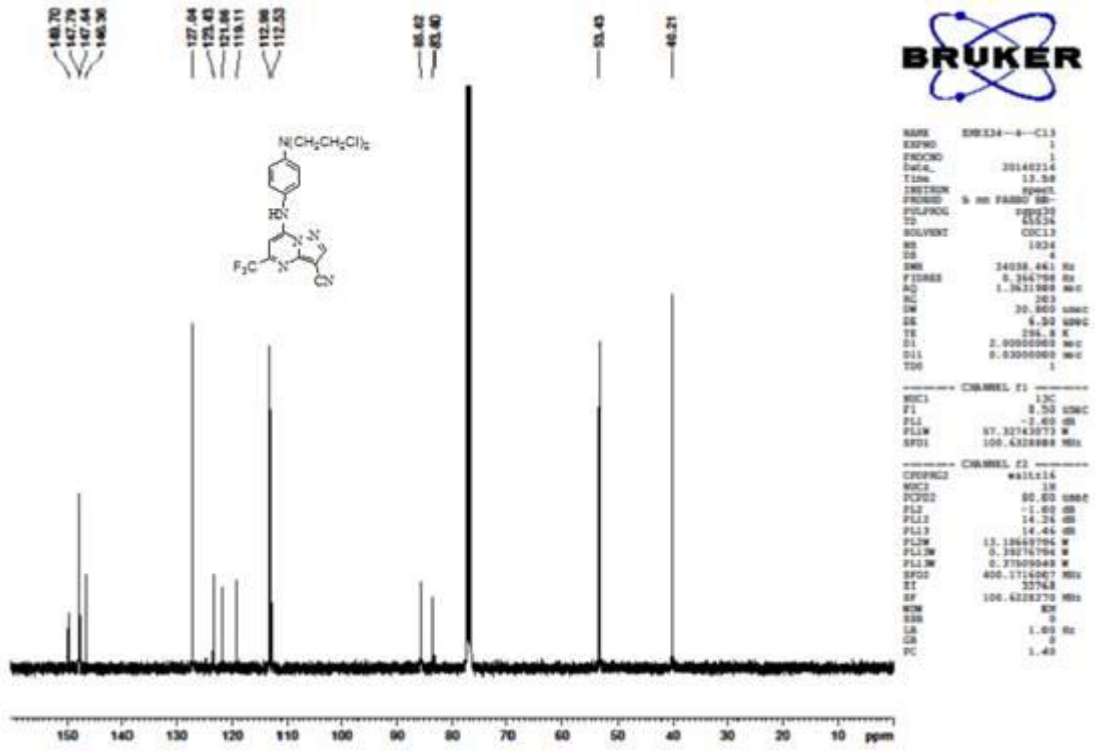
^{13}C NMR for compound **9f**



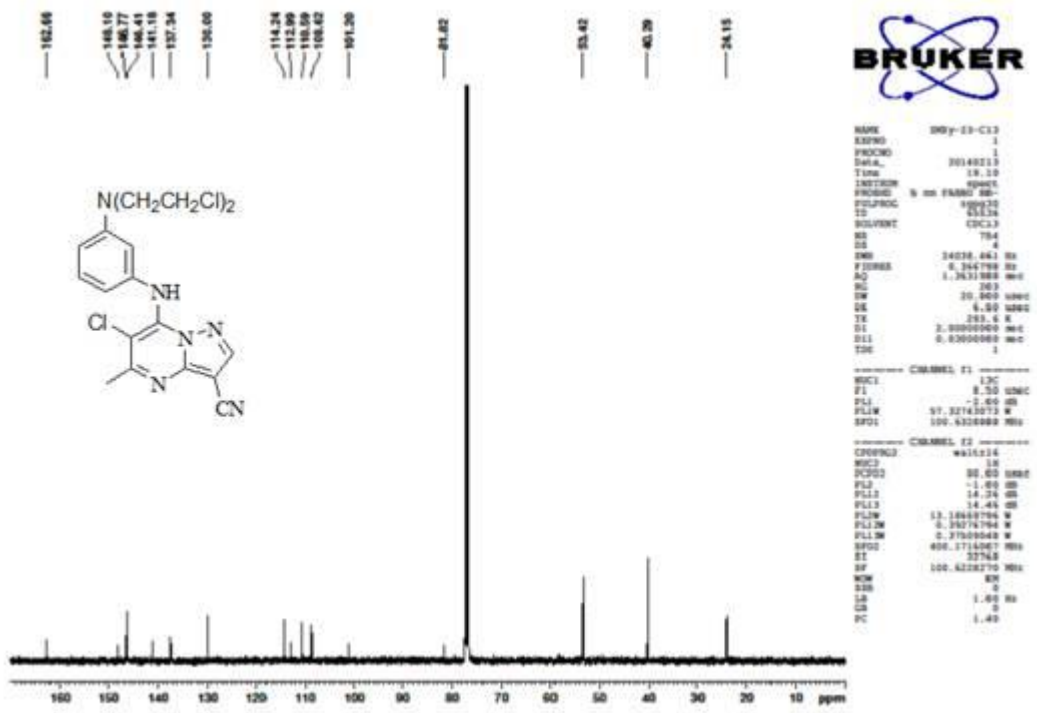
^{13}C NMR for compound **8g**



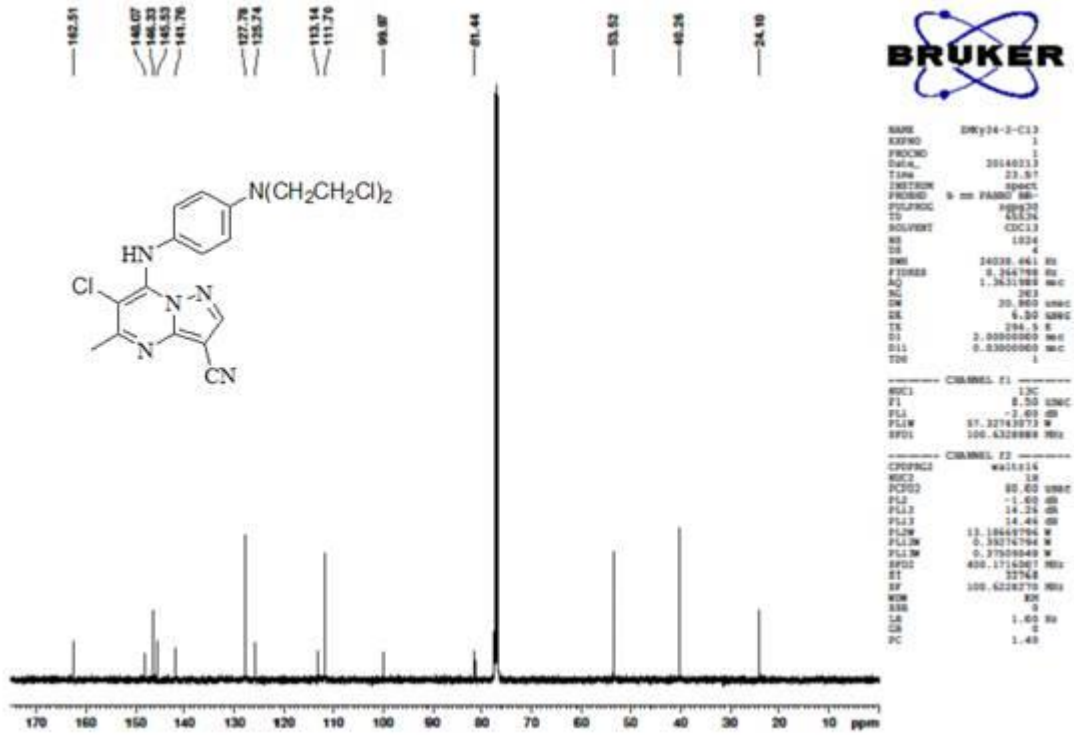
^{13}C NMR for compound **9g**



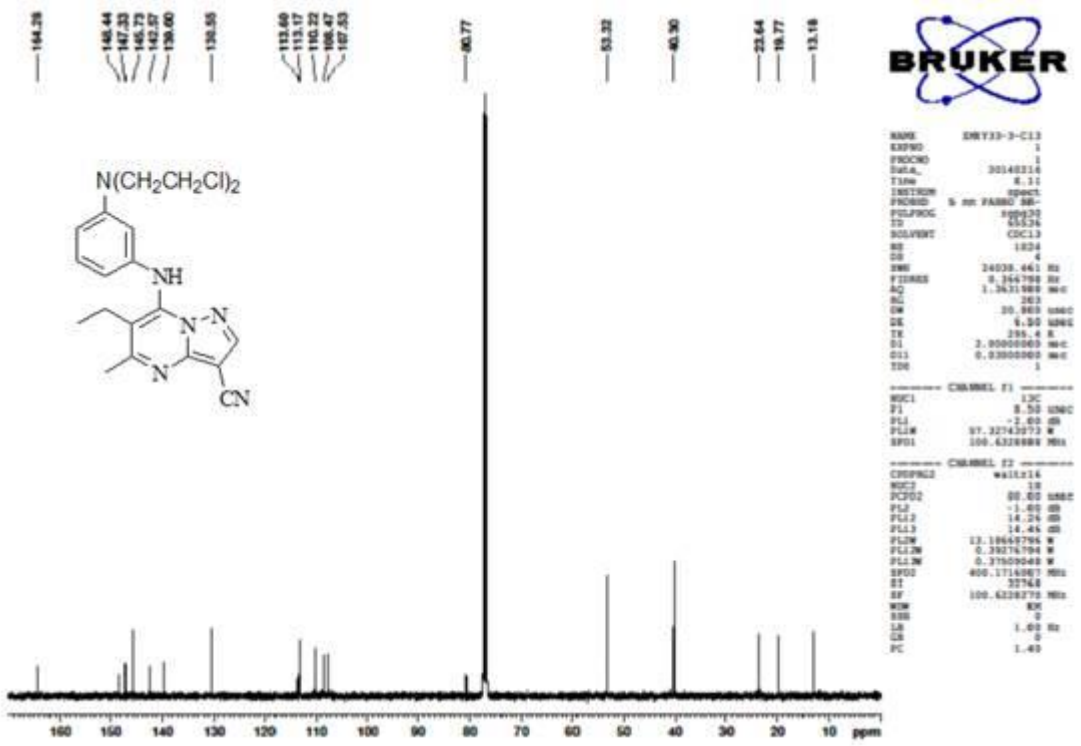
^{13}C NMR for compound **8h**



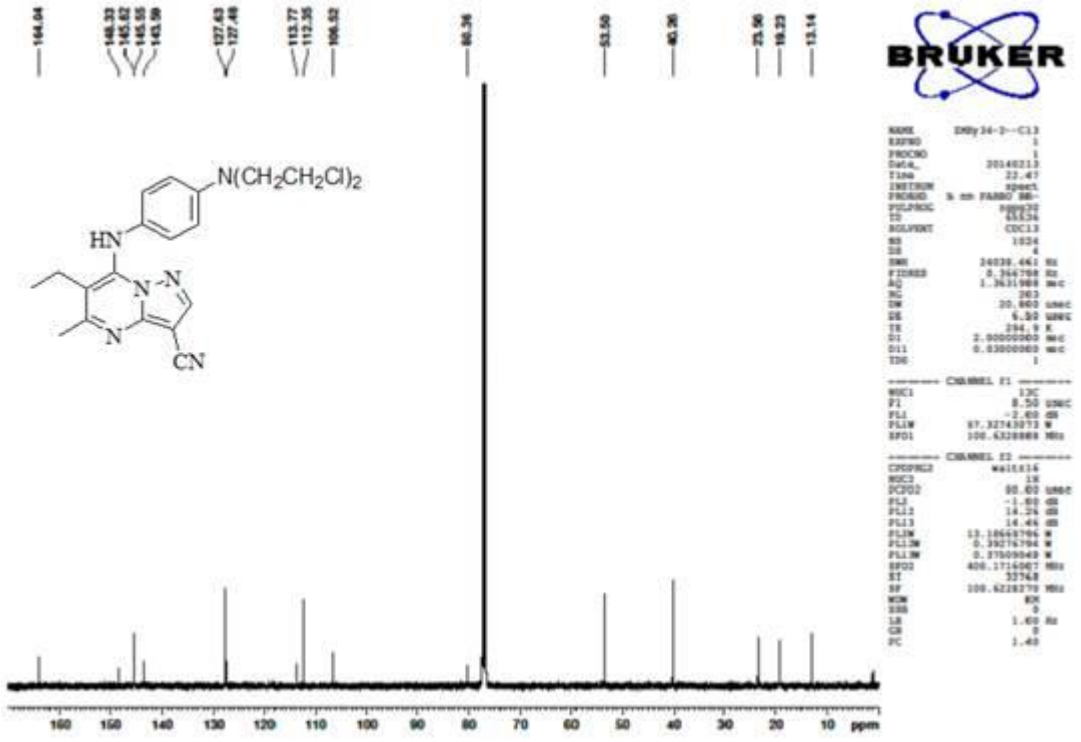
^{13}C NMR for compound **9h**



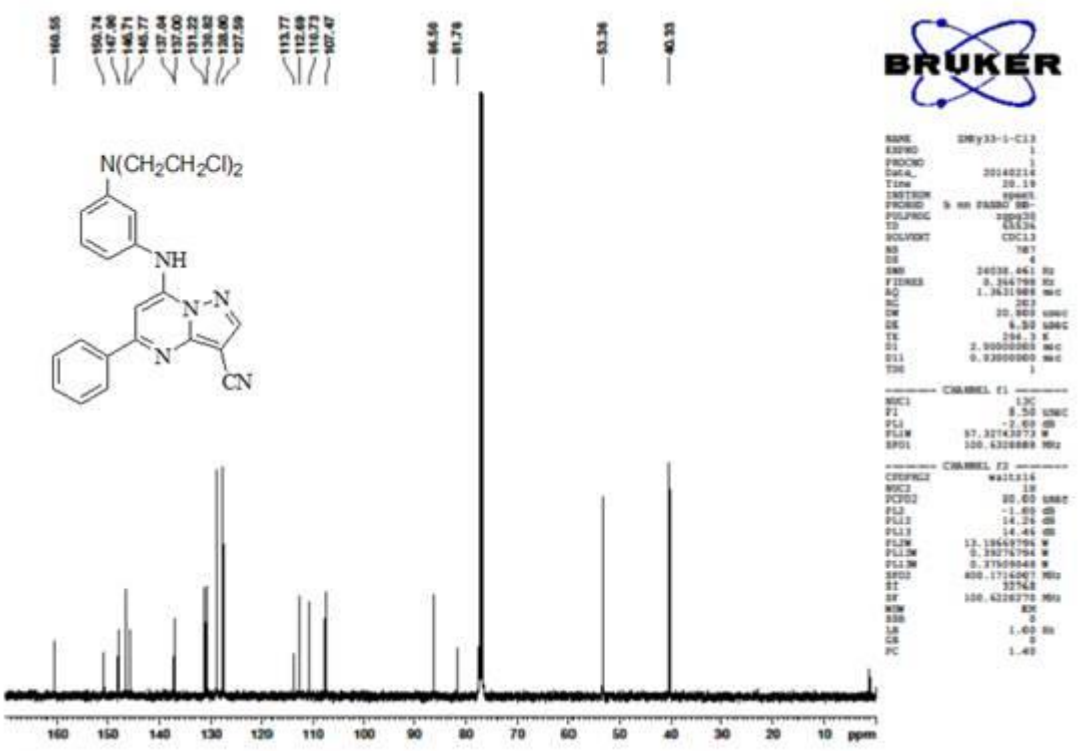
^{13}C NMR for compound **8i**



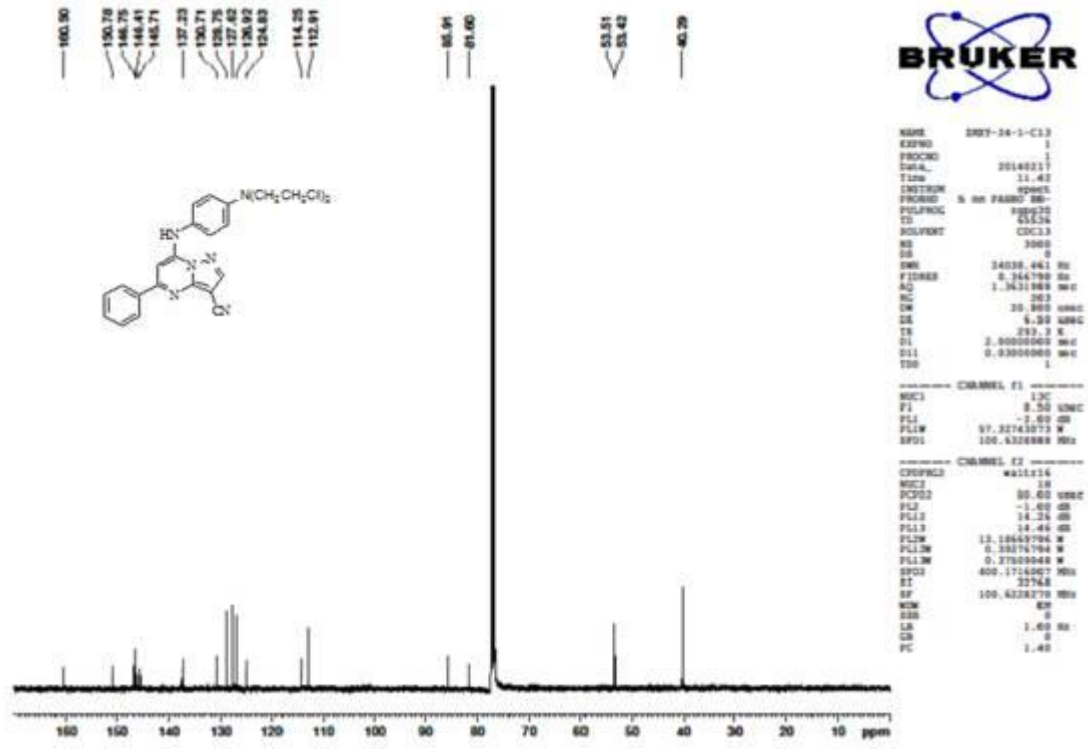
^{13}C NMR for compound **9i**



^{13}C NMR for compound **8j**

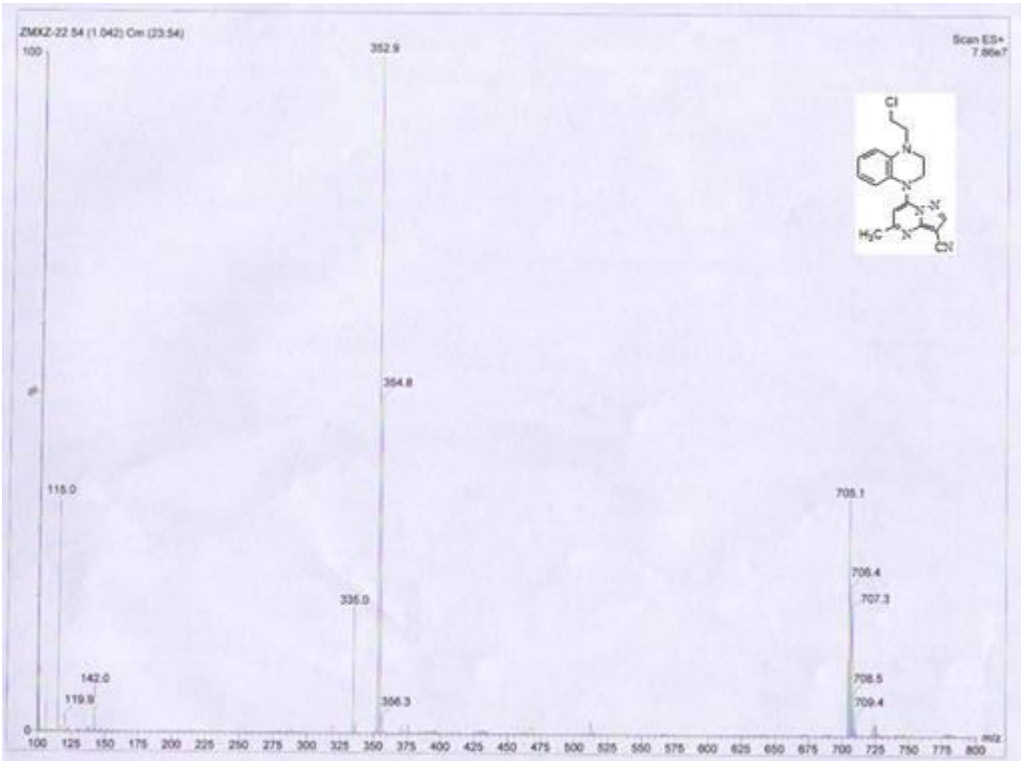


^{13}C NMR for compound **9j**

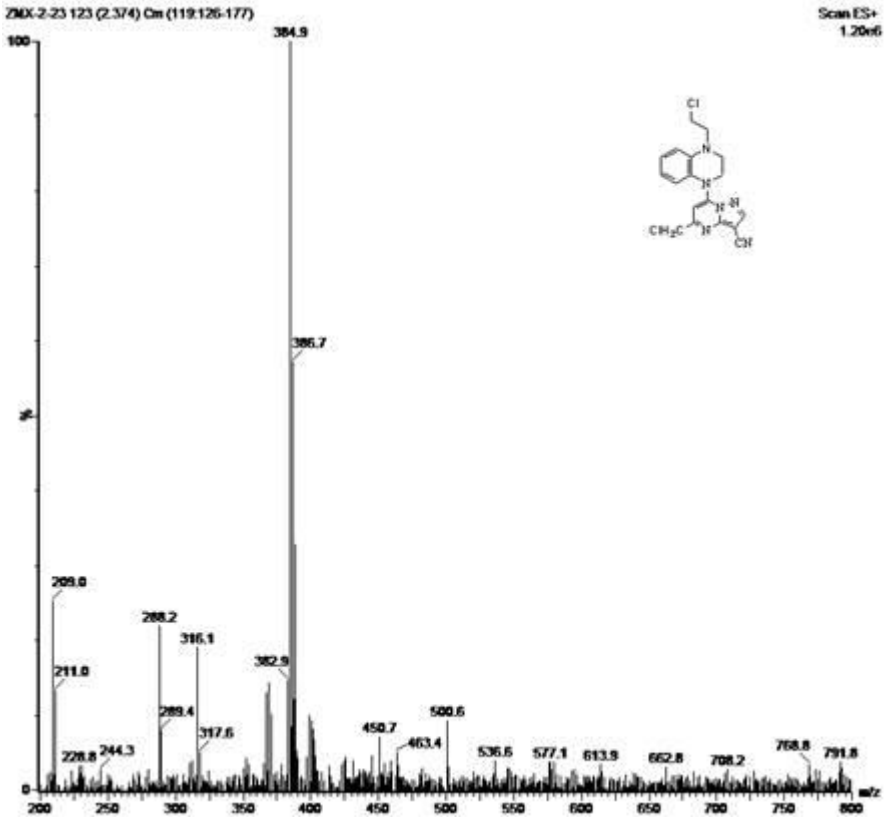


5. MS of target compounds

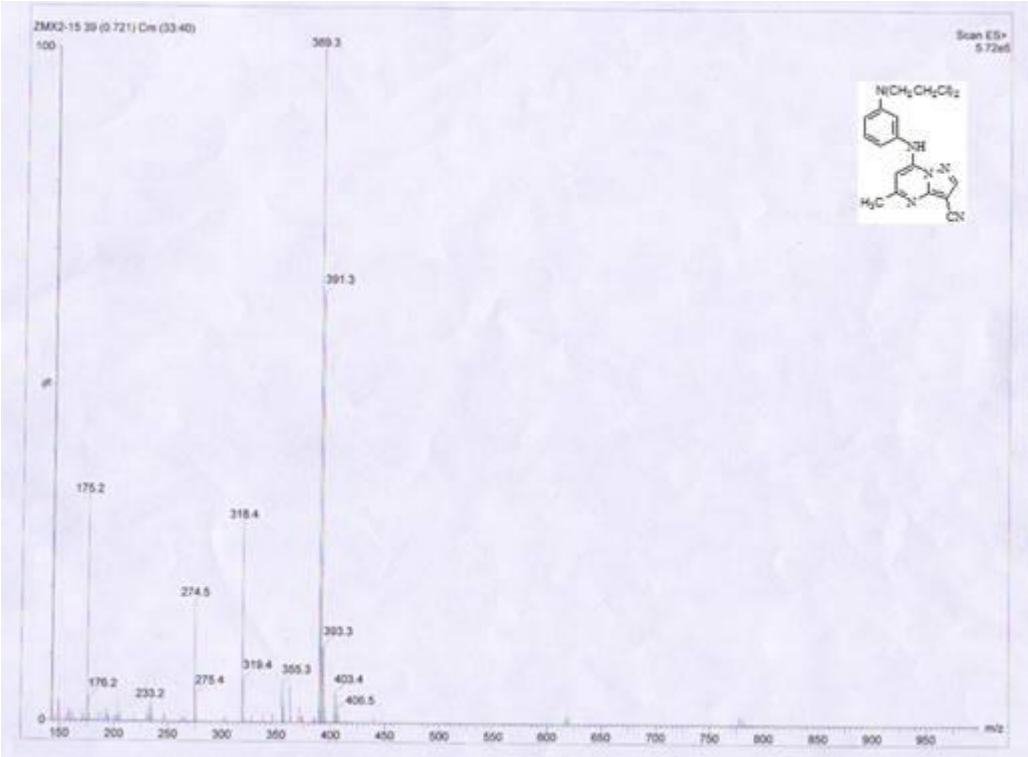
MS for compound **7m**



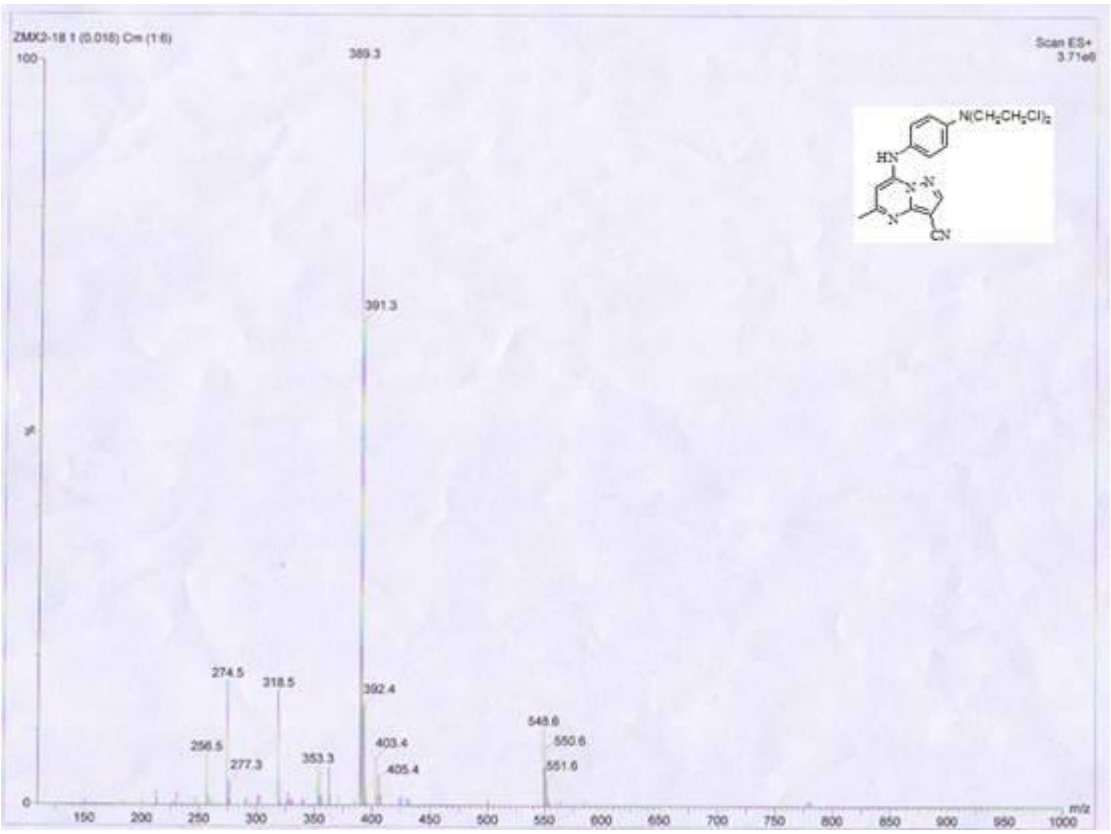
MS for compound **7n**



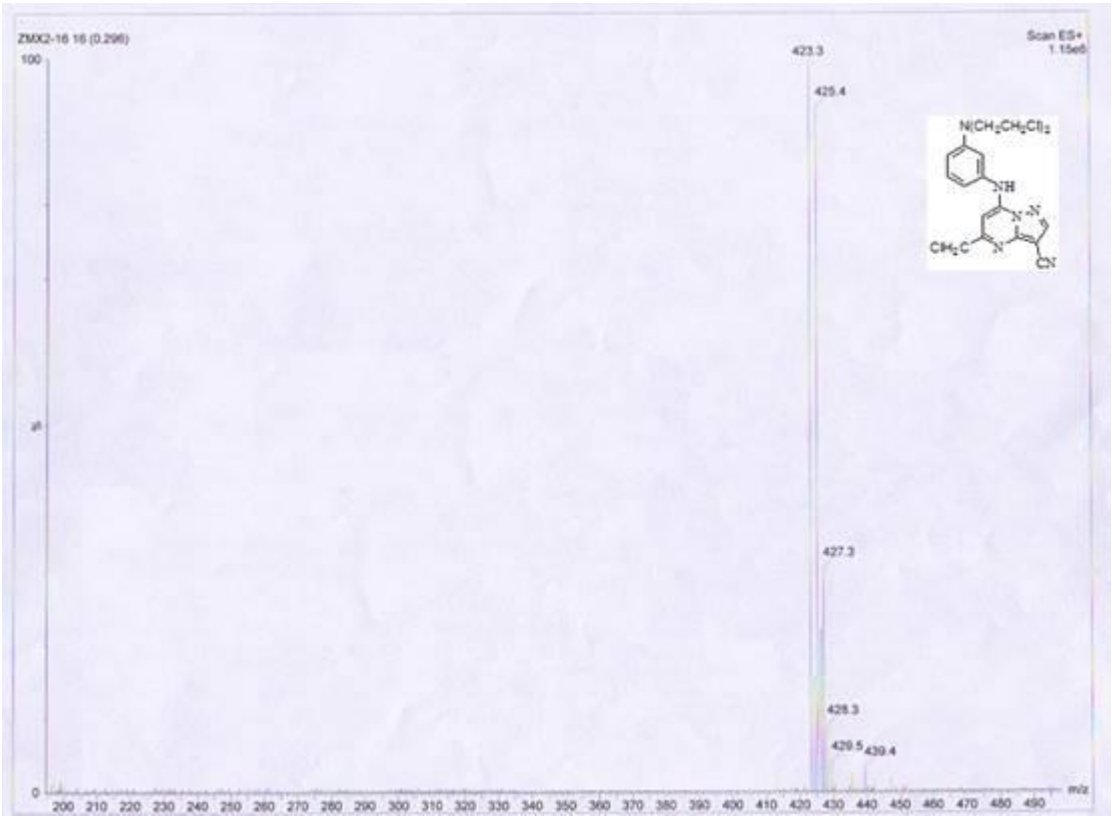
MS for compound **8a**



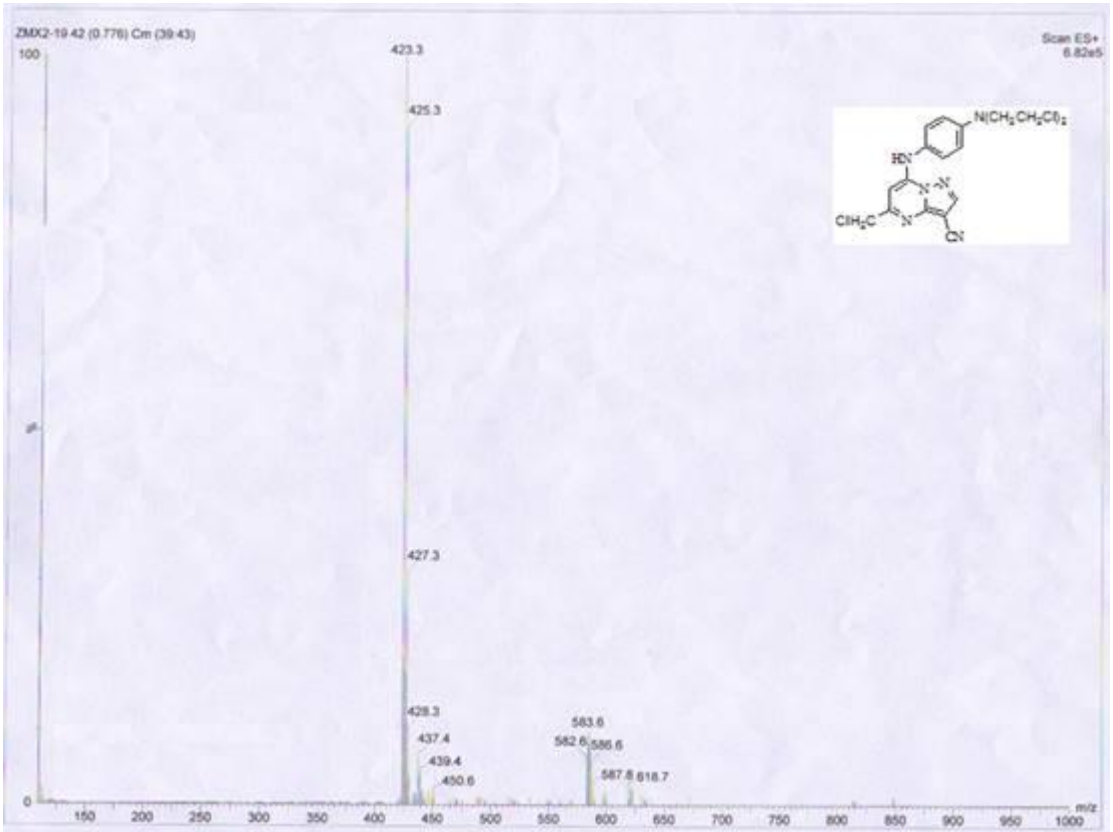
MS for compound **9a**



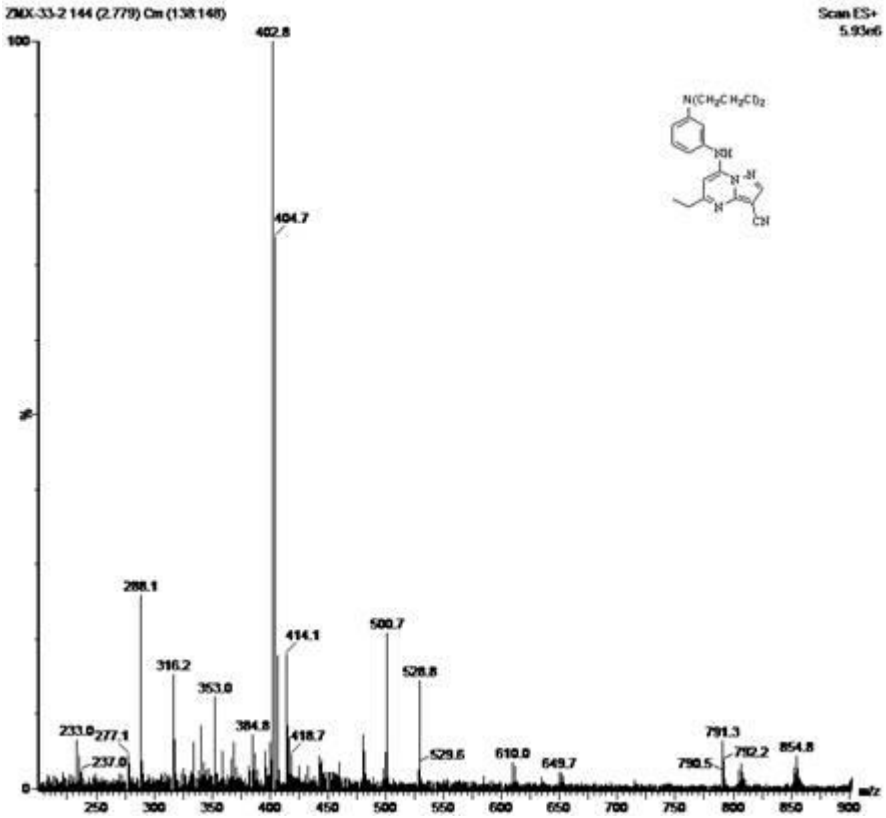
MS for compound **8b**



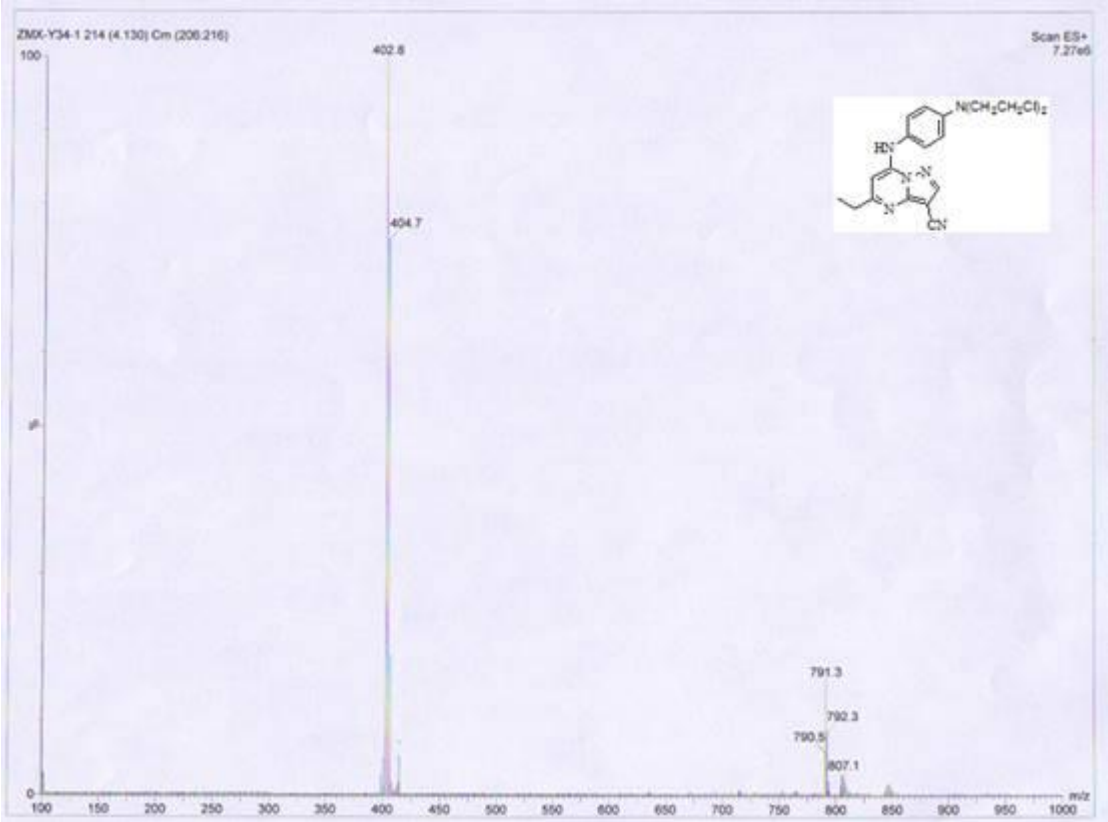
MS for compound **9b**



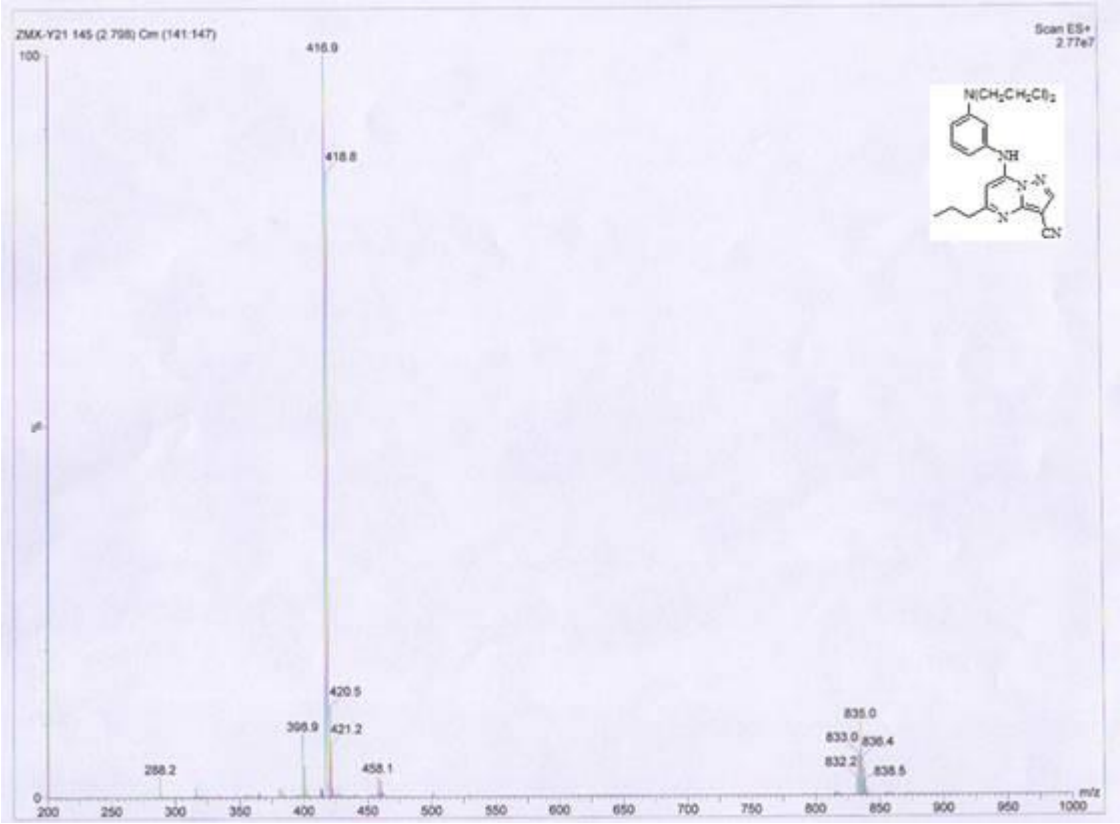
MS for compound **8c**



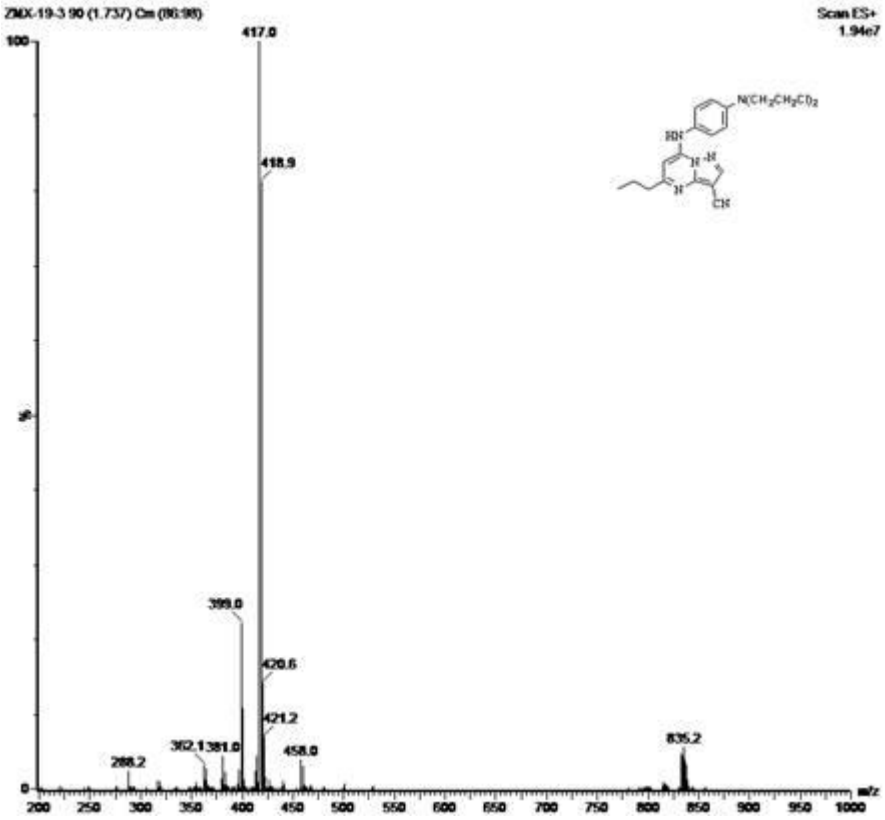
MS for compound **9c**



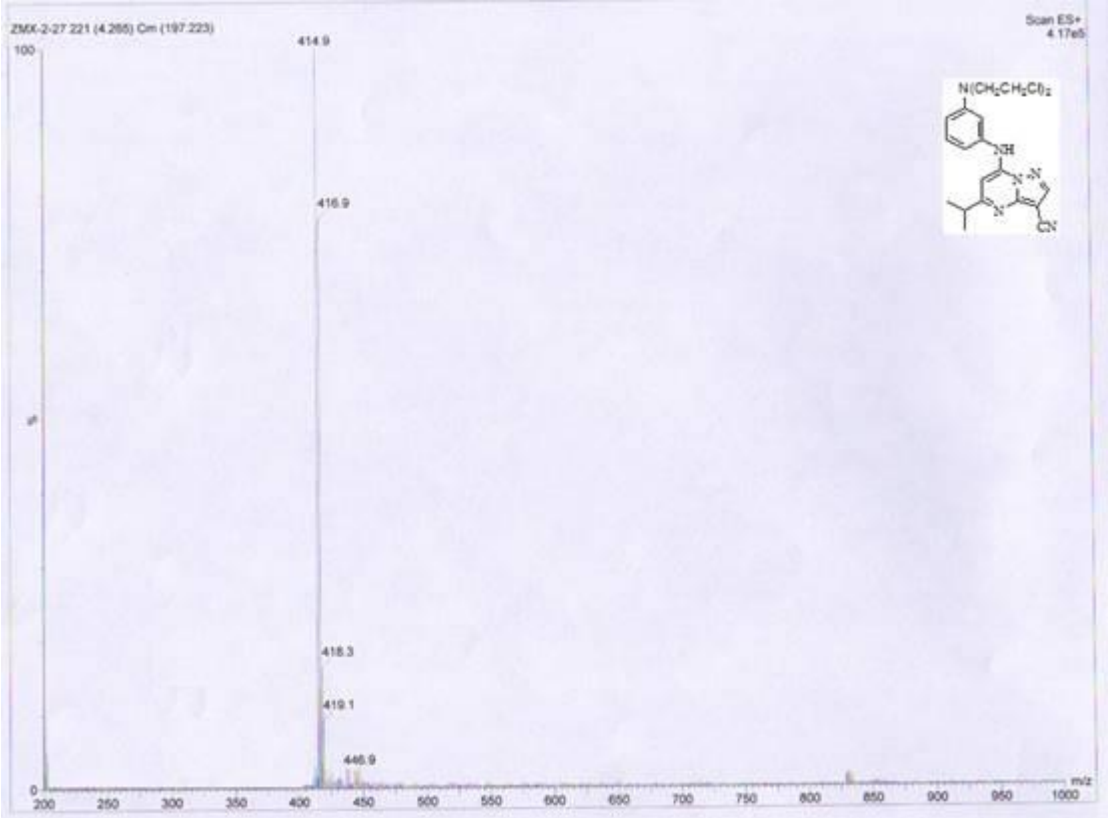
MS for compound **8d**



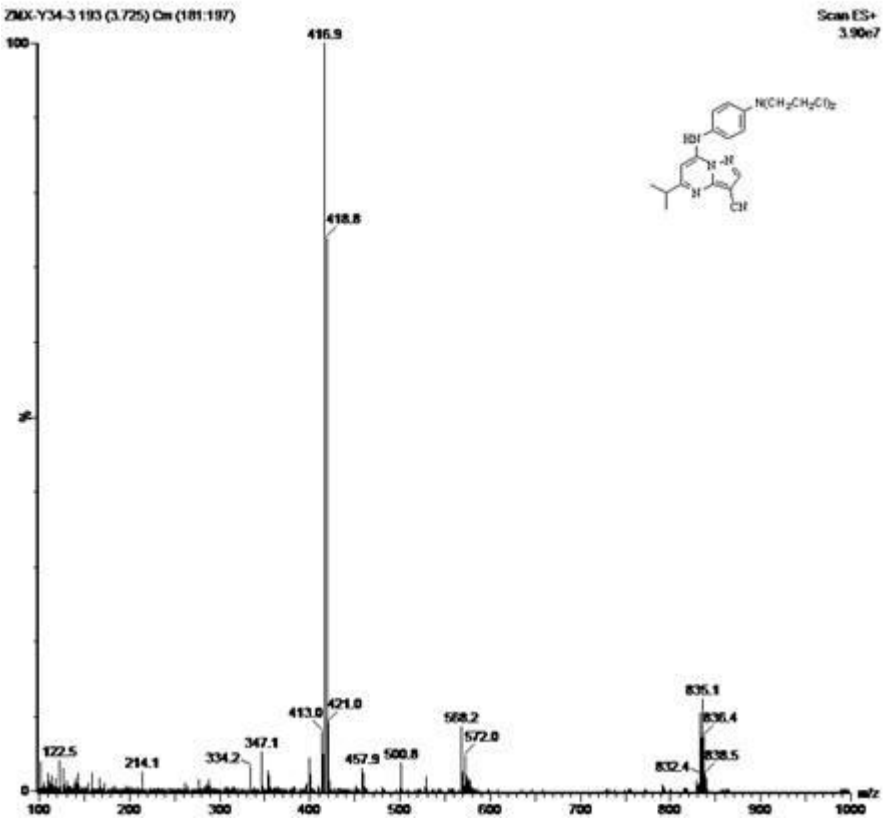
MS for compound **9d**



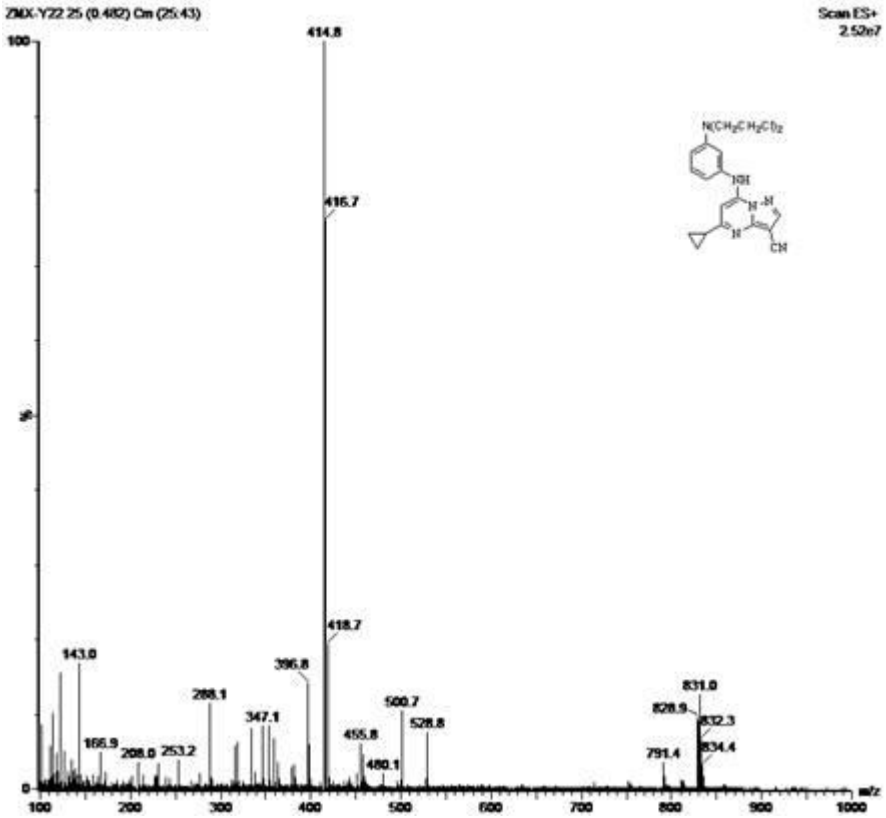
MS for compound **8e**



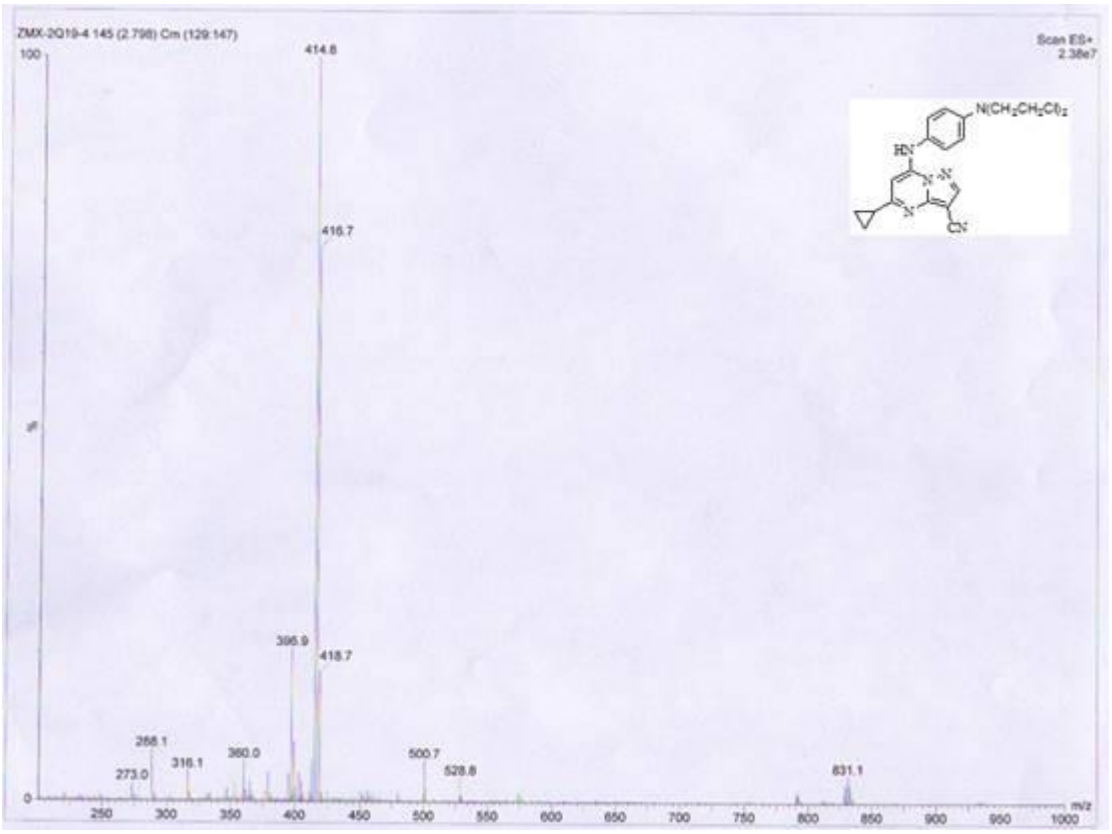
MS for compound **9e**



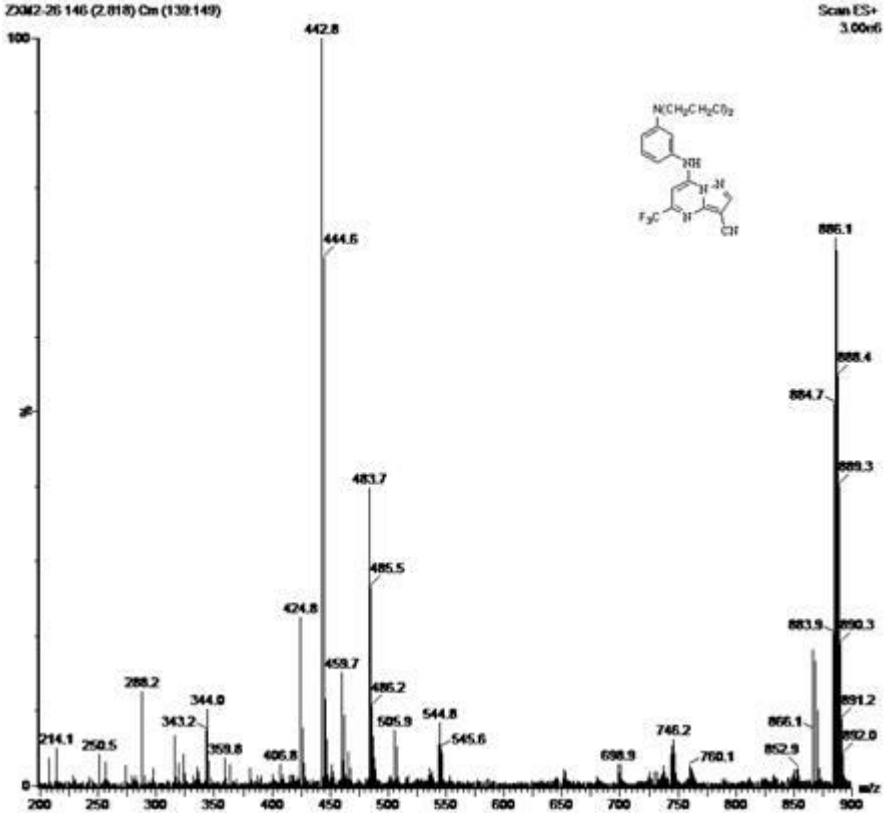
MS for compound **8f**



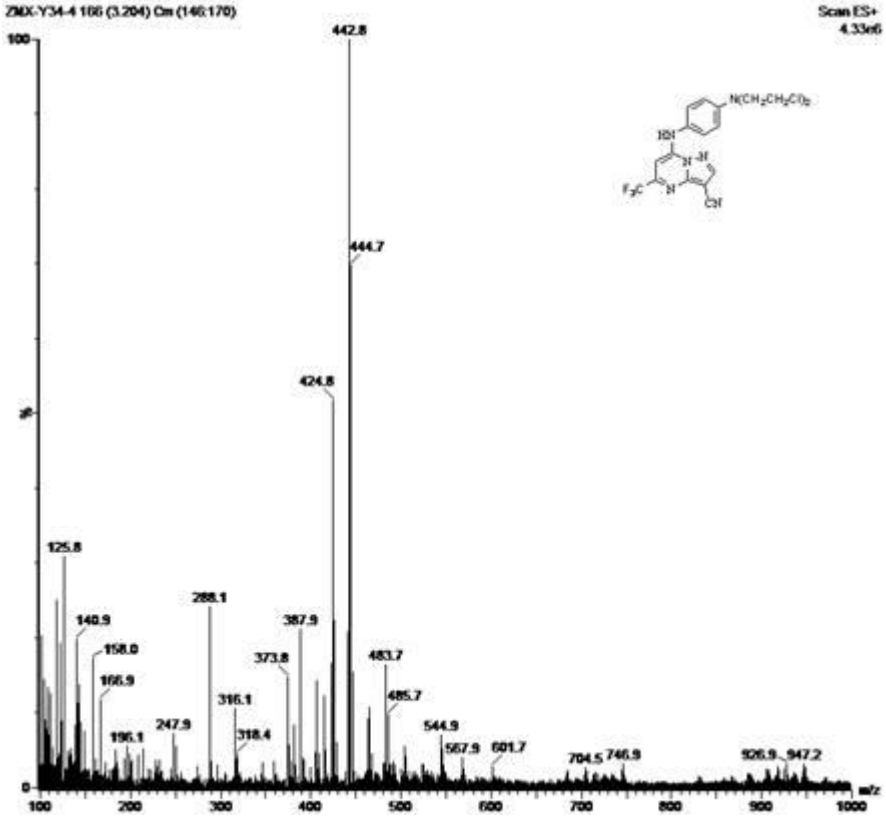
MS for compound **9f**



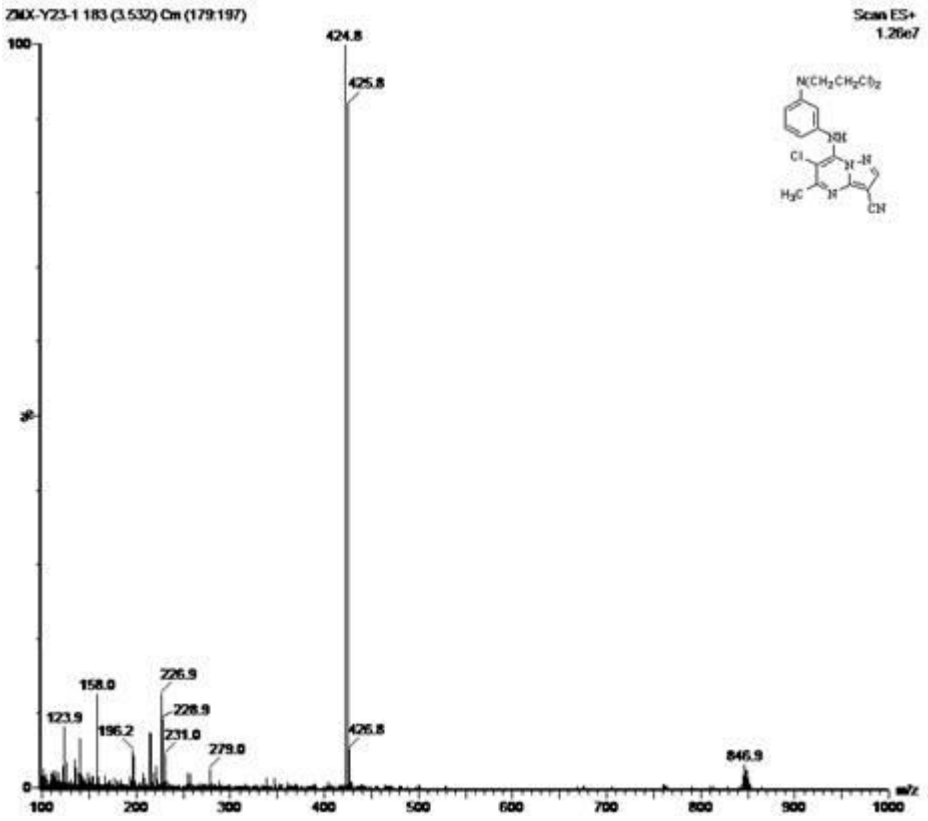
MS for compound **8g**



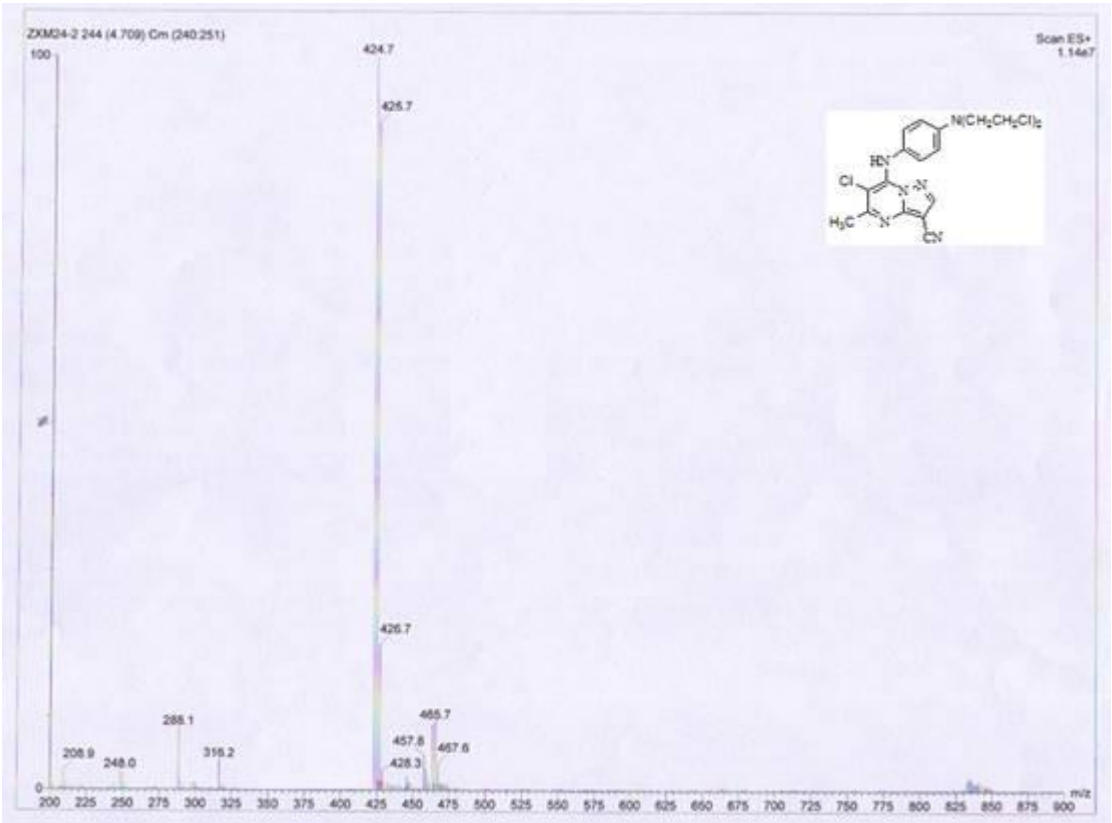
MS for compound **9g**



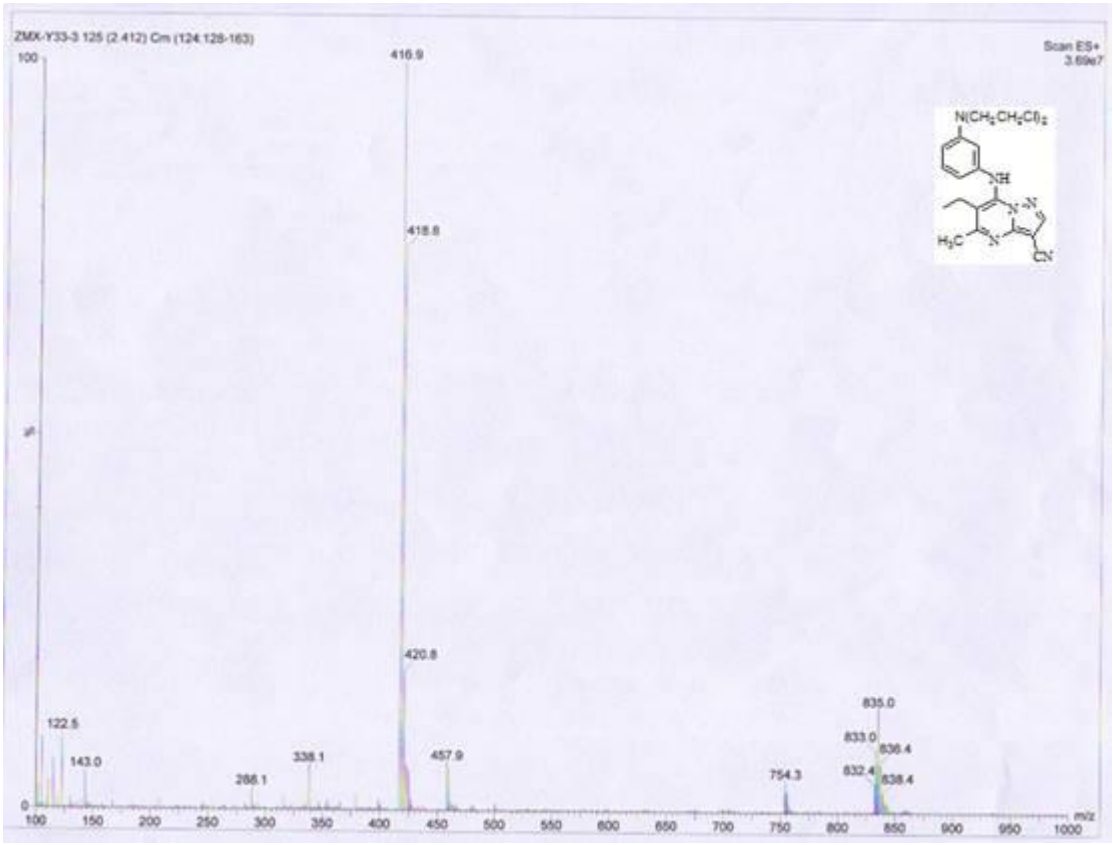
MS for compound **8h**



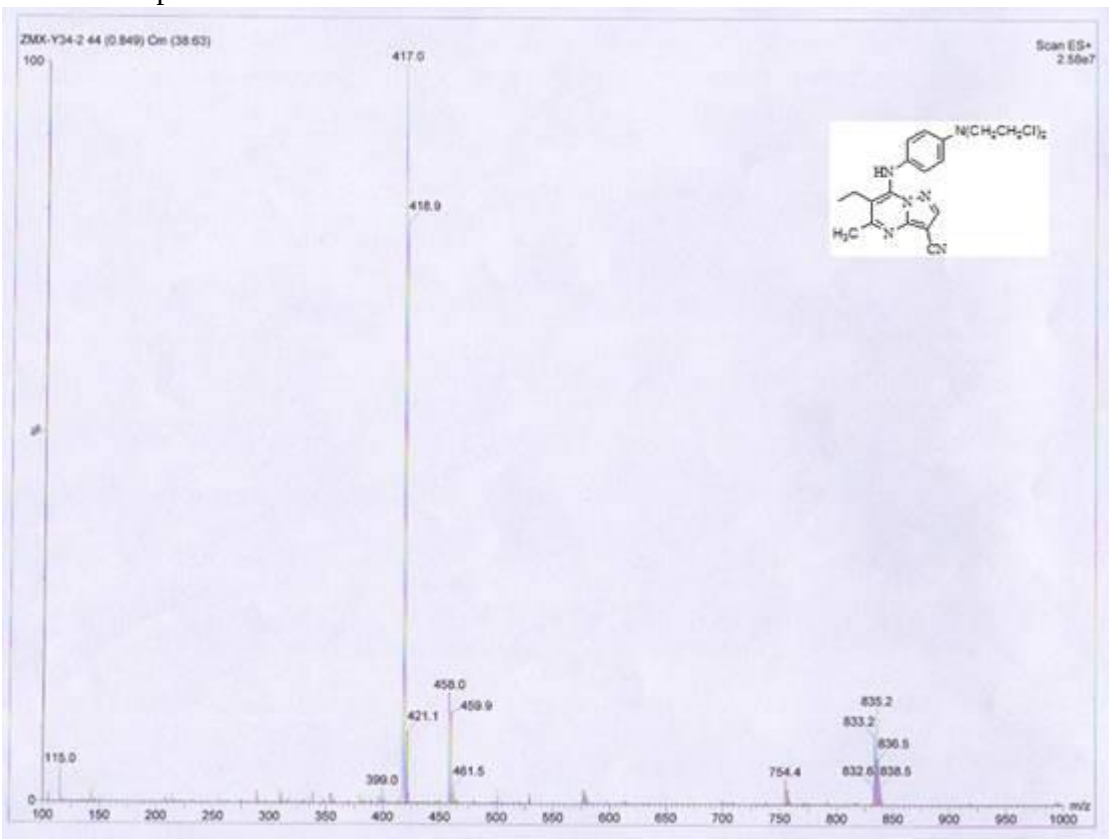
MS for compound **9h**



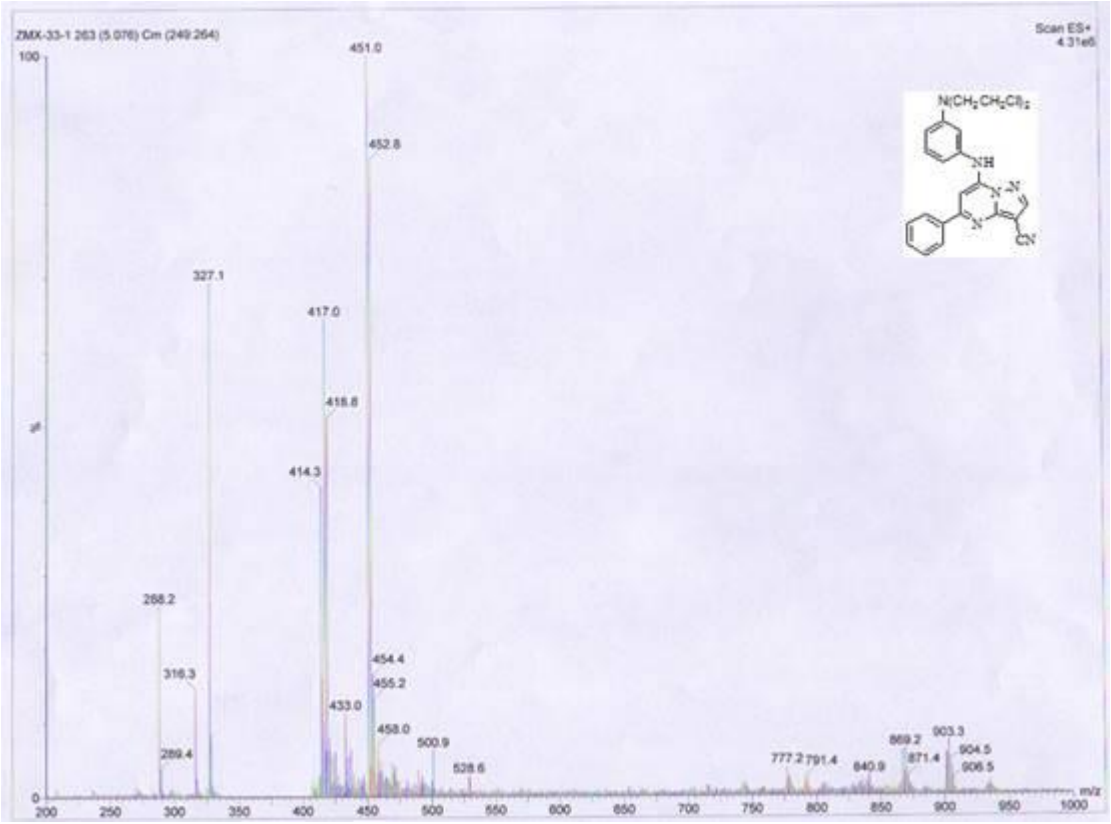
MS for compound **8i**



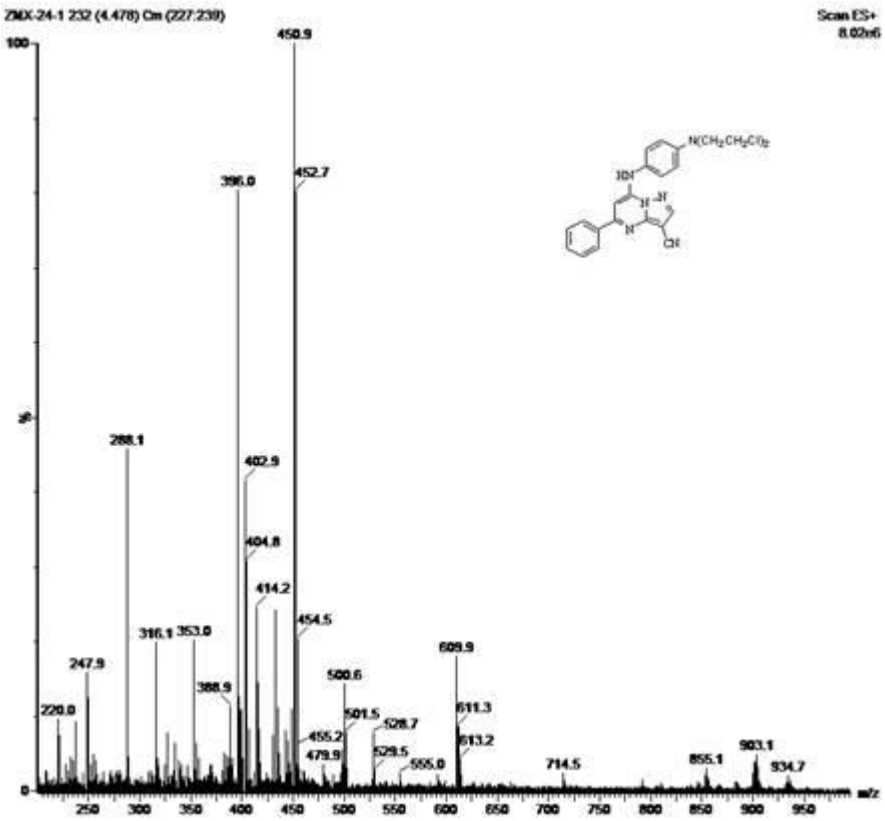
MS for compound **9i**



MS for compound **8j**

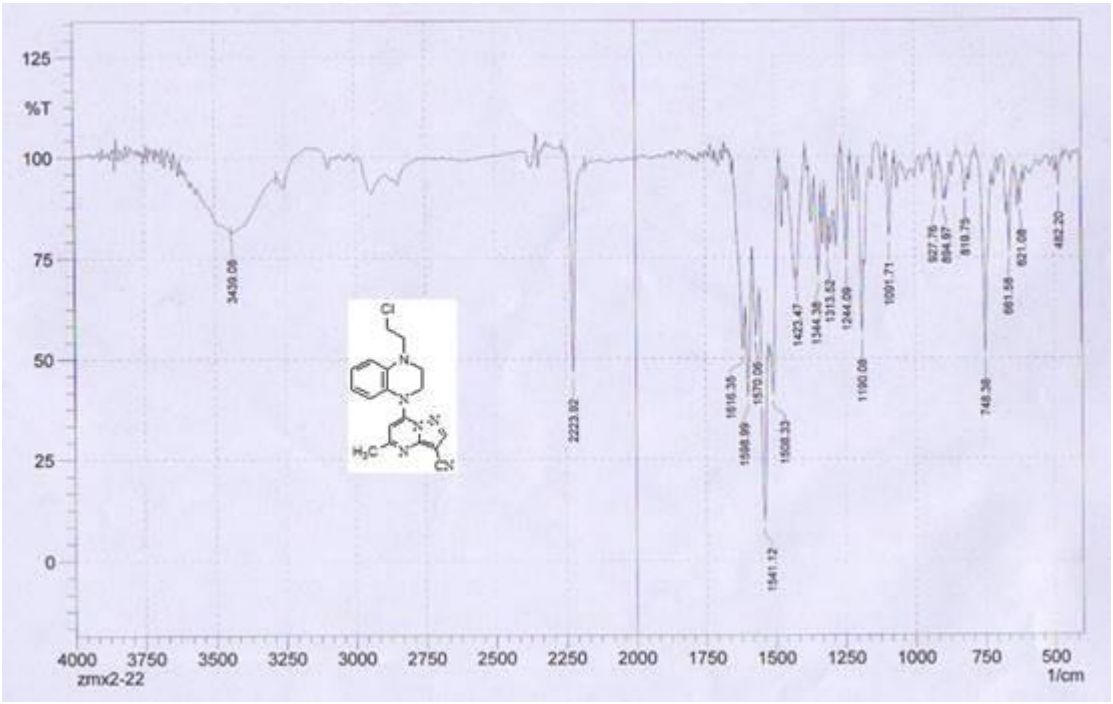


MS for compound **9j**

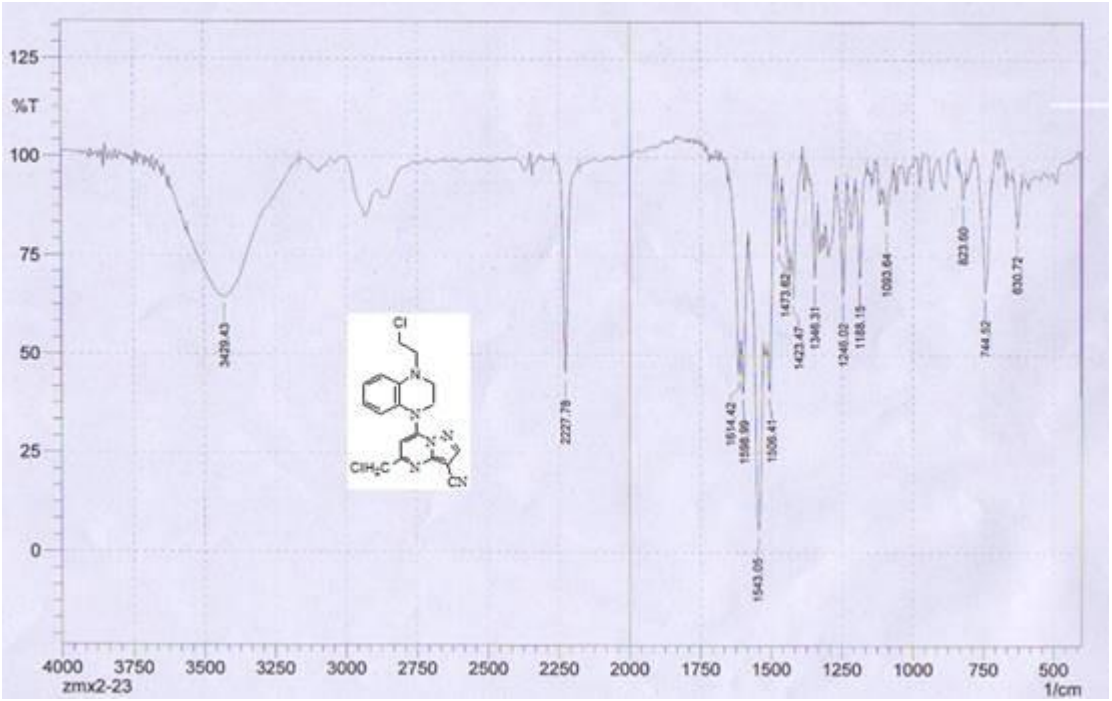


6. IR of target compounds

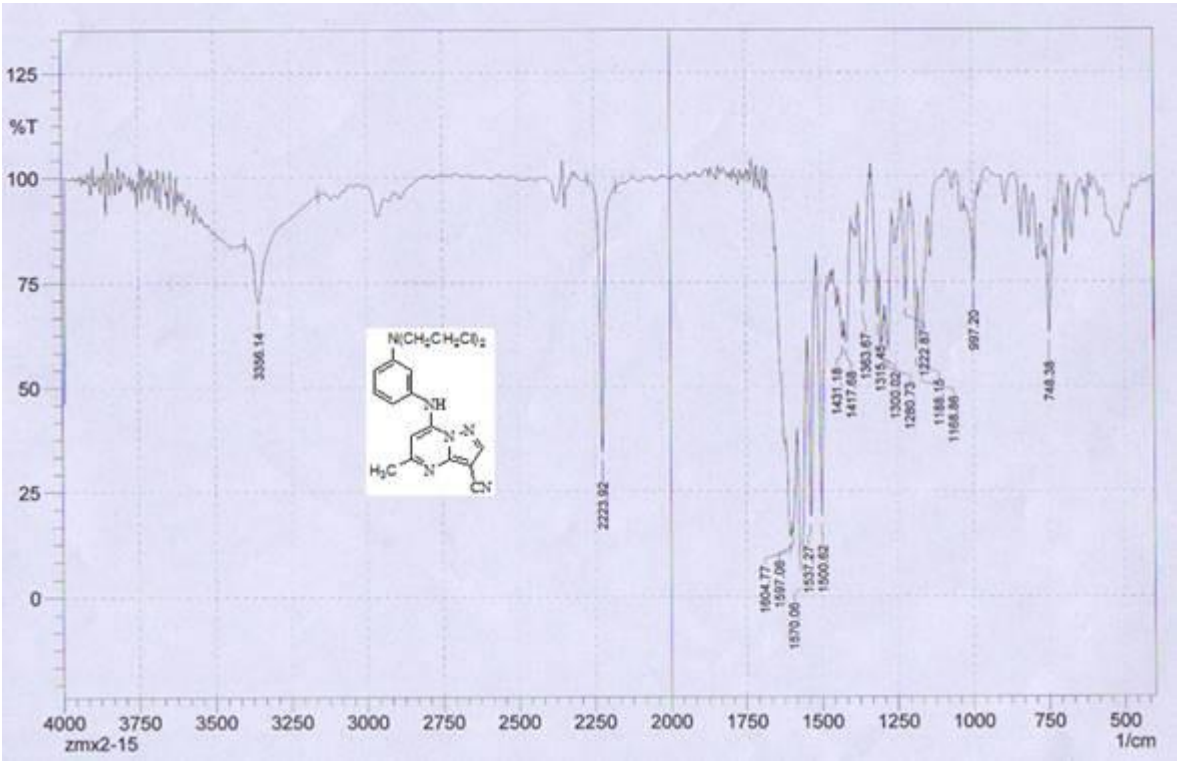
IR for compound **7m**



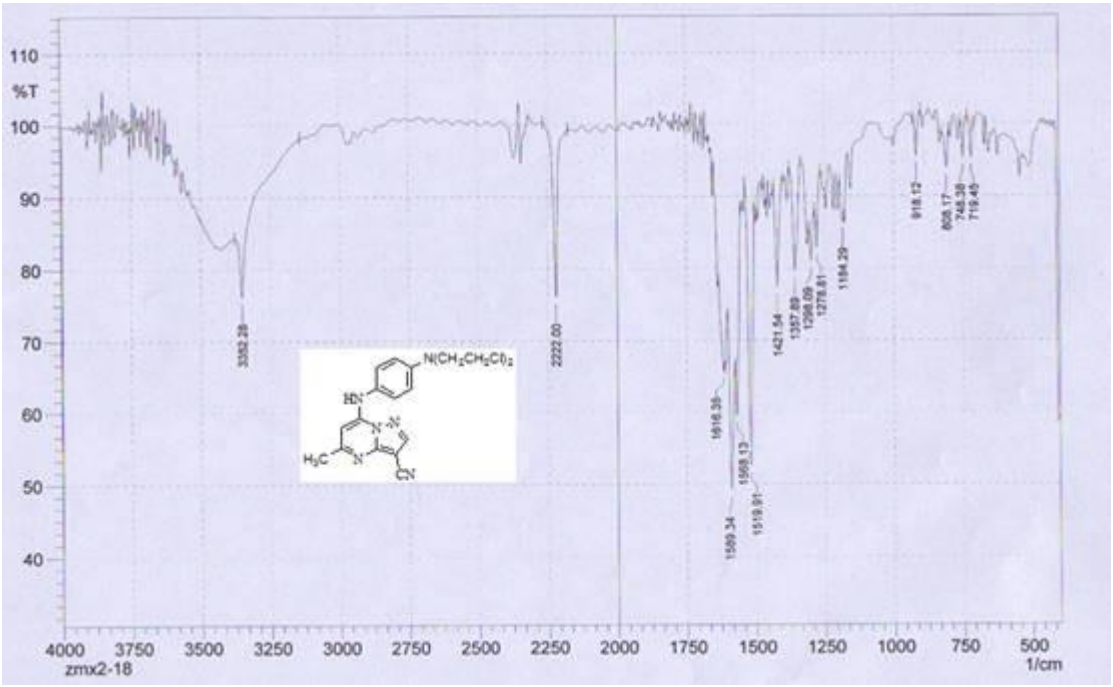
IR for compound **7n**



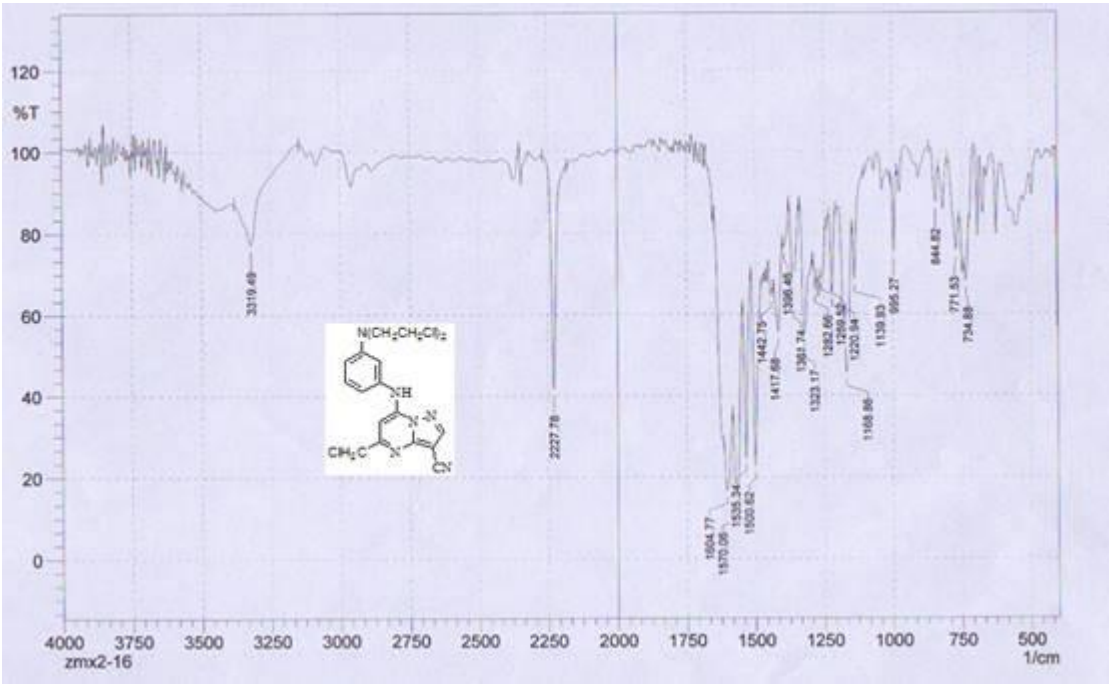
IR for compound **8a**



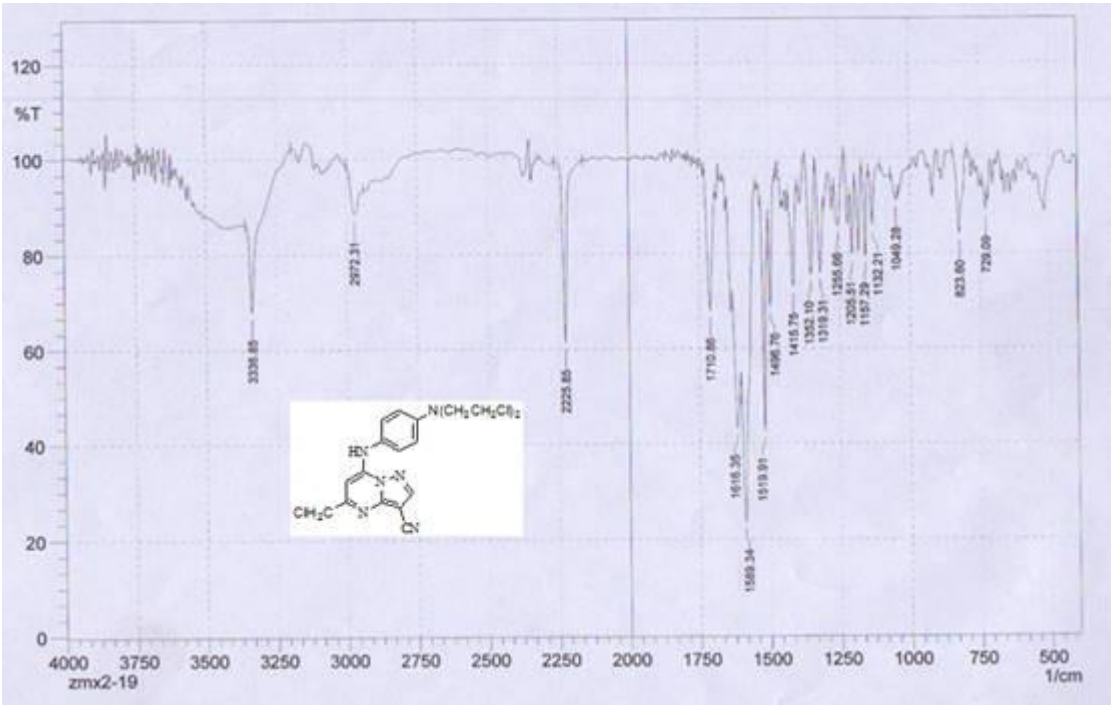
IR for compound **9a**



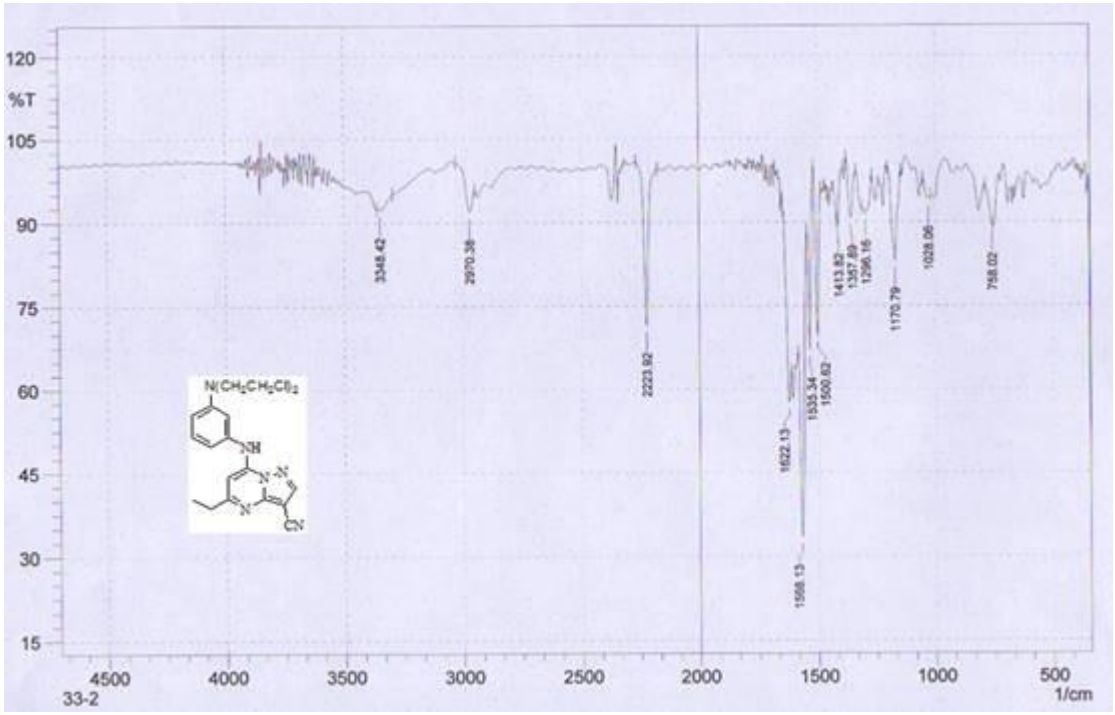
IR for compound **8b**



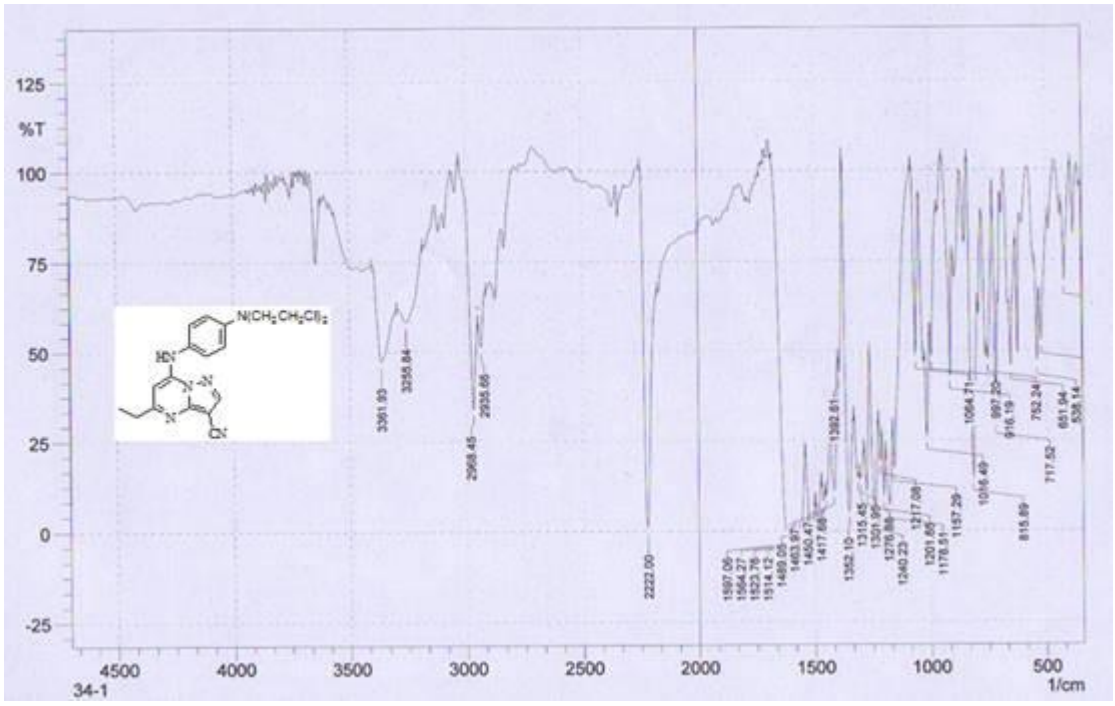
IR for compound **9b**



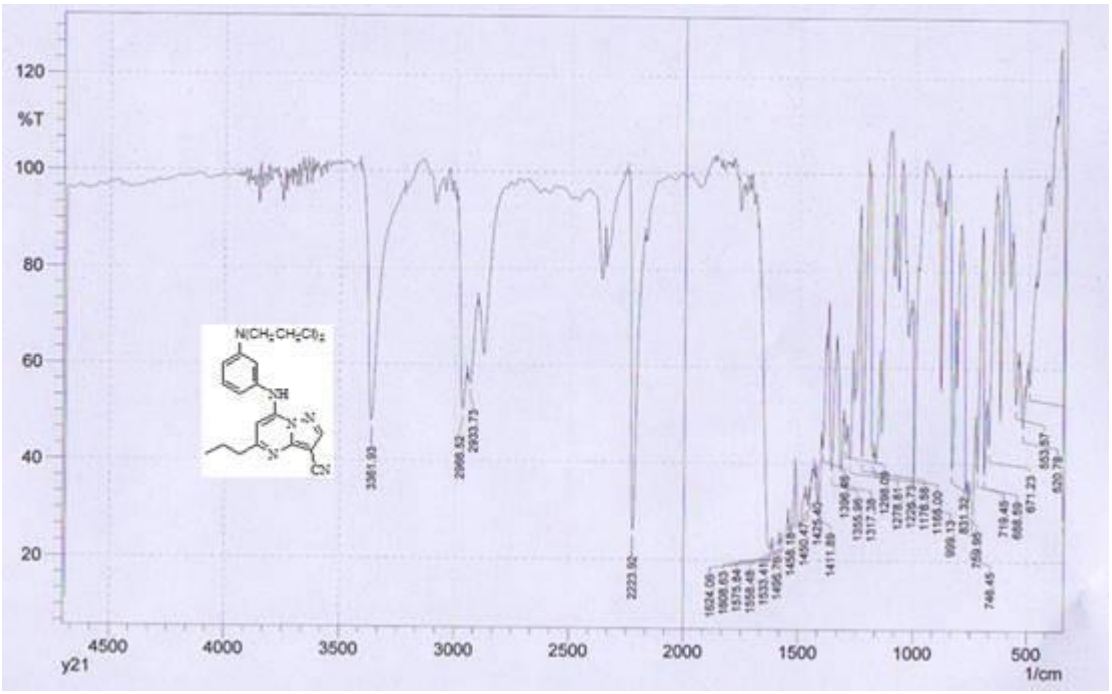
IR for compound **8c**



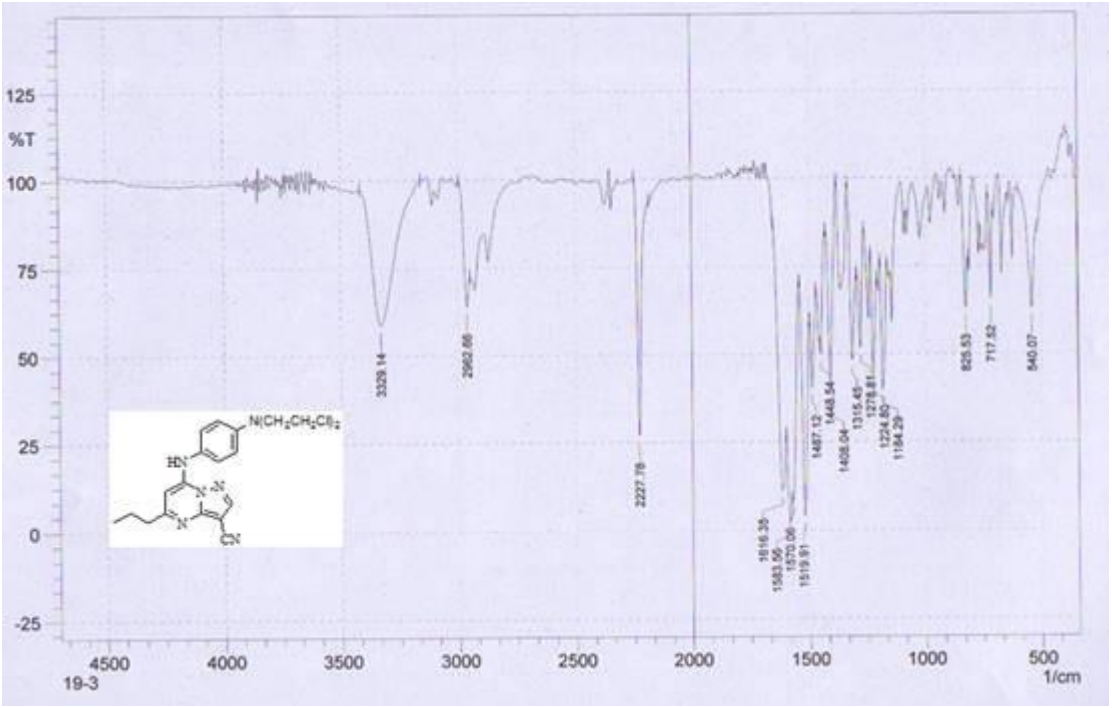
IR for compound **9c**



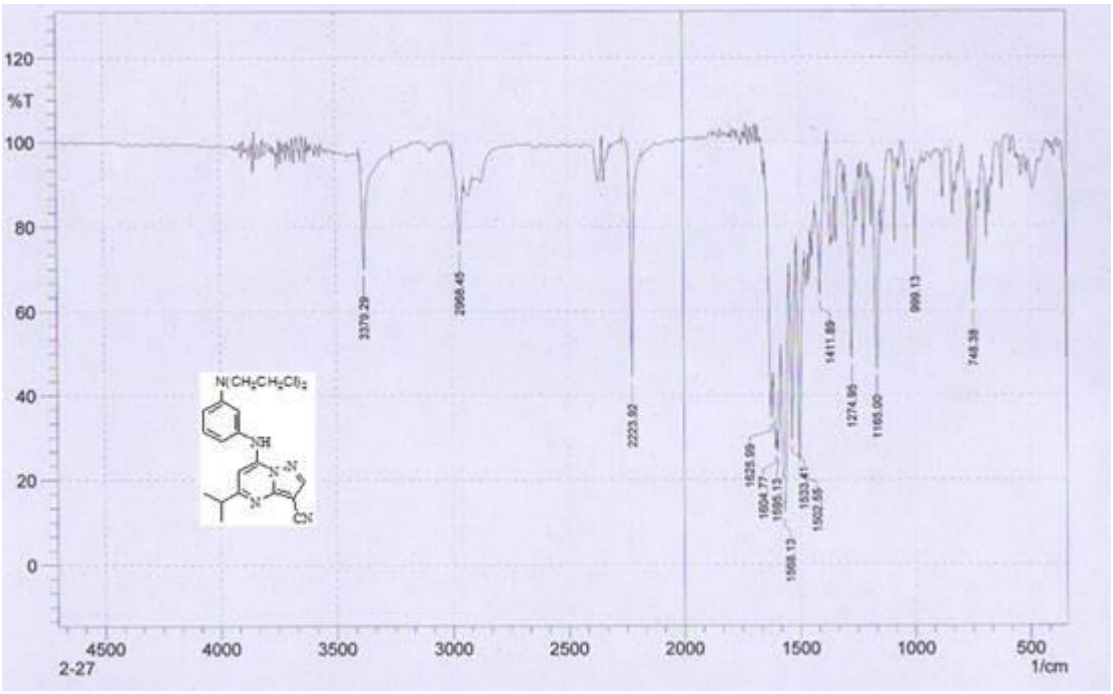
IR for compound **8d**



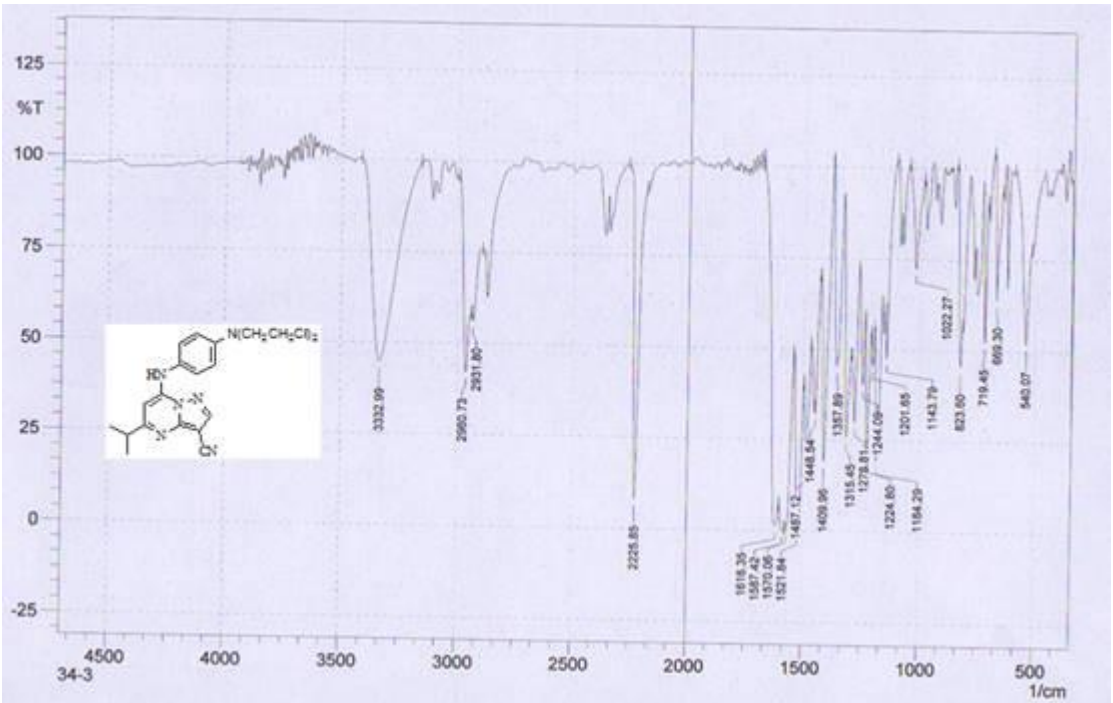
IR for compound **9d**



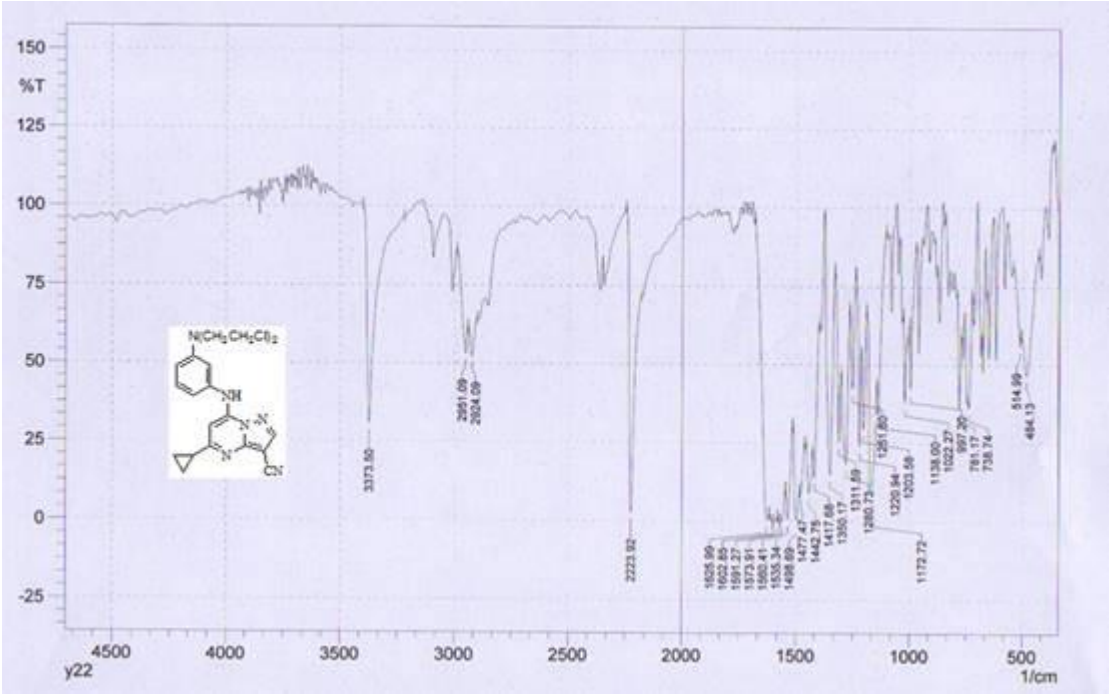
IR for compound **8e**



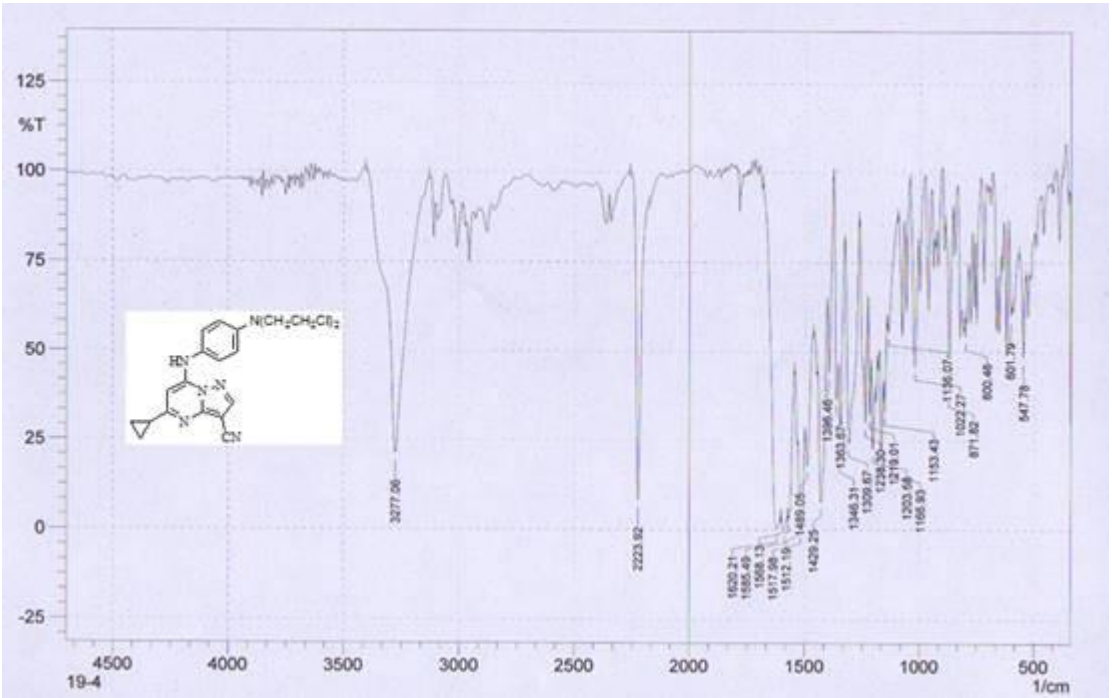
IR for compound **9e**



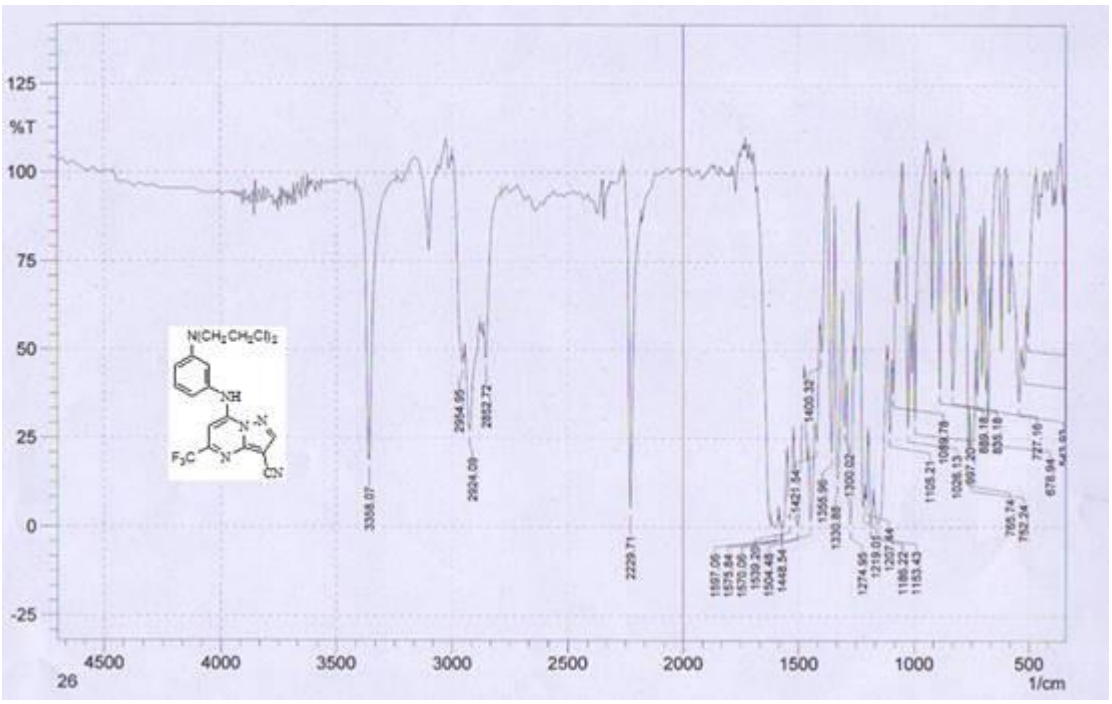
IR for compound **8f**



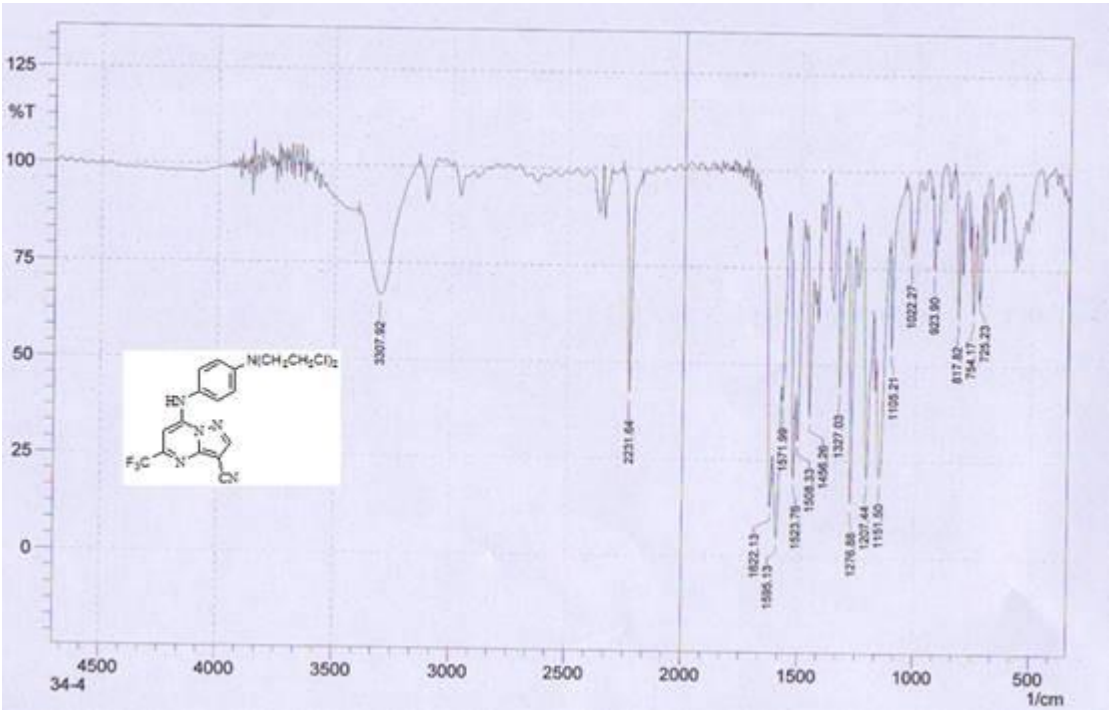
IR for compound **9f**



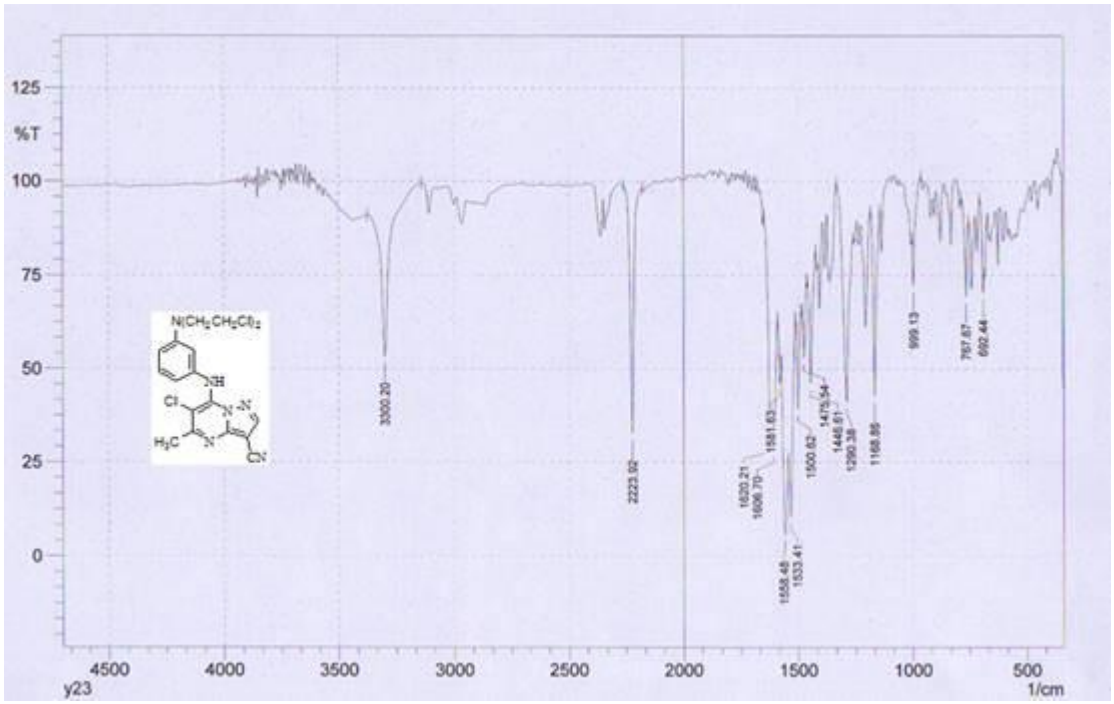
IR for compound **8g**



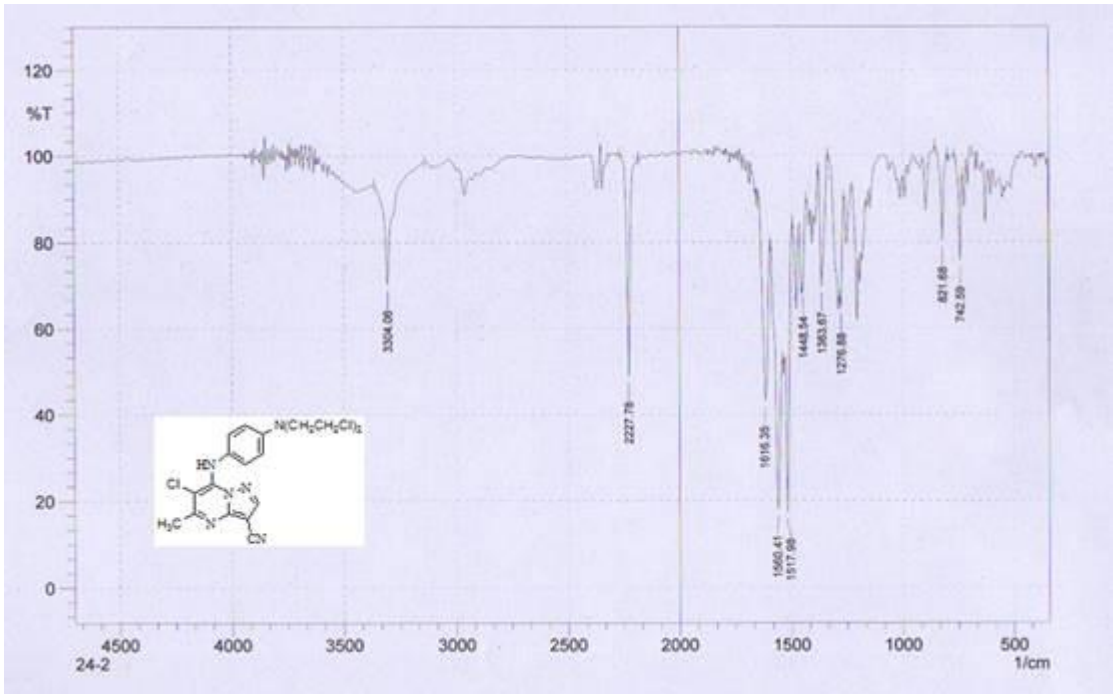
IR for compound **9g**



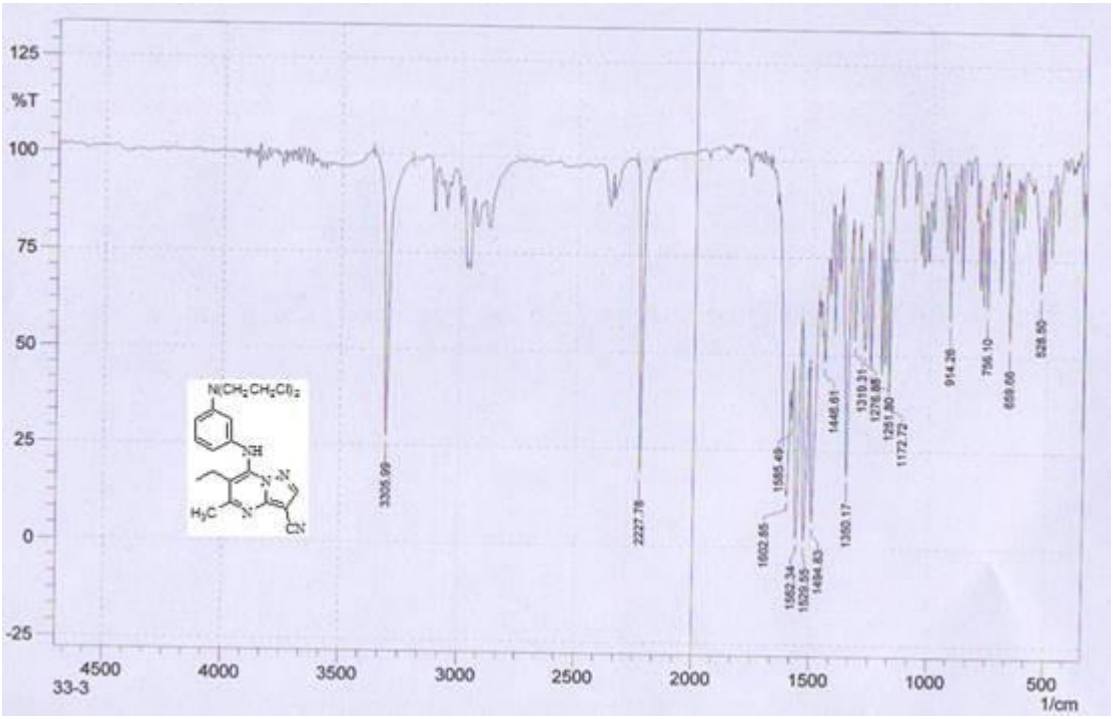
IR for compound **8h**



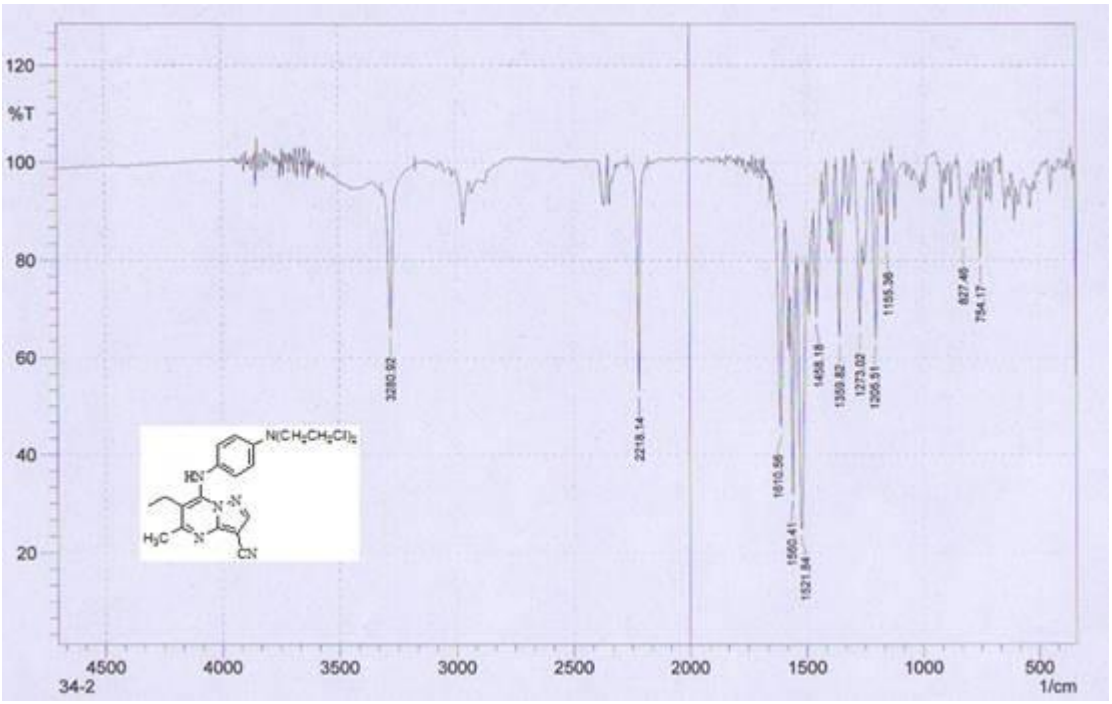
IR for compound **9h**



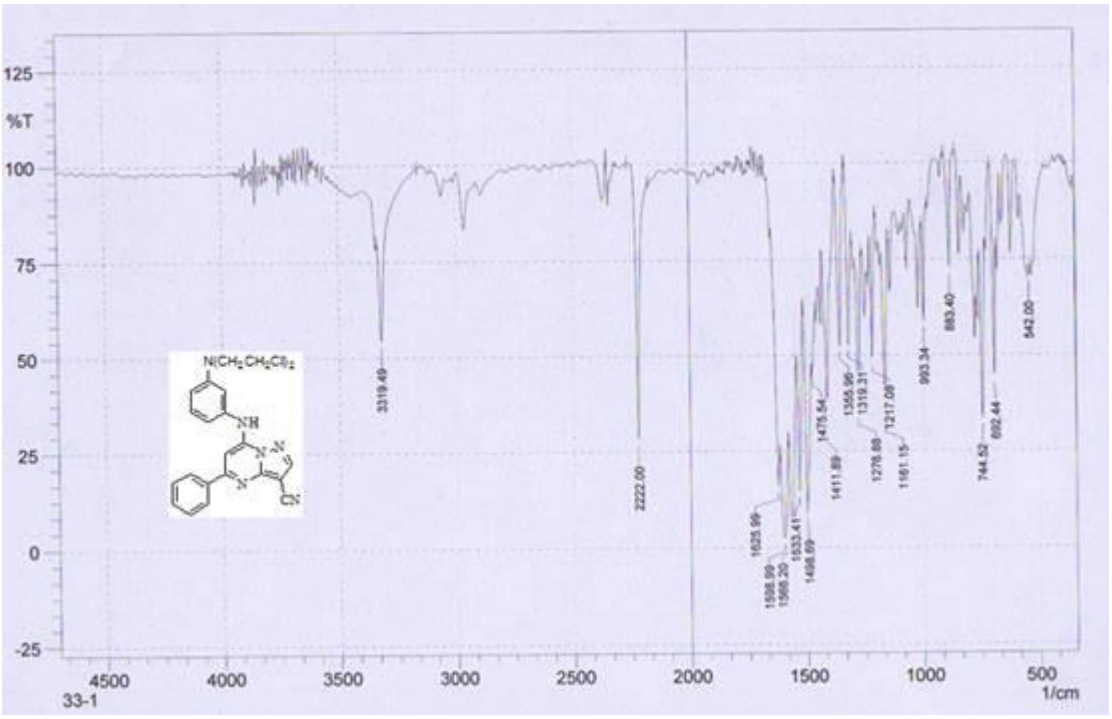
IR for compound **8i**



IR for compound **9i**



IR for compound **8j**



IR for compound **9j**