Electronic Supplementary Material (ESI) for New Journal of Chemistry.
This journal is © The Royal Society of Chemistry and the Centre National de la Recherche Scientifique 2018

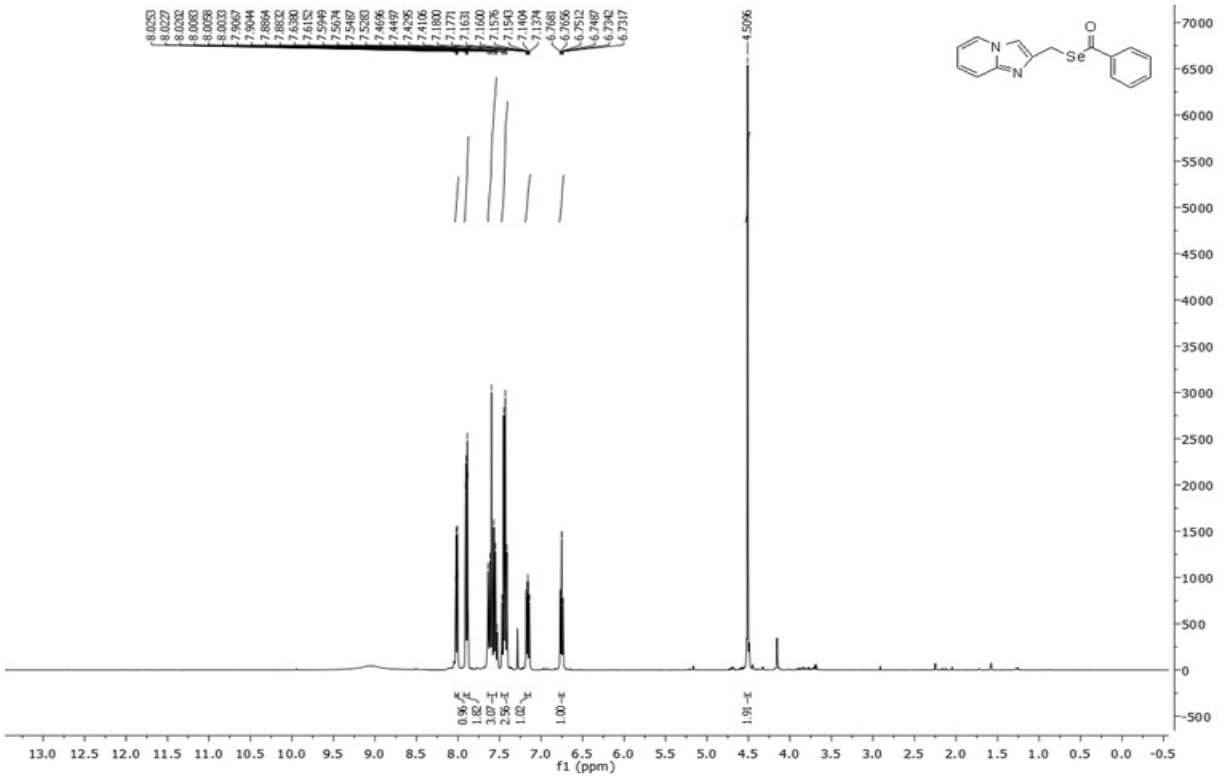
Synthesis and characterization of fused imidazole heterocyclic selenoesters and their application for chemical detoxification of $HgCl_2$

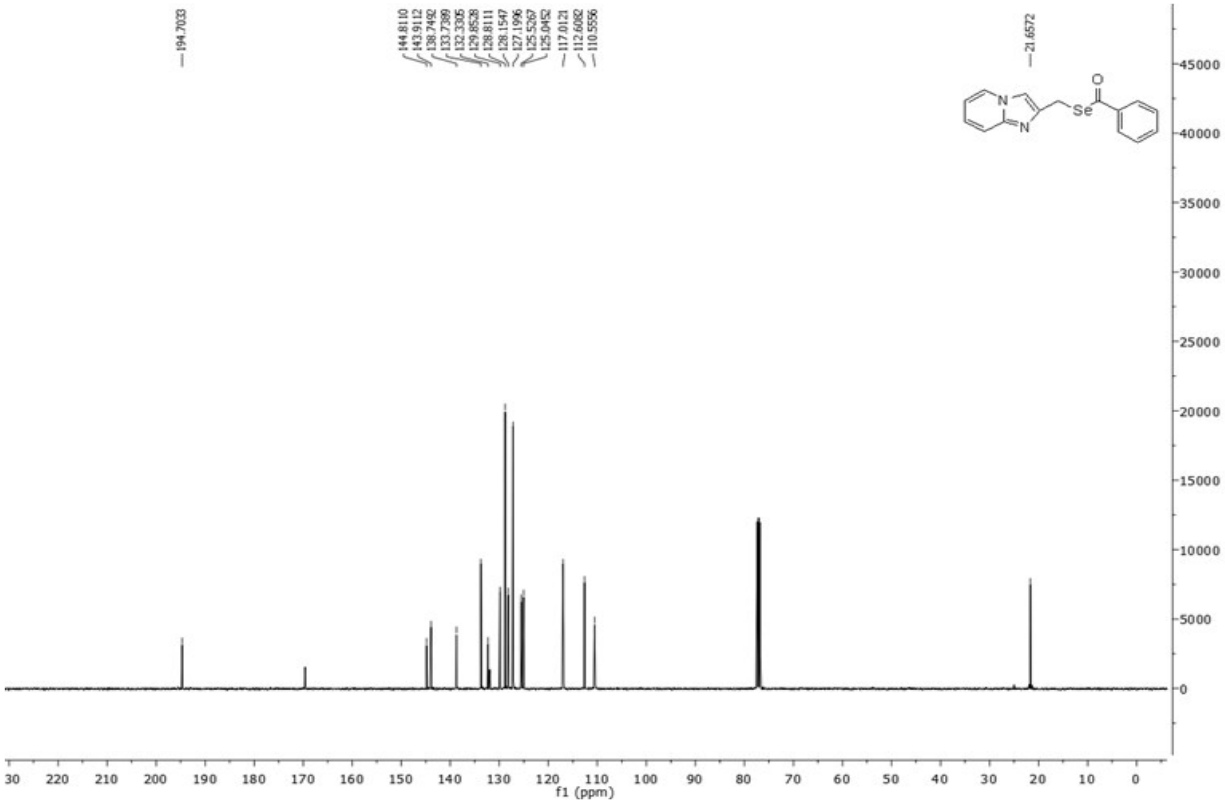
Nidhi Sharma,[a] Sanjeev Kumar,[a] K. K. Bhasin,*[a] S. K. Mehta*[a]

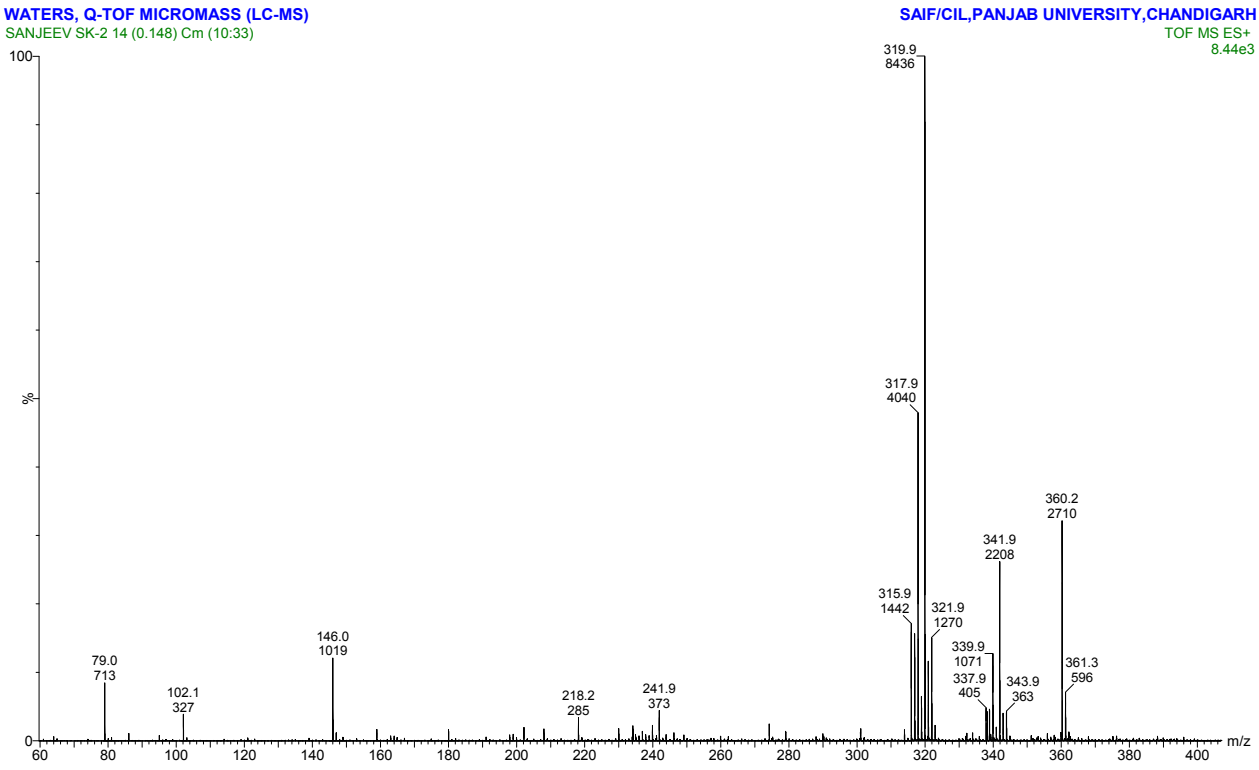
[a]*Department of Chemistry and Centre for Advanced Studies in Chemistry, Panjab University, Chandigarh, 160014, India*

Table of Contents

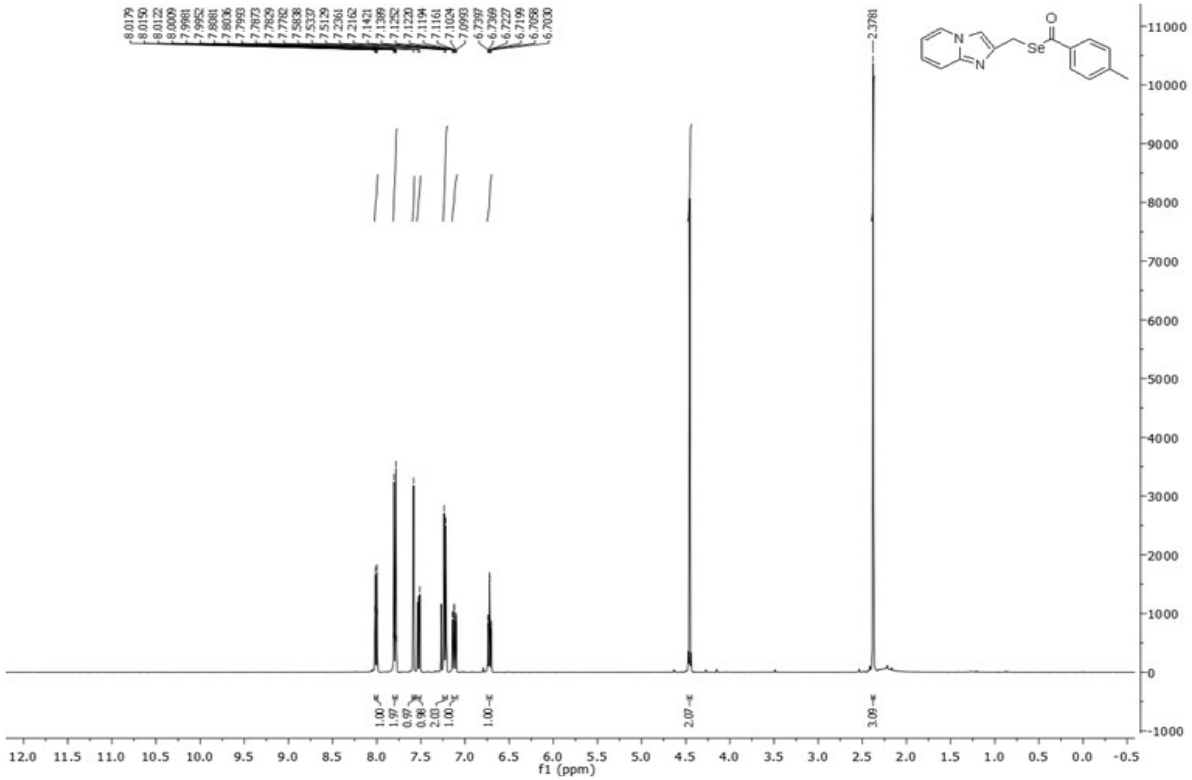
***Se*-(imidazo[1,2-*a*]pyridin-2-ylmethyl) benzoselenoate (6a) ^{1}H, ^{13}C, Mass Spectra**

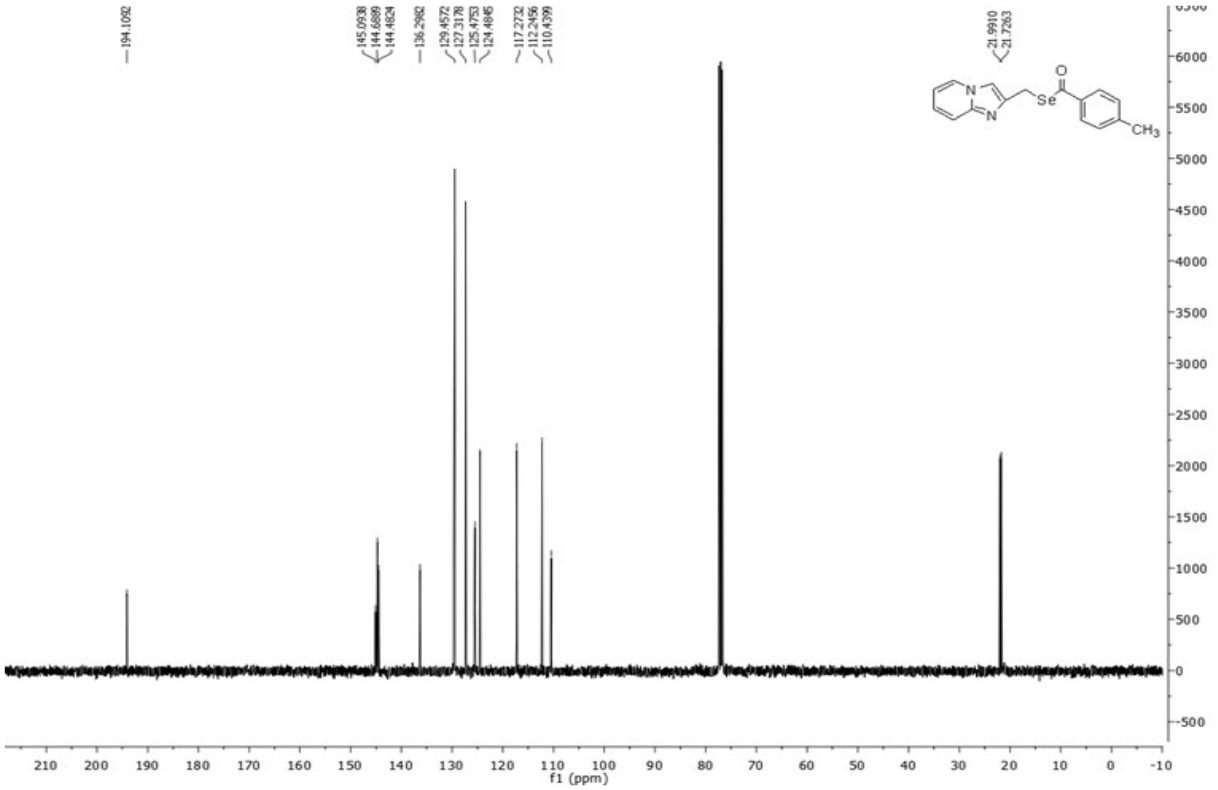


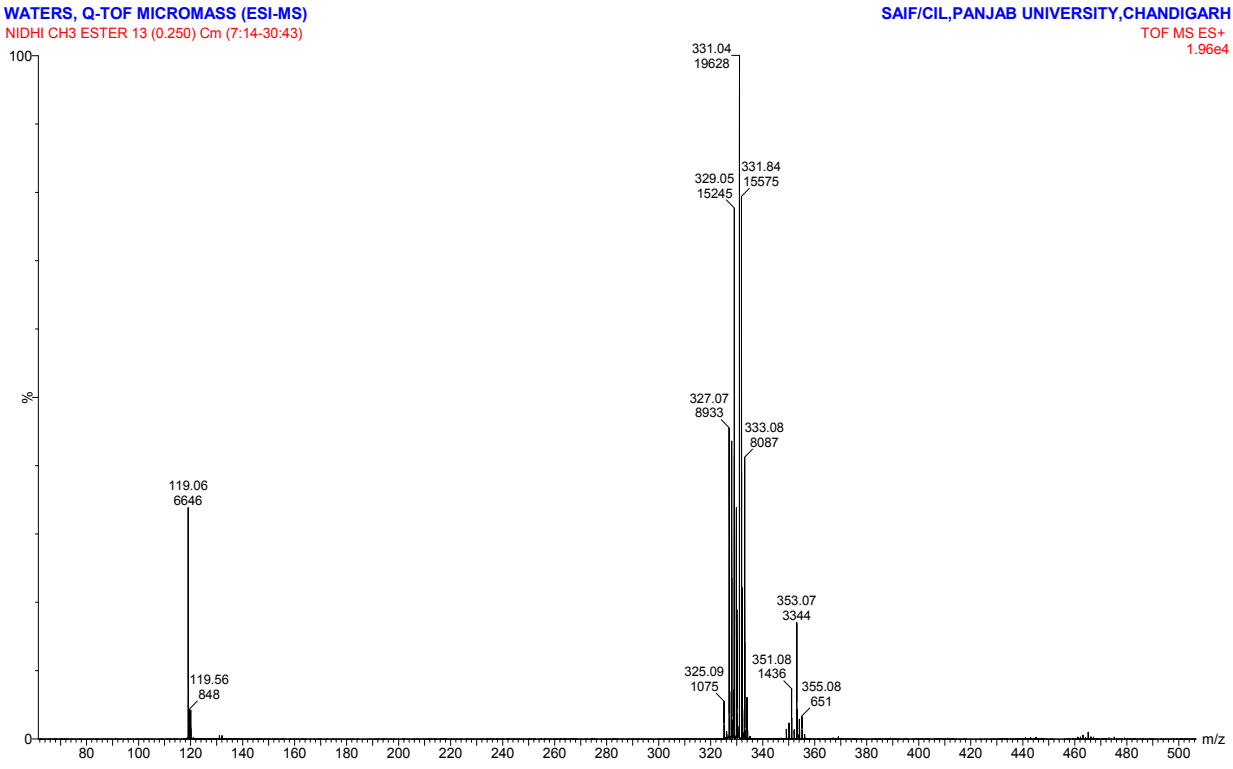




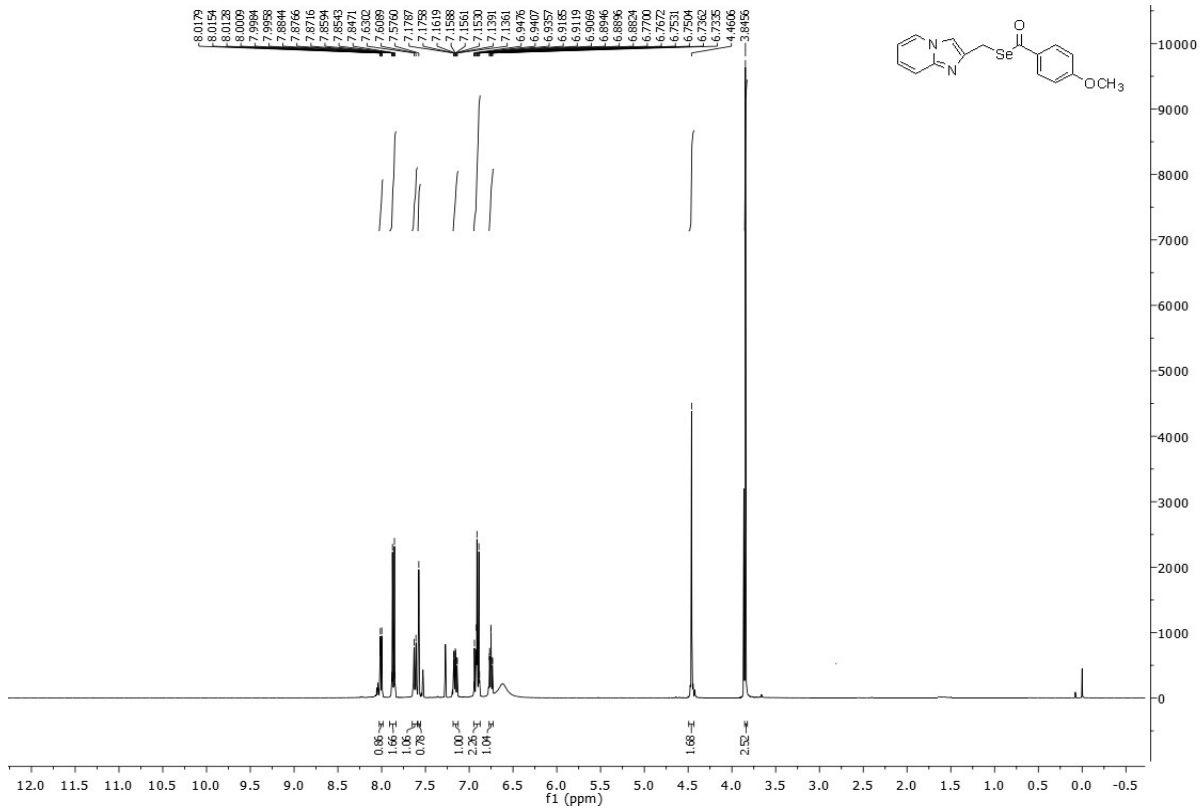
***Se*-(imidazo[1,2-*a*]pyridin-2-ylmethyl) 4-methylbenzoselenoate (6b) ^{1}H, ^{13}C, Mass Spectra**

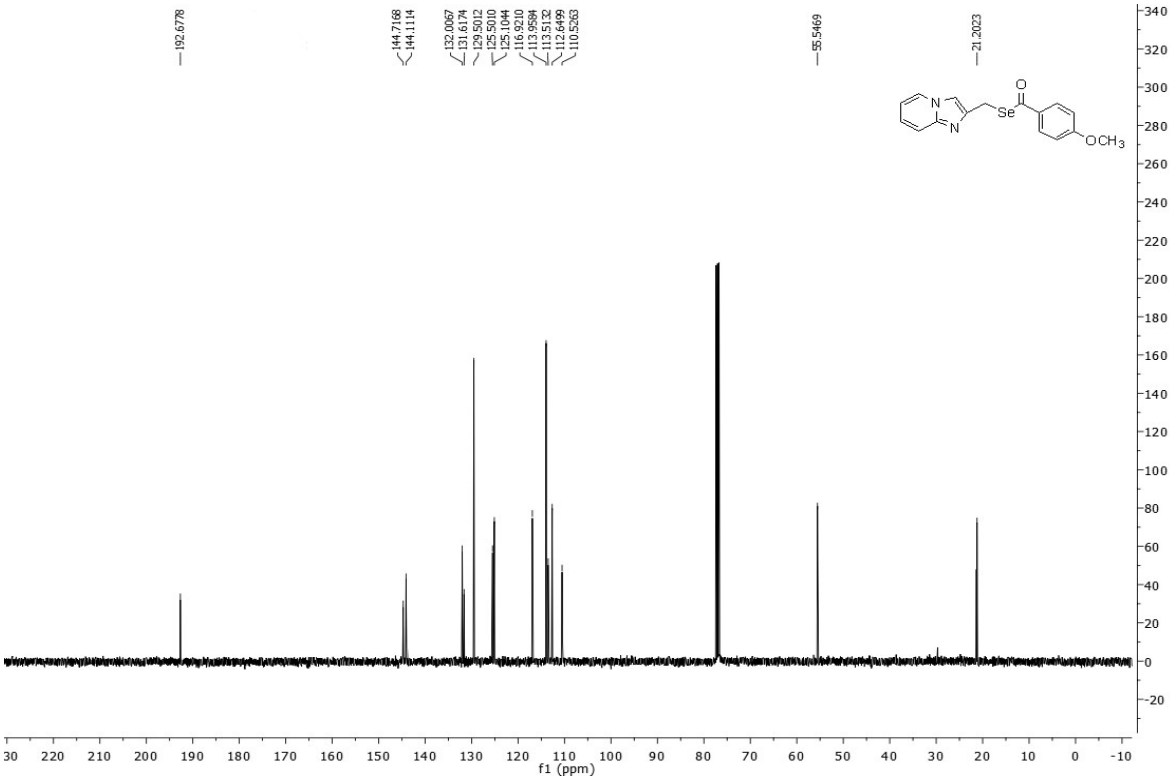


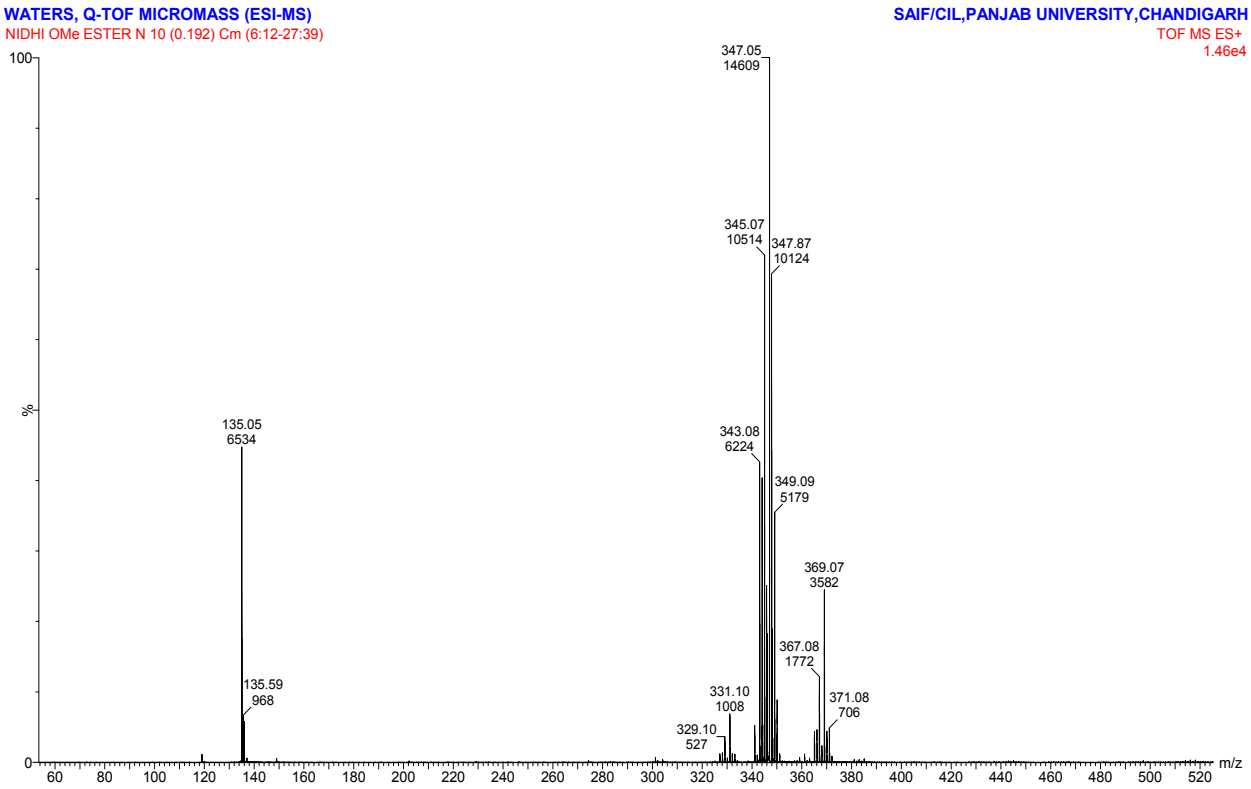

194.1092
145.0938
144.6889
144.4824
136.2982
129.4572
127.3178
125.4753
124.4845
117.2732
112.2456
110.4399
21.9910
21.7263
Se
O
N
N
CH3
f1 (ppm)


WATERS, Q-TOF MICROMASS (ESI-MS)
NIDHI CH3 ESTER 13 (0.250) Cm (7:14-30:43)
SAIF/CIL,PANJAB UNIVERSITY,CHANDIGARH
TOF MS ES+
1.96e4
331.04
19628
331.84
15575
329.05
15245
327.07
8933
333.08
8087
119.06
6646
119.56
848
353.07
3344
351.08
1436
325.09
1075
355.08
651
%
m/z

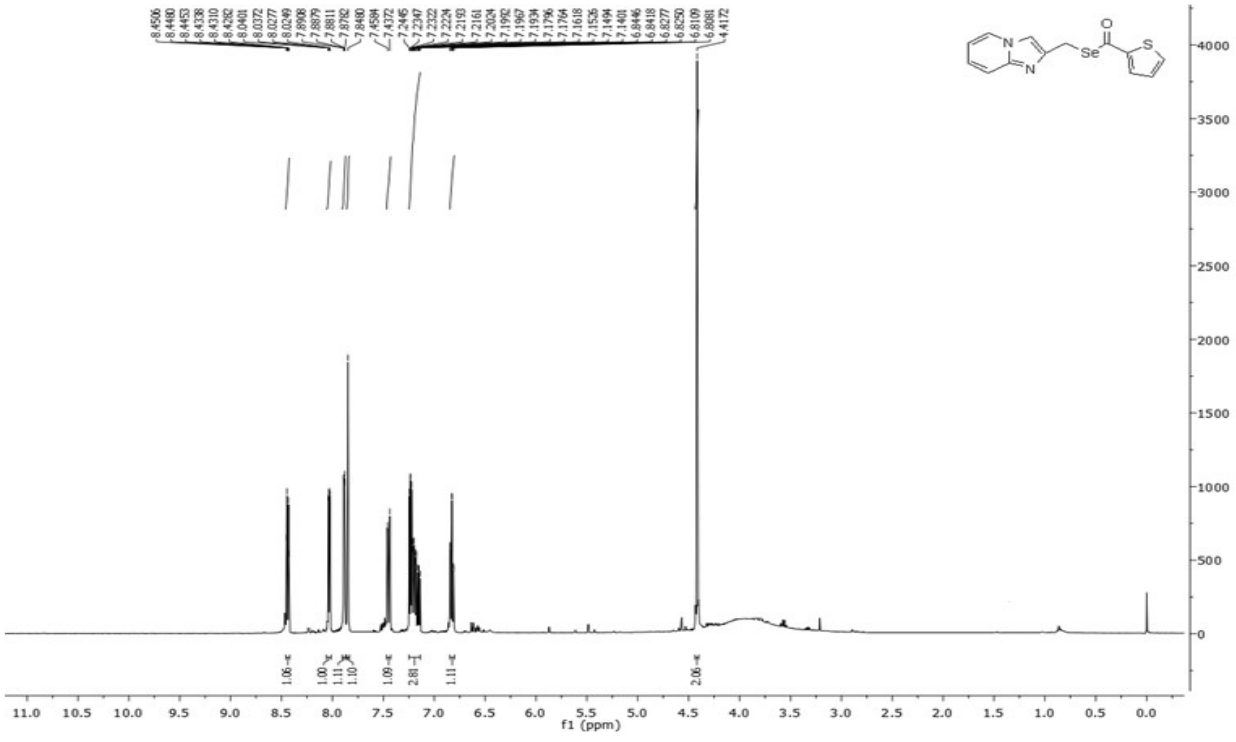
***Se*-(imidazo[1,2-*a*]pyridin-2-ylmethyl) 4-methoxybenzoselenoate (6c) ^{1}H, ^{13}C, Mass Spectra**

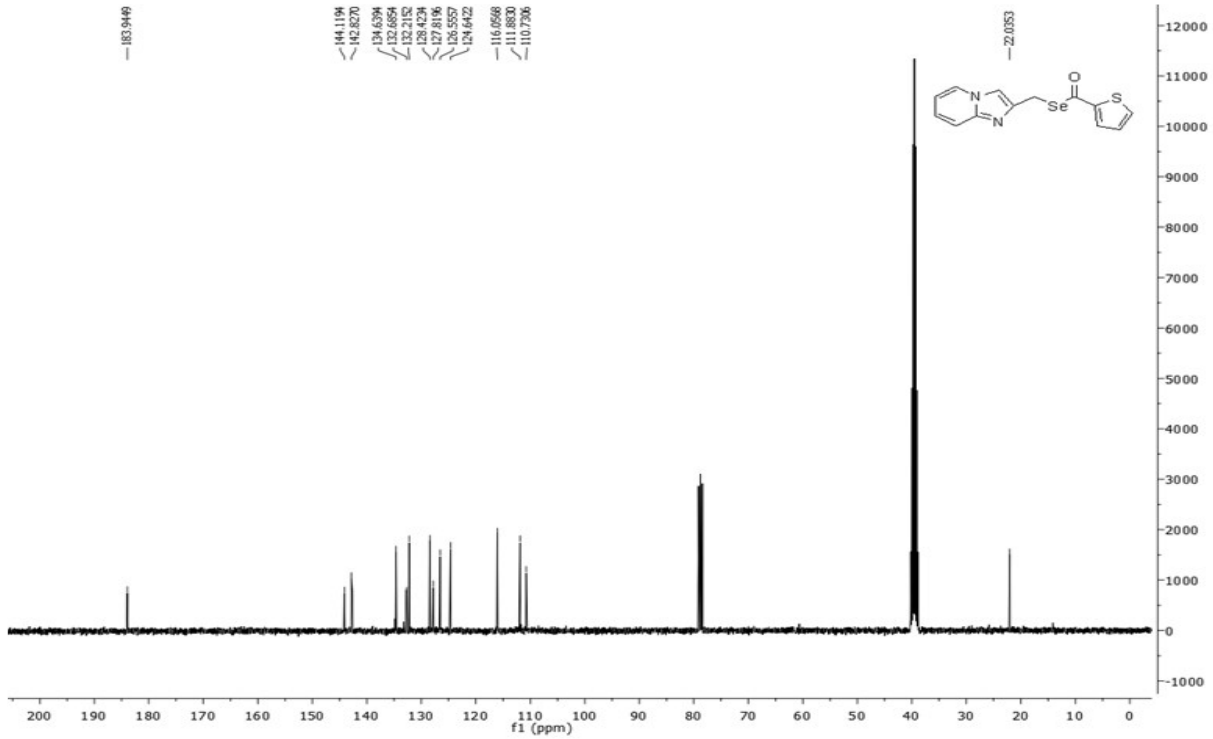






***Se*-(imidazo[1,2-*a*]pyridin-2-ylmethyl) thiophene-2-carboselenoate (6d) ^{1}H, ^{13}C, Mass Spectra**



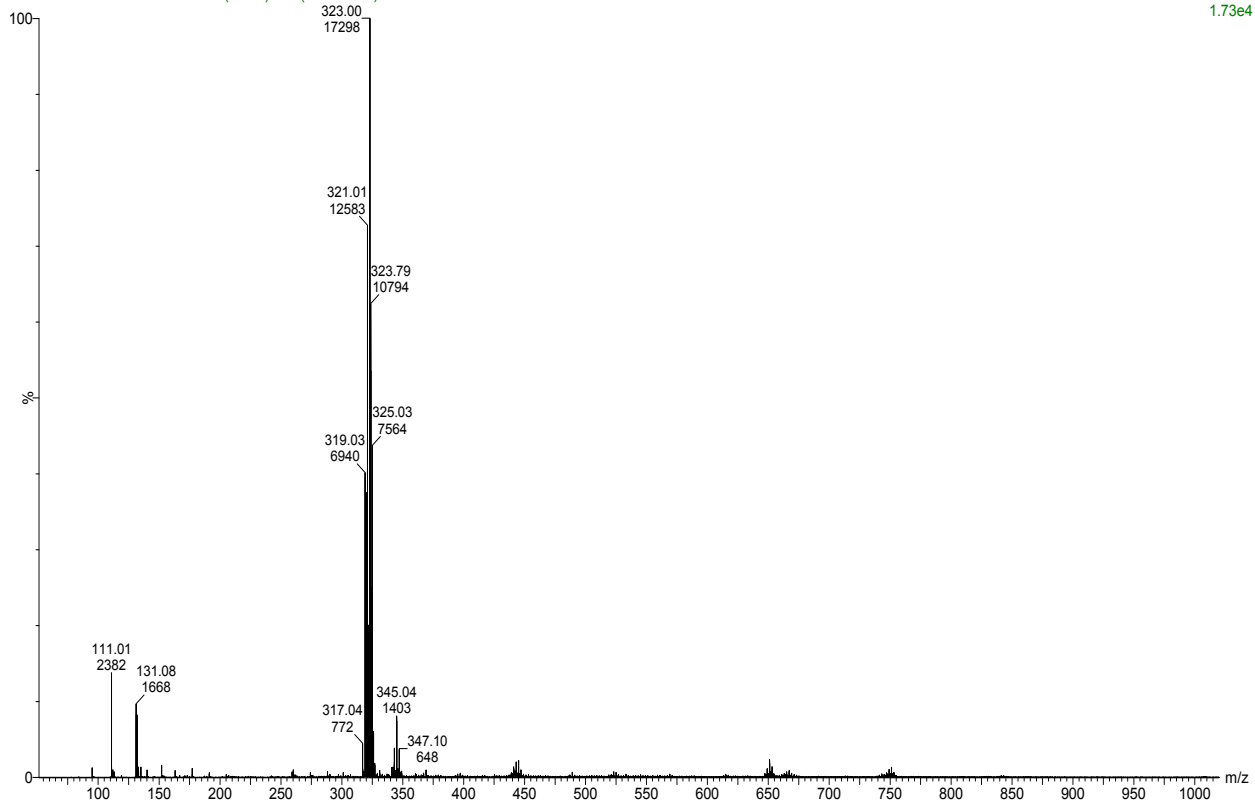


WATERS, Q-TOF MICROMASS (ESI-MS)

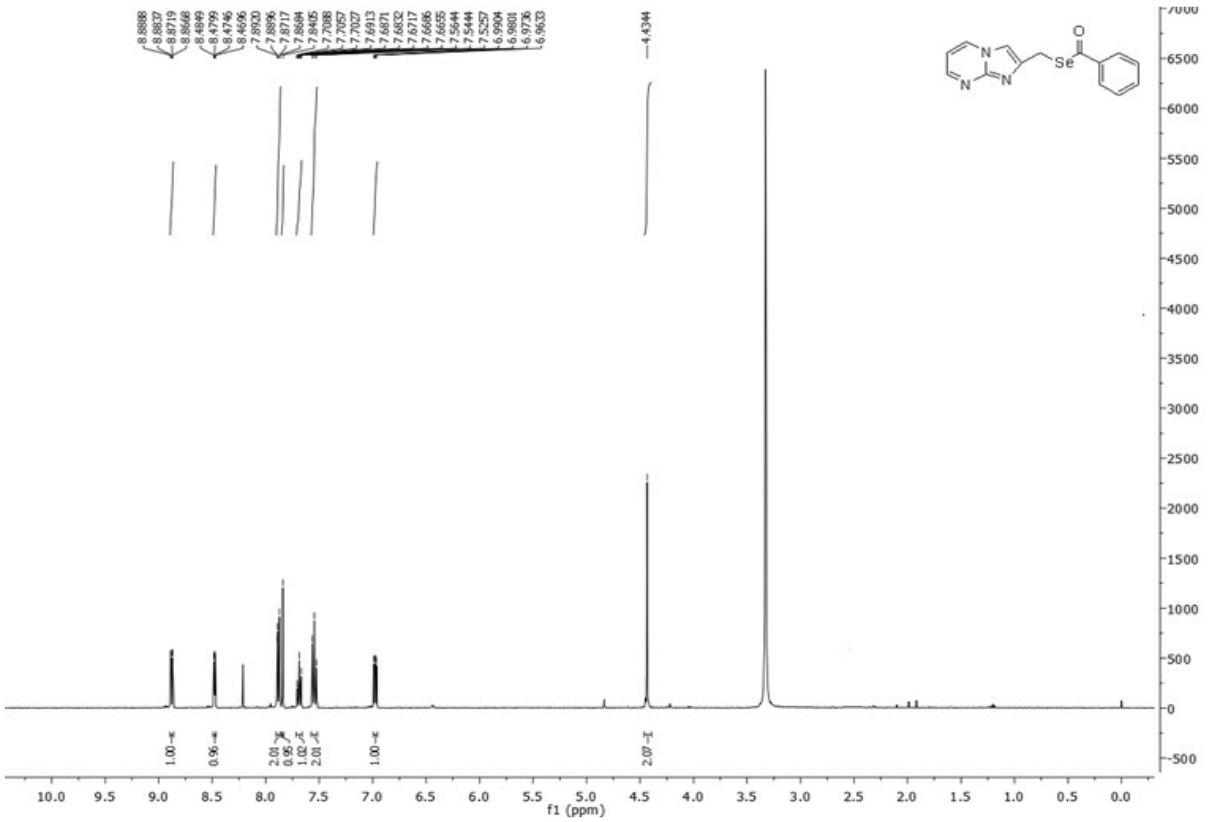
NIDHI THIOPHENE ESTER N 10 (0.192) Cm (7:14-27:35)

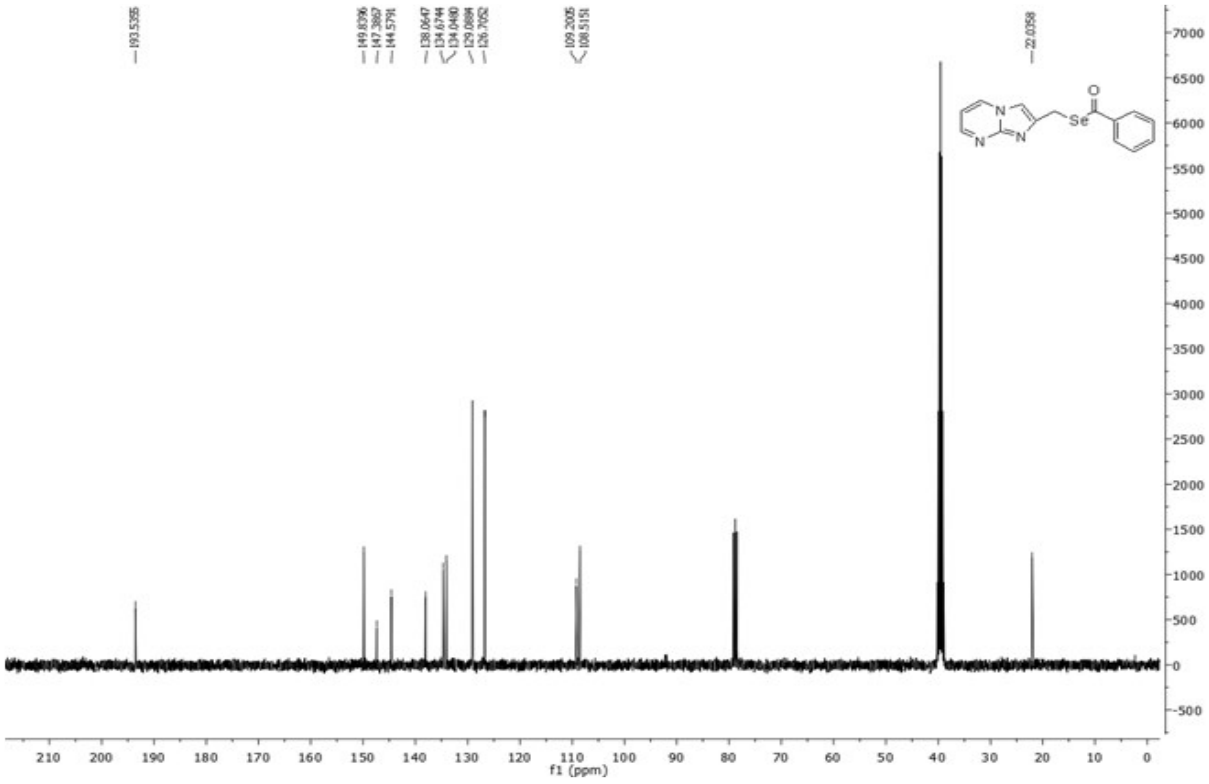
SAIF/CIL,PANJAB UNIVERSITY,CHANDIGARH

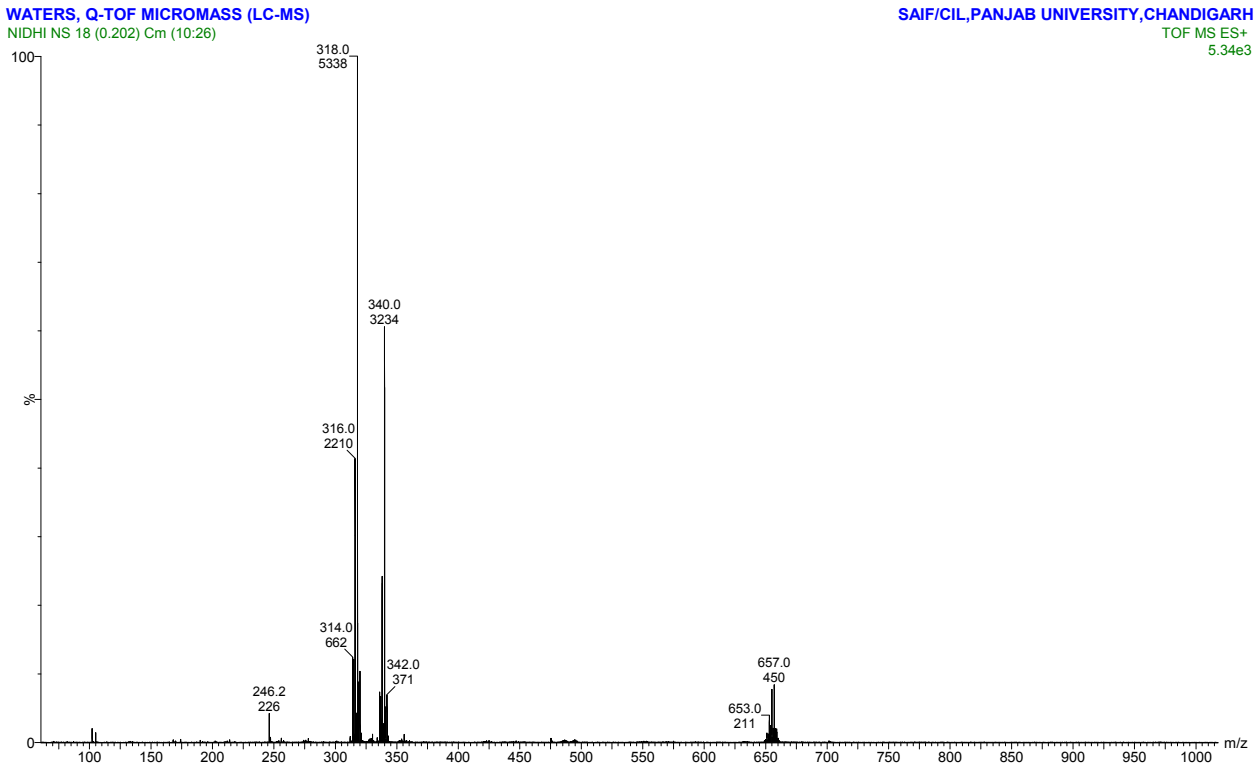
TOF MS ES+
1.73e4



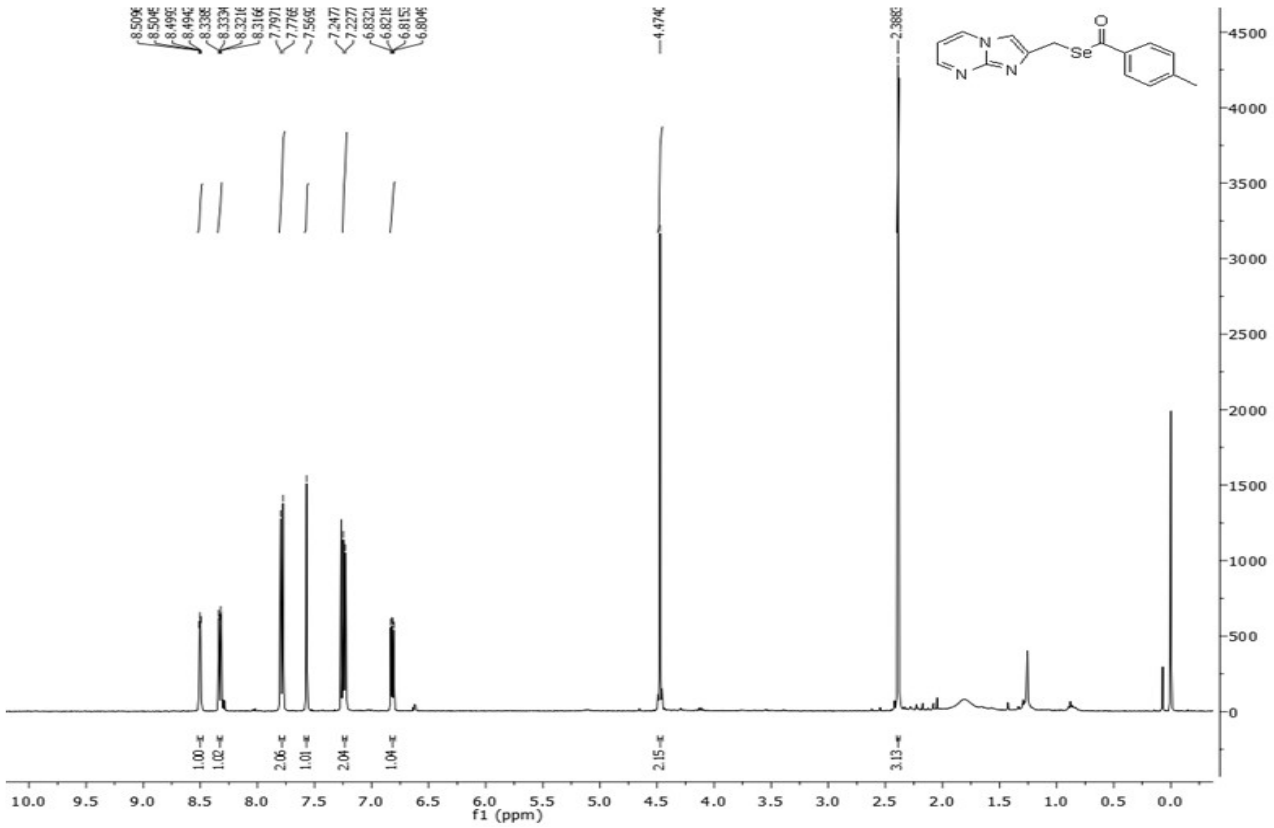
***Se*-(imidazo[1,2-*a*]pyrimidin-2-ylmethyl) benzoselenoate (6e) ^{1}H, ^{13}C, Mass Spectra**

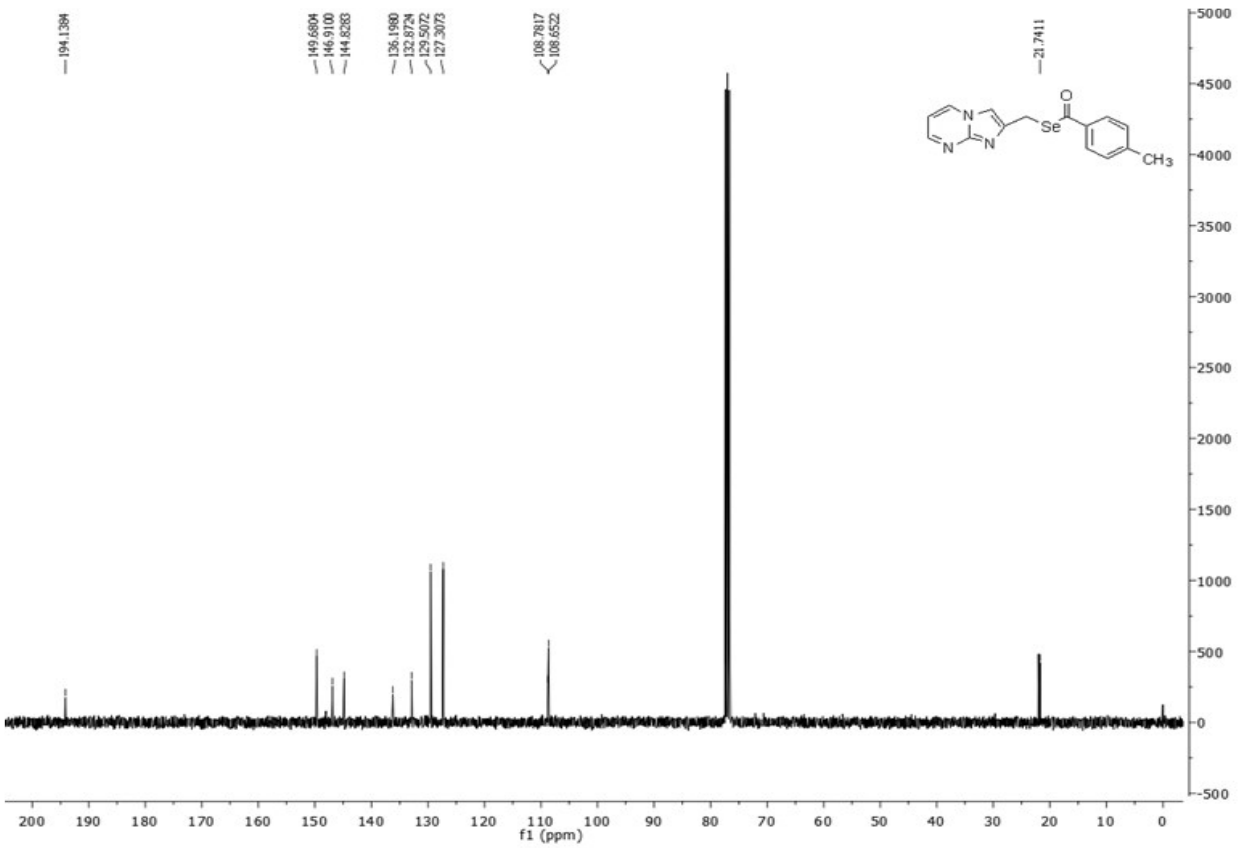






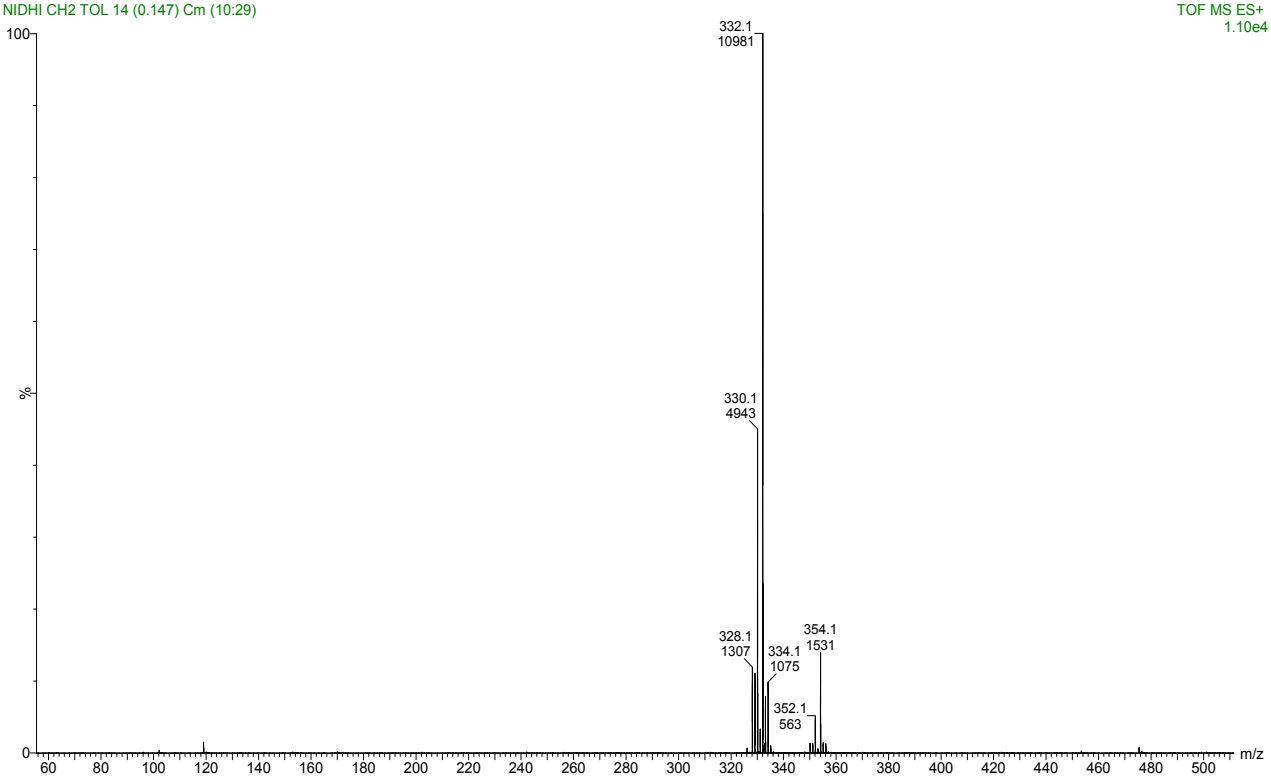
***Se*-(imidazo[1,2-*a*]pyrimidin-2-ylmethyl) 4-methylbenzoselenoate (6f) ^{1}H, ^{13}C, Mass Spectra**



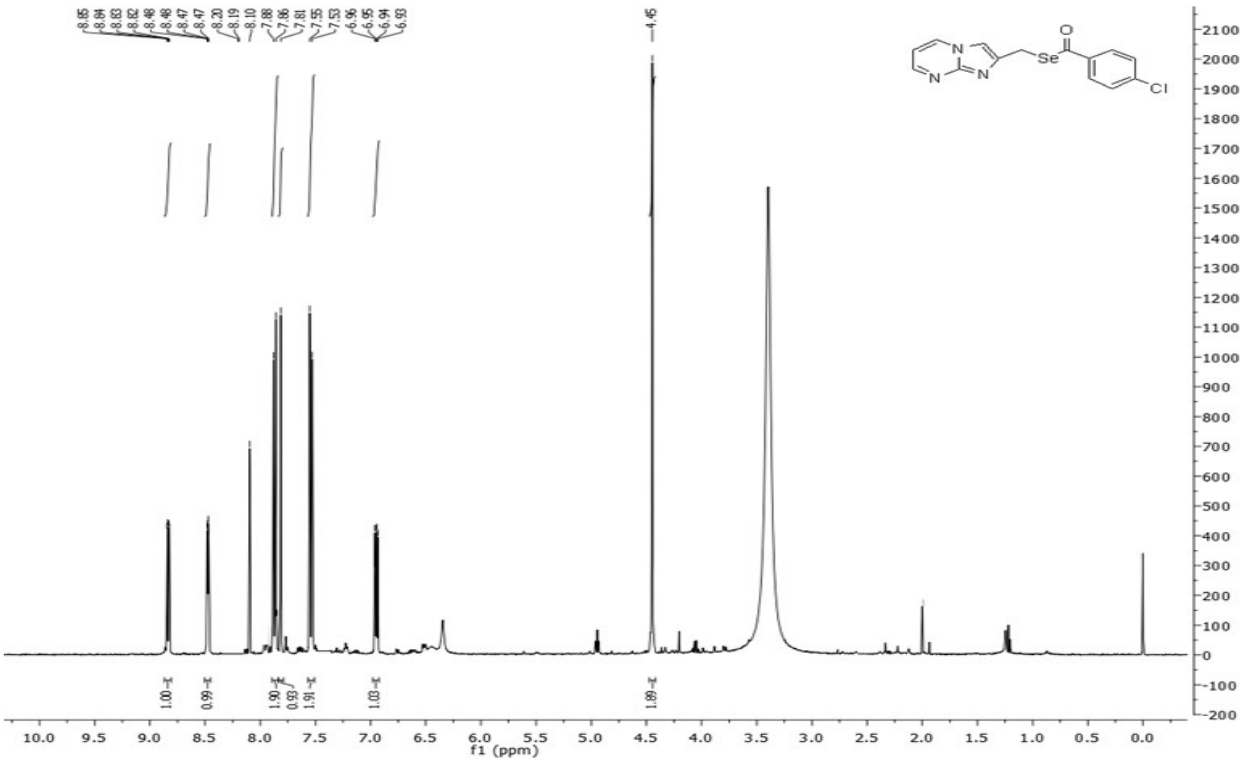


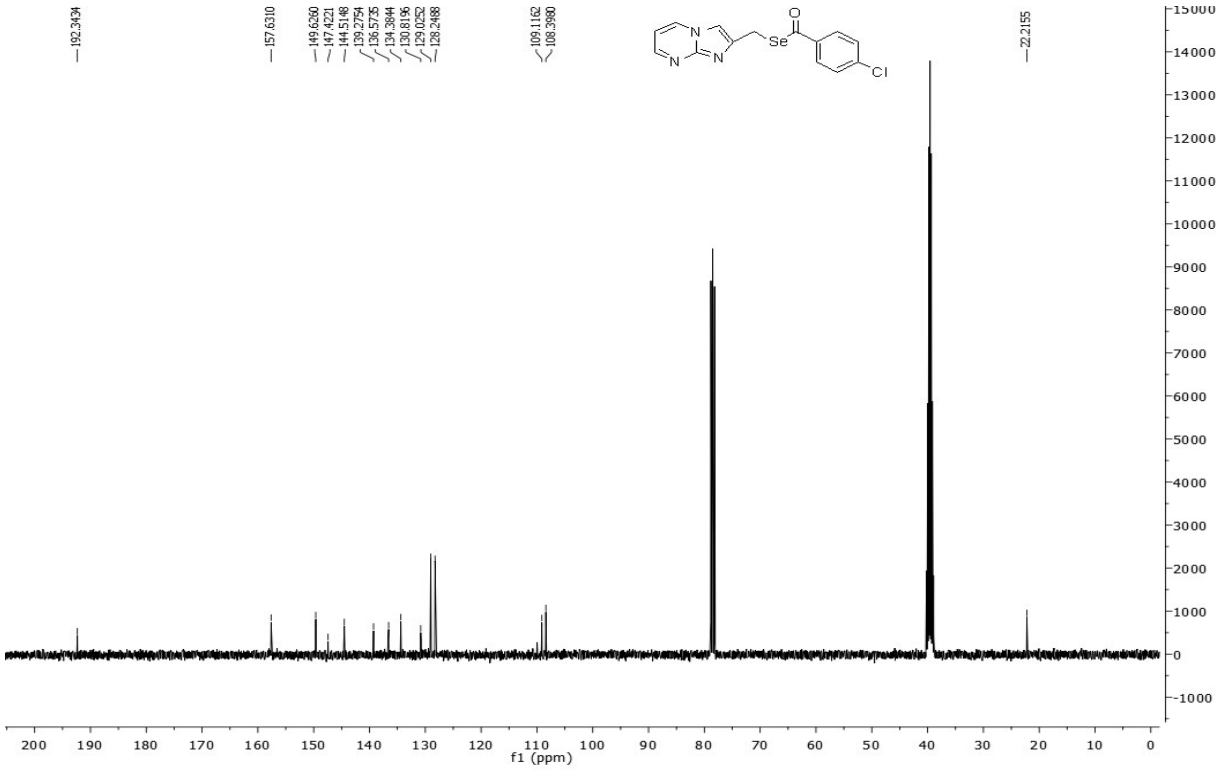
WATERS, Q-TOF MICROMASS (LC-MS)
NIDHI CH2 TOL 14 (0.147) Cm (10:29)

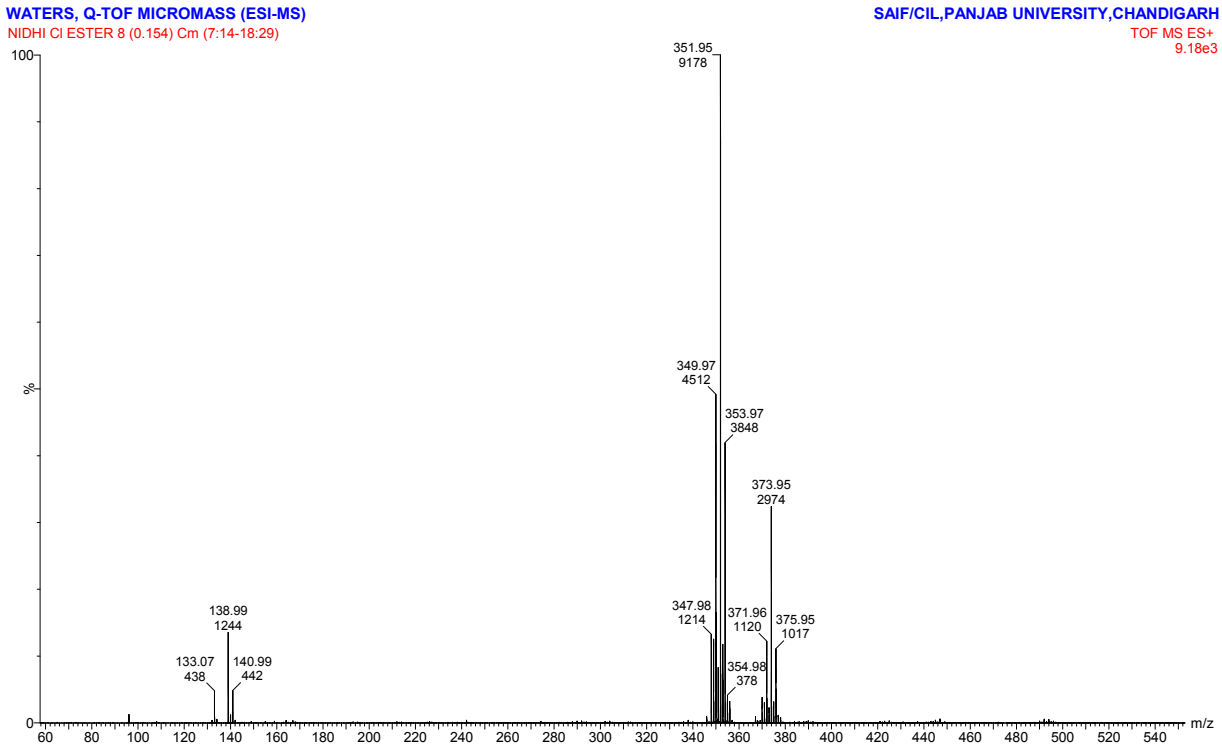
SAIF/CIL,PANJAB UNIVERSITY,CHANDIGARH
TOF MS ES+
1.10e4



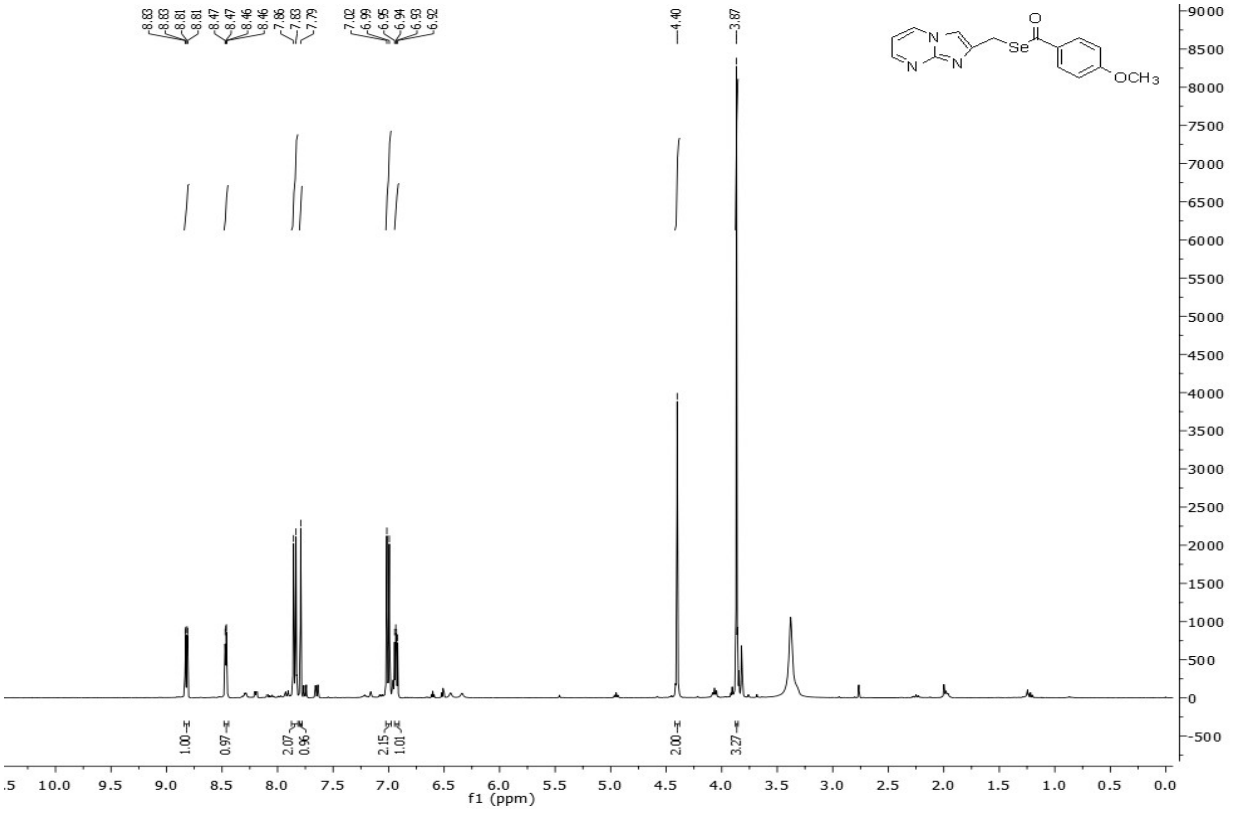
***Se*-(imidazo[1,2-*a*]pyrimidin-2-ylmethyl) 4-chlorobenzoselenoate (6g) ^{1}H, ^{13}C, Mass Spectra**

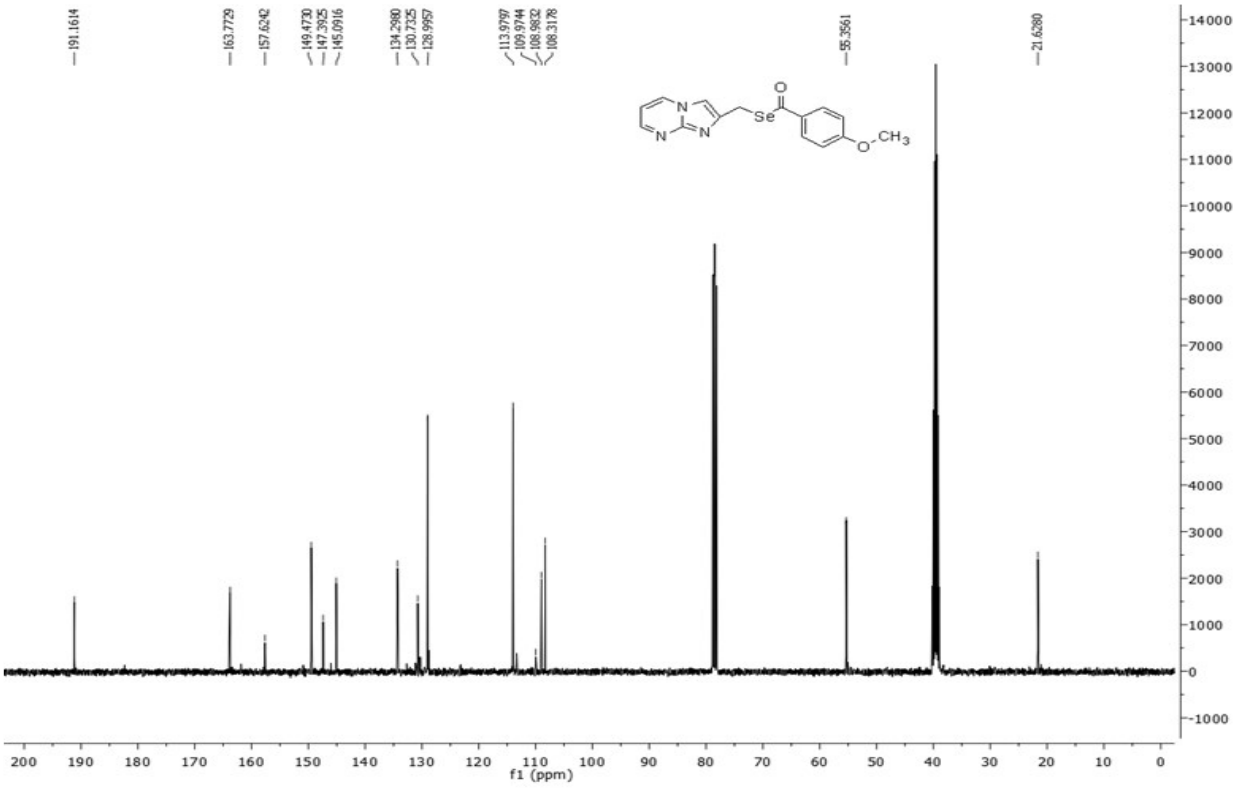






***Se*-(imidazo[1,2-*a*]pyrimidin-2-ylmethyl) 4-methoxybenzoselenoate (6h) ^{1}H, ^{13}C, Mass Spectra**



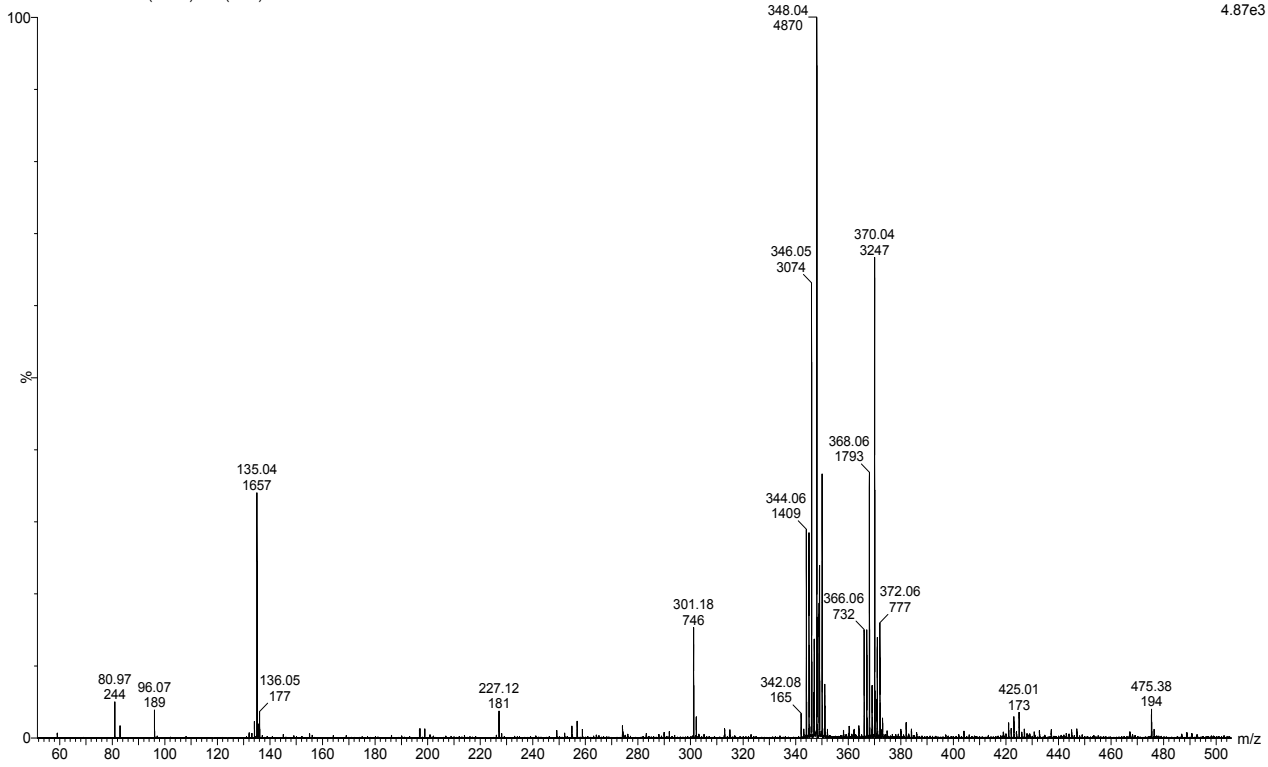


WATERS, Q-TOF MICROMASS (ESI-MS)

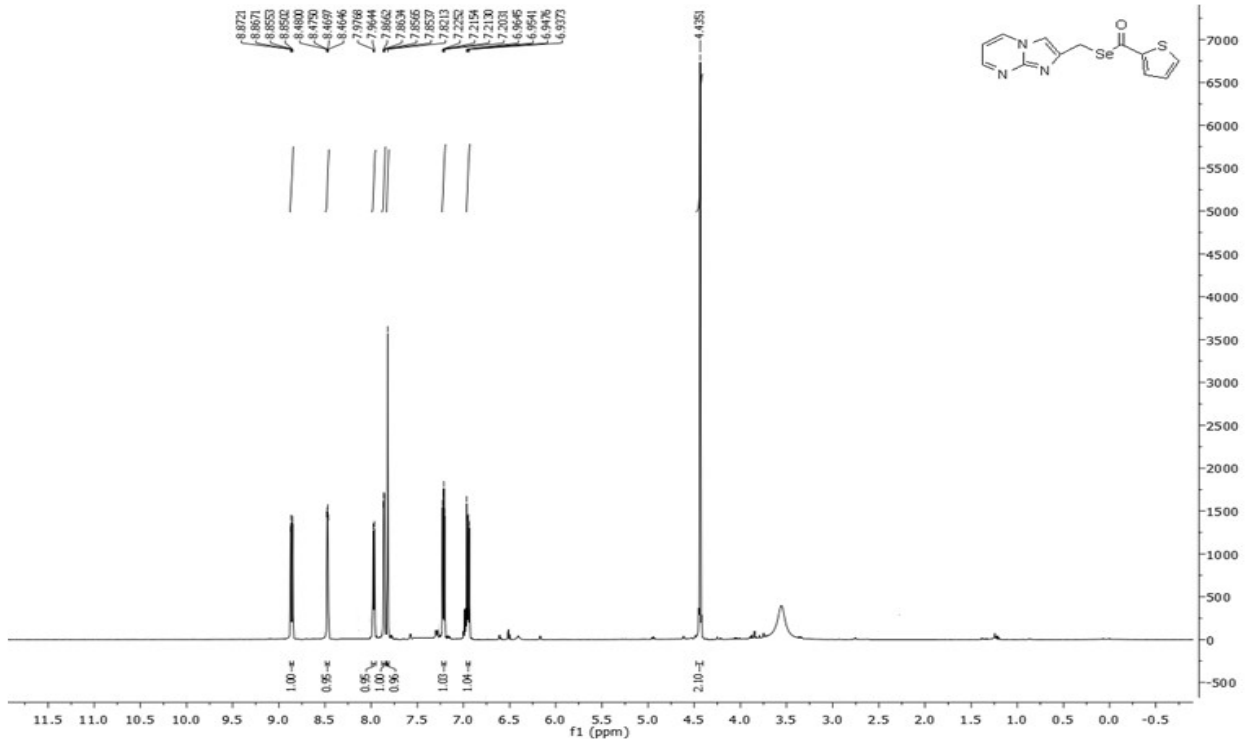
NIDHI OMe ESTER 8 (0.154) Cm (8:11)

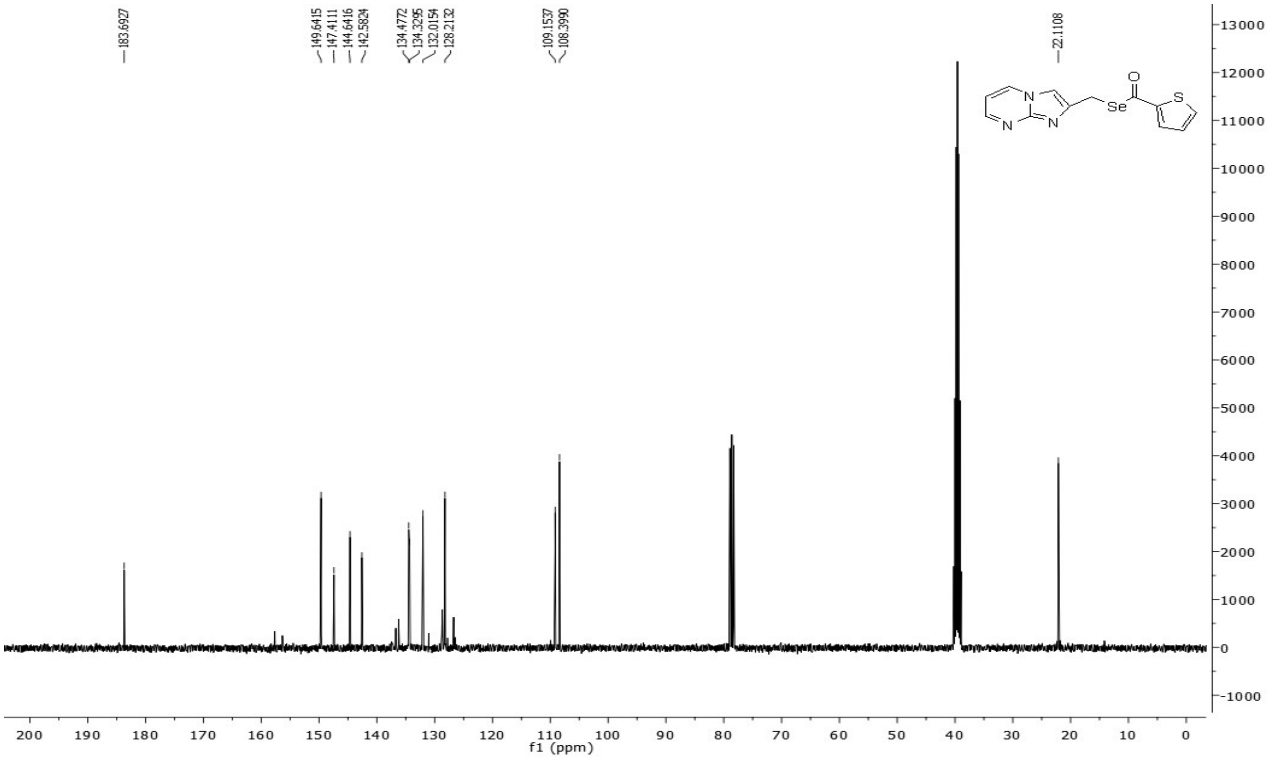
SAIF/CIL,PANJAB UNIVERSITY,CHANDIGARH

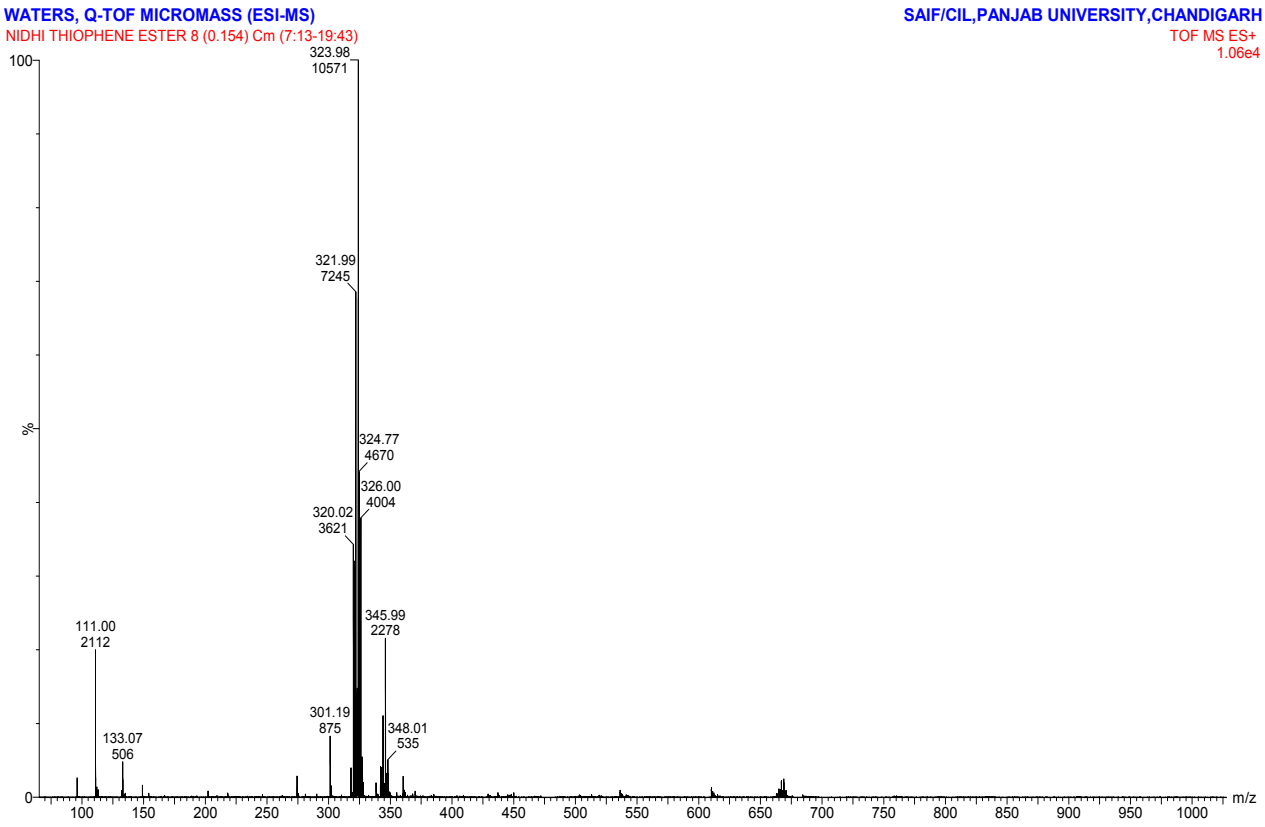
TOF MS ES+
4.87e3



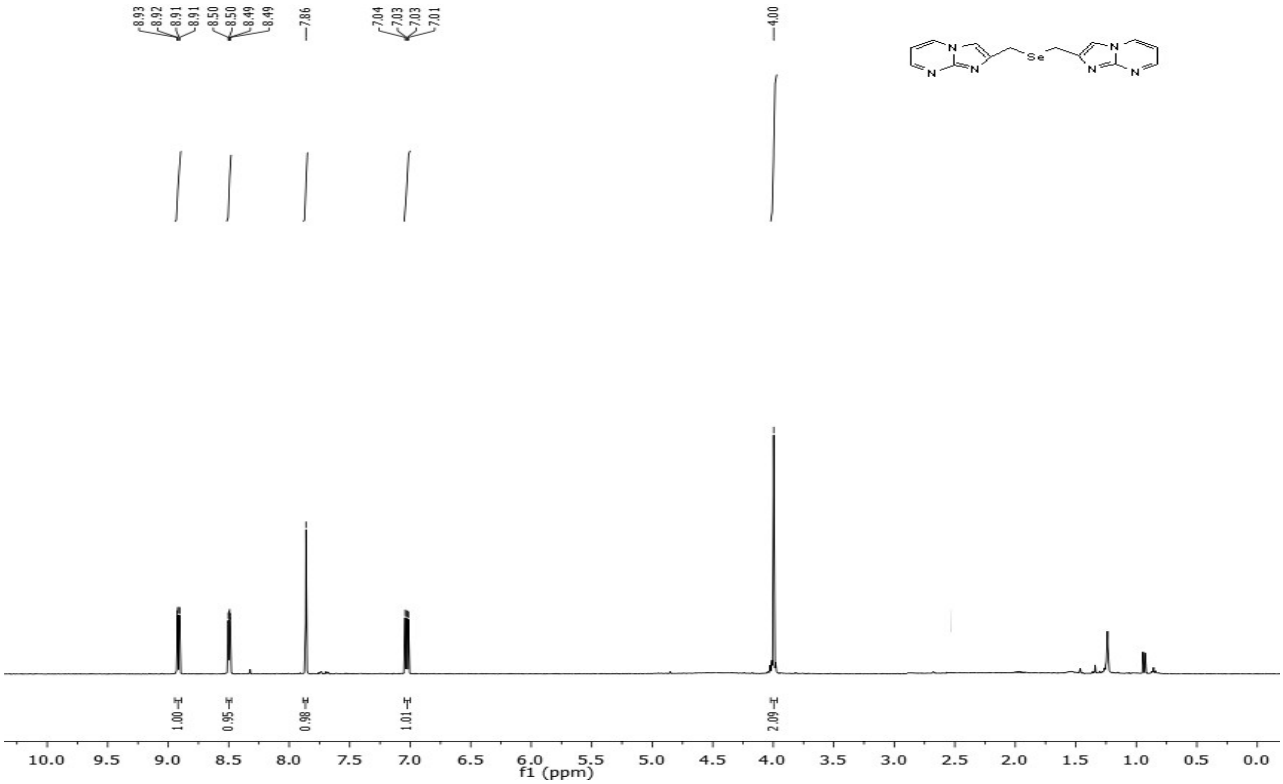
***Se*-(imidazo[1,2-*a*]pyrimidin-2-ylmethyl) thiophene-2-carboselenoate (6i) ^{1}H, ^{13}C, Mass Spectra**

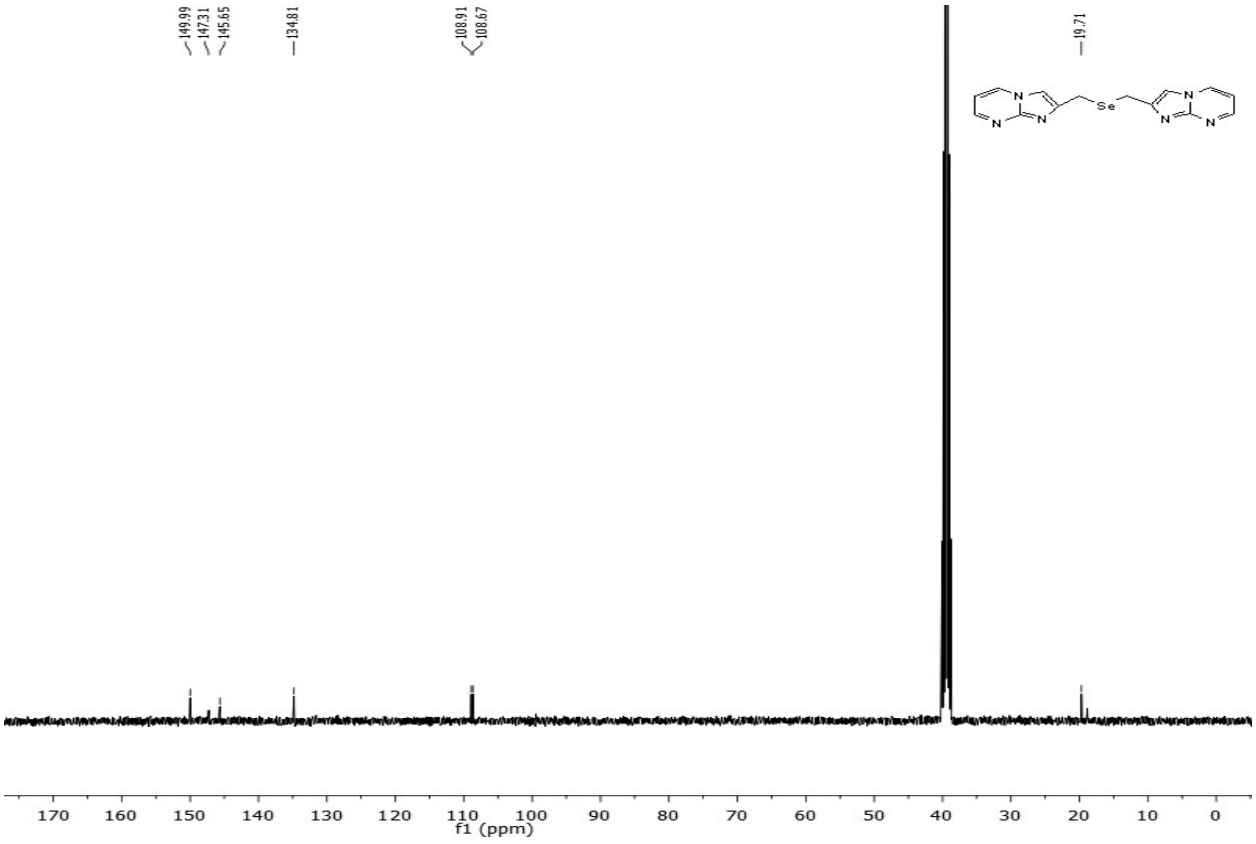






Bis(imidazo[1,2-*a*]pyrimidin-2-ylmethyl)selane (8) ^{1}H, ^{13}C, Mass Spectra





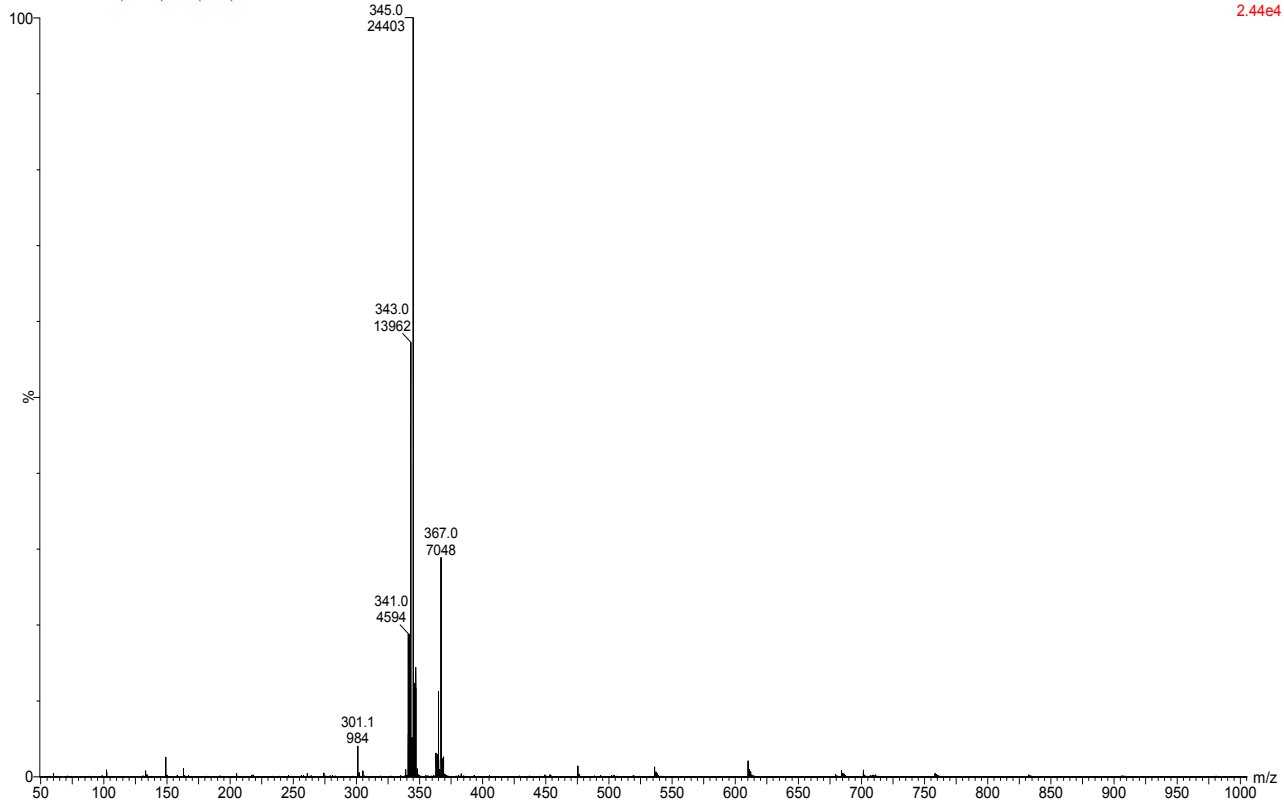
WATERS, Q-TOF MICROMASS (LC-MS)

NIDHI IMPSe 16 (0.169) Cm (8:35)

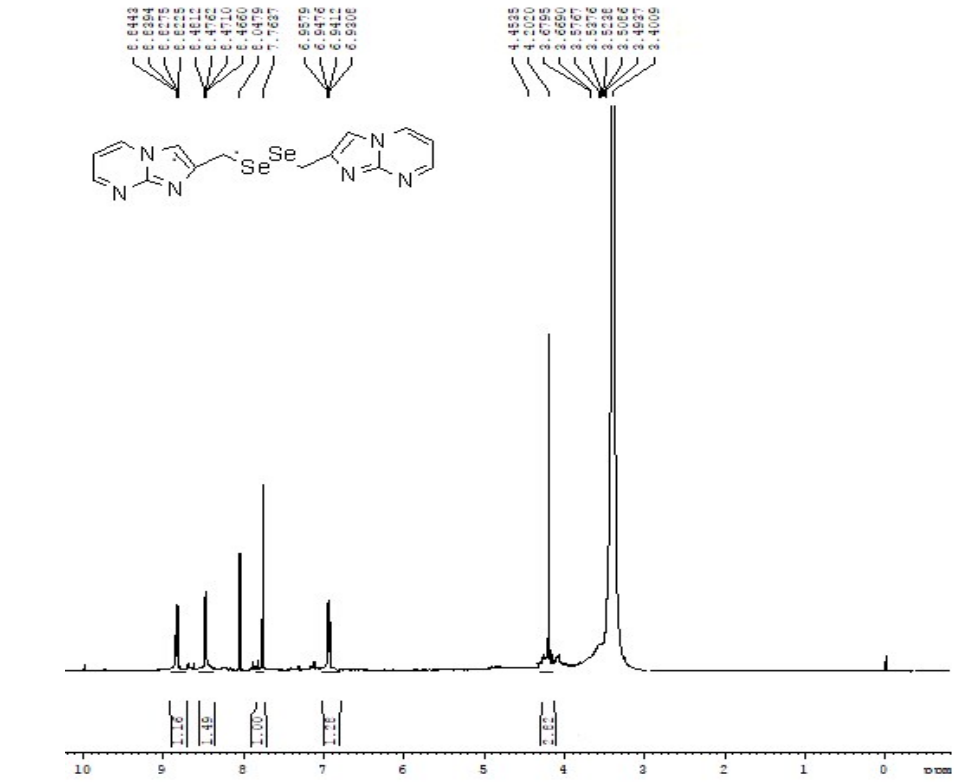
SAIF/CIL,PANJAB UNIVERSITY,CHANDIGARH

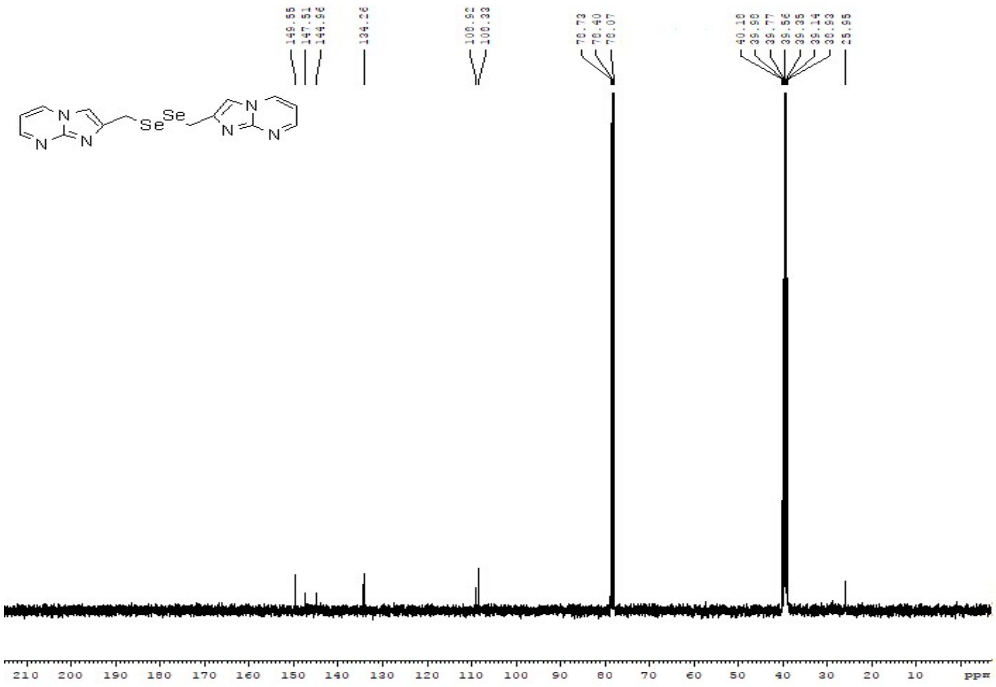
TOF MS ES+

2.44e4

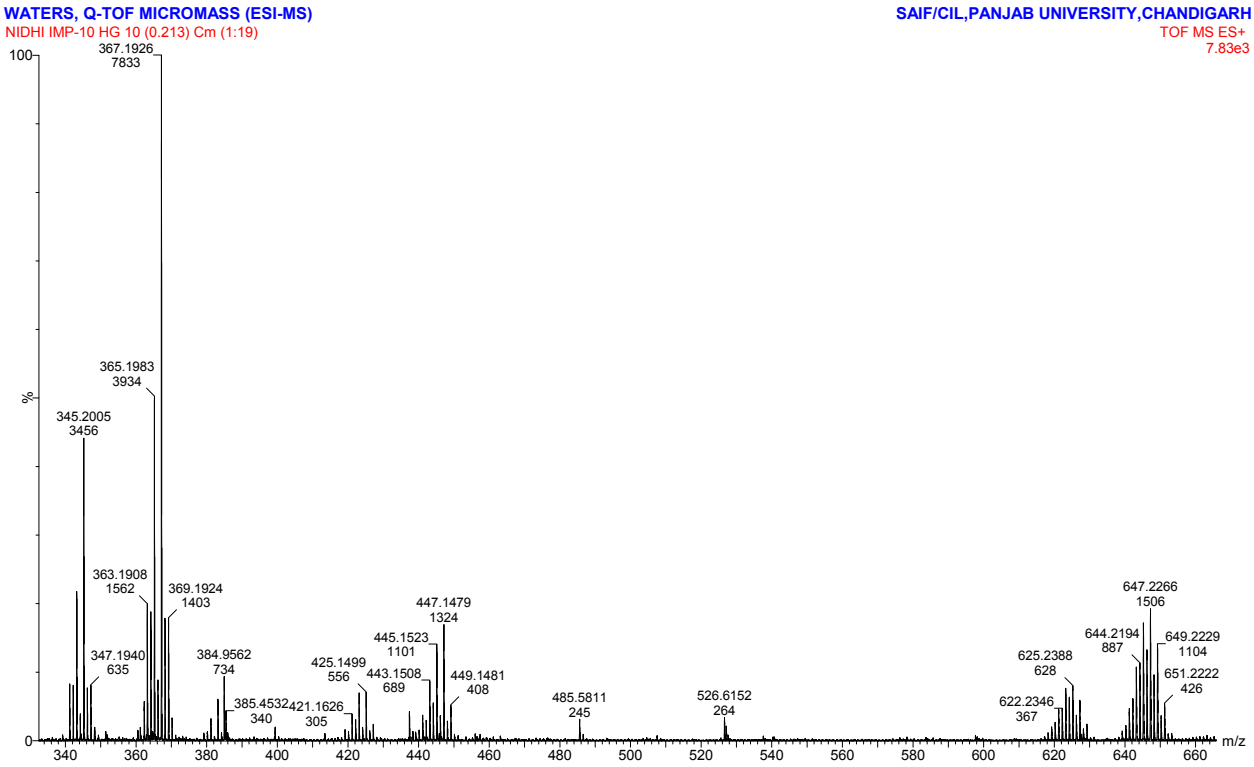


Bis(imidazo[1,2-*a*]pyrimidin-2-ylmethyl)diselenide (9) ^{1}H and ^{13}C NMR Spectra

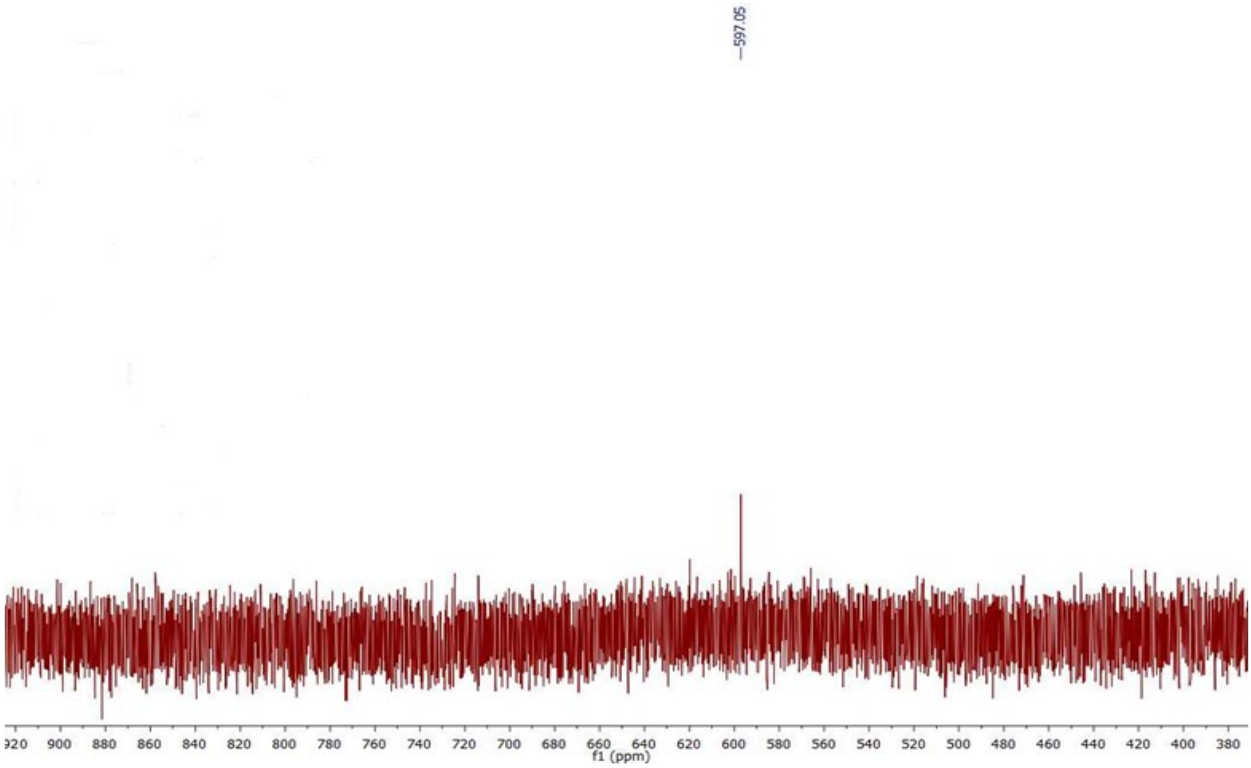




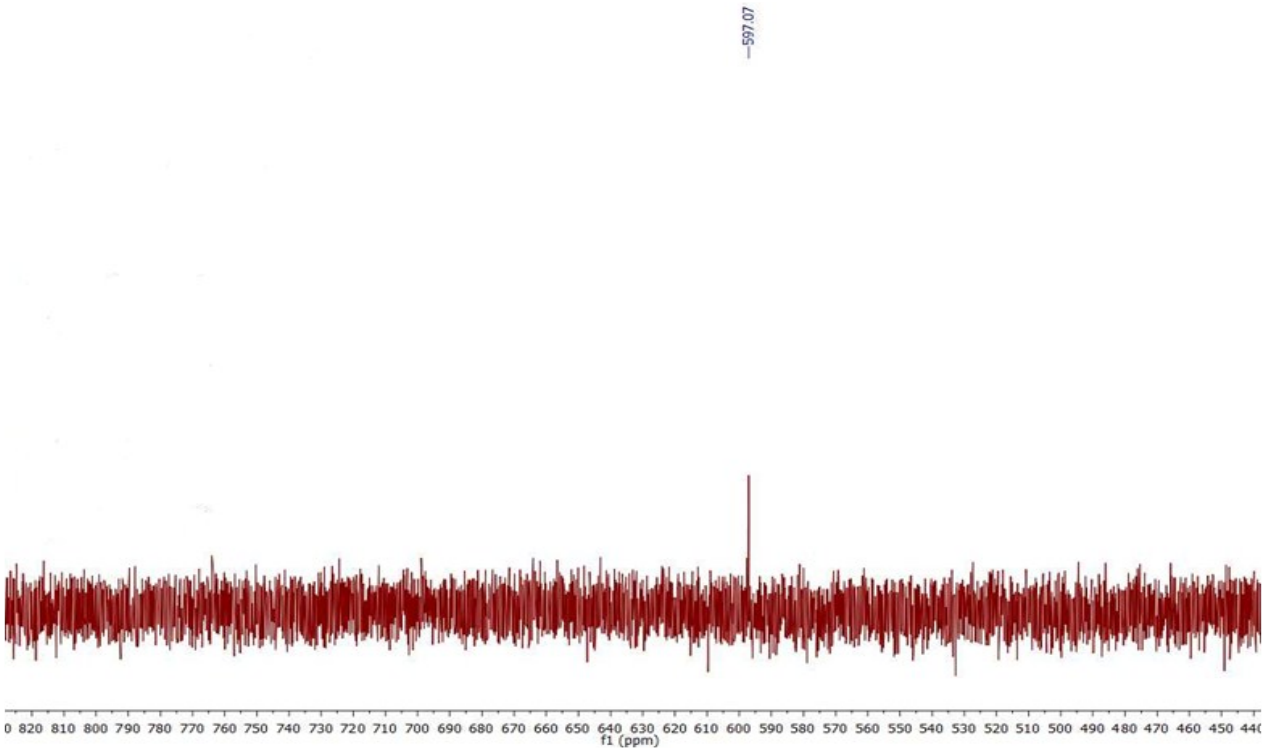
Bis(imidazo[1,2-*a*]pyrimidin-2-ylmethyl)diselenide (9) and bis((imidazo[1,2-*a*]pyrimidin-2-ylmethyl)selanyl)mercury (10) mass spectrum



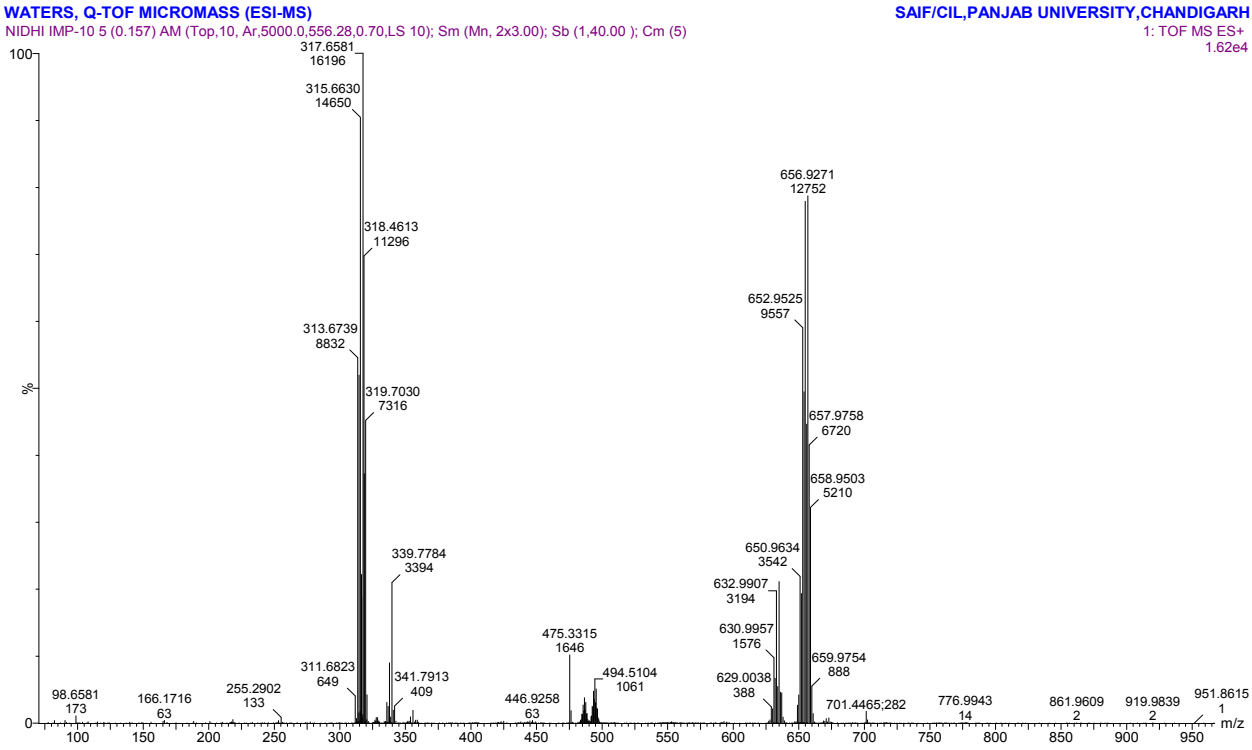
***Se*-(imidazo[1,2-*a*]pyridin-2-ylmethyl) benzoselenoate (6a) ^{77}Se NMR**



***Se*-(imidazo[1,2-*a*]pyrimidin-2-ylmethyl) benzoselenoate (6e) ^{77}Se NMR**



***Se*-(imidazo[1,2-*a*]pyridin-2-ylmethyl) benzoselenoate (6a) HRMS**



***Se*-(imidazo[1,2-*a*]pyrimidin-2-ylmethyl) benzoselenoate (6e) HRMS**

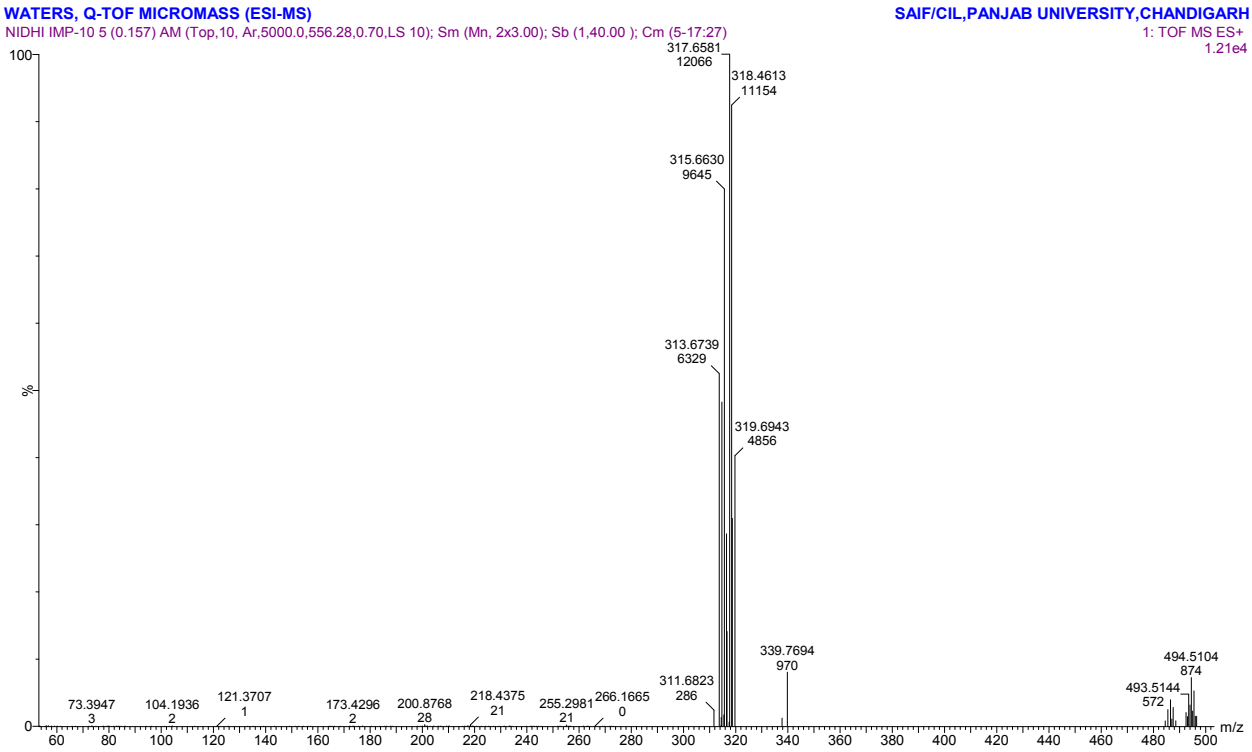
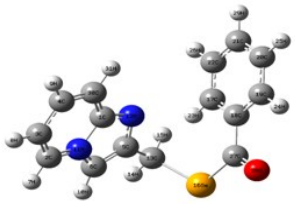
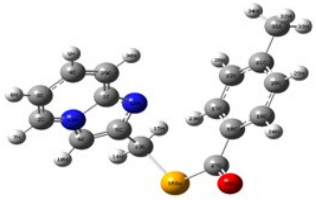
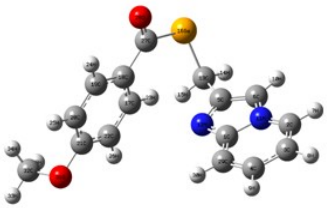
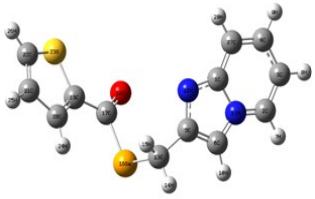
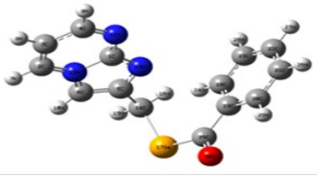
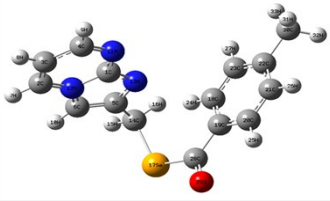
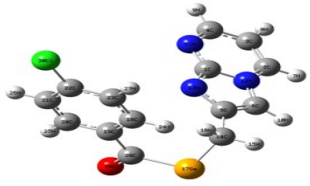


Table S1 Optimized structures of compounds **6a-i** and **8a-b** with DFT

Compound	Optimized structure
6a	
6b	
6c	
6d	
6e	
6f	
6g	

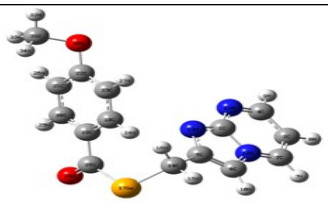
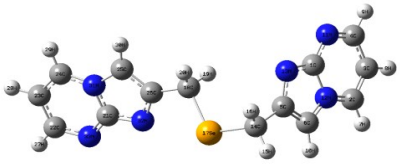
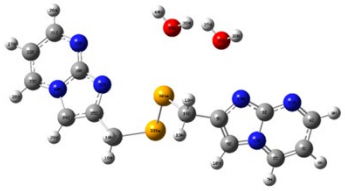
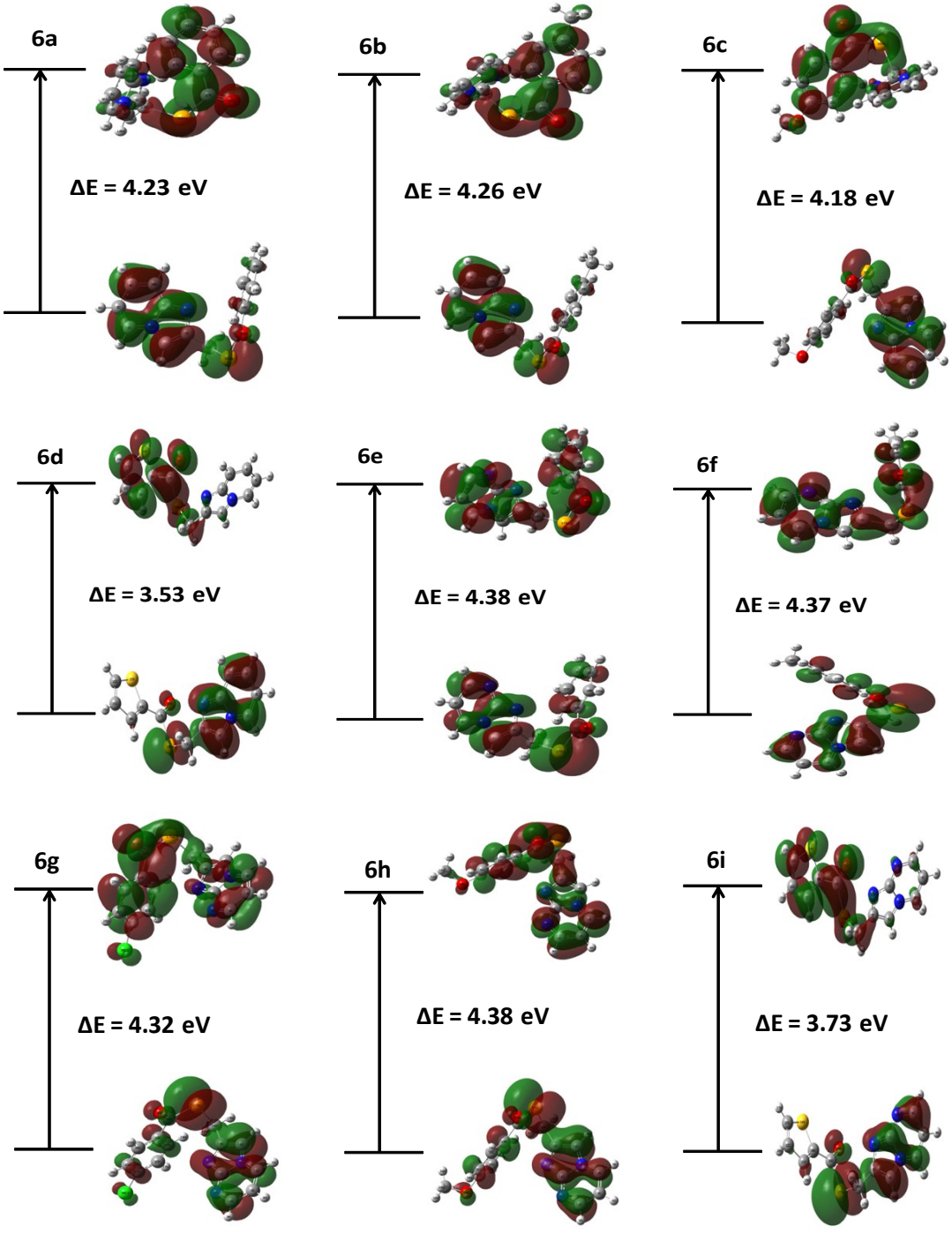
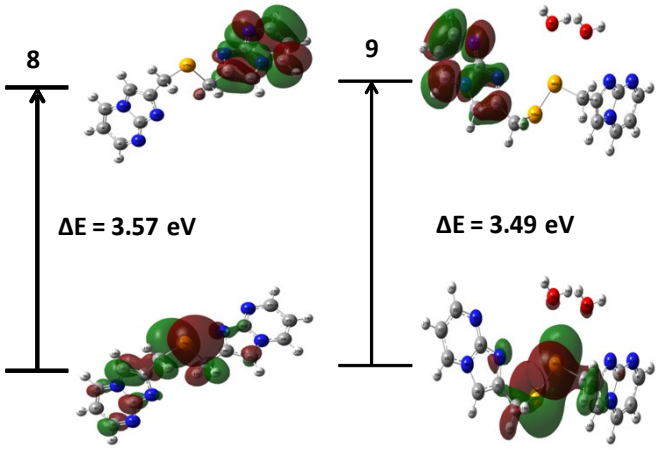
6h	
6i	
8	
9	

Table S2 Theoretical parameters calculated by DFT studies for compounds **6a-i** and **8-9**

Compound	Energy (a. u.)	Band gap (eV)	CH_2-Se-C-O Bond angle (°)
6a	-3162.87	4.23	149.99
6b	-3202.18	4.26	150.00
6c	-3277.38	4.18	149.99
6d	-3483.62	3.53	90.00
6e	-3178.92	4.38	150.00
6f	-3218.23	4.37	150.00
6g	-3638.51	4.32	150.00
6h	-3293.43	4.38	150.00
6i	-3499.66	3.73	90.00
8	-3268.54	3.57	-
9	-5820.70	3.49	-

Fig. S1 HOMO-LUMO diagrams of compounds **6a-i** and **8-9**




8
9
ΔE = 3.57 eV
ΔE = 3.49 eV