Electronic Supplementary Material (ESI) for RSC Advances.

Synthesis, structural analysis, antimicrobial evaluation and synergistic studies of imidazo[1,2-a]pyrimidine chalcogenides

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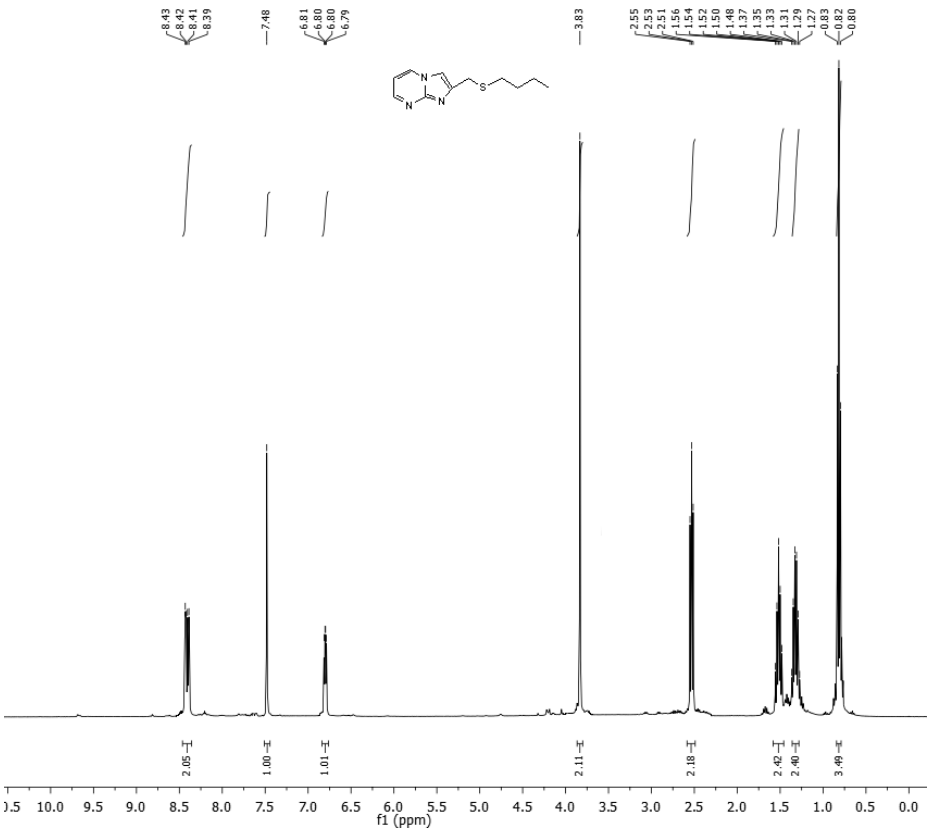
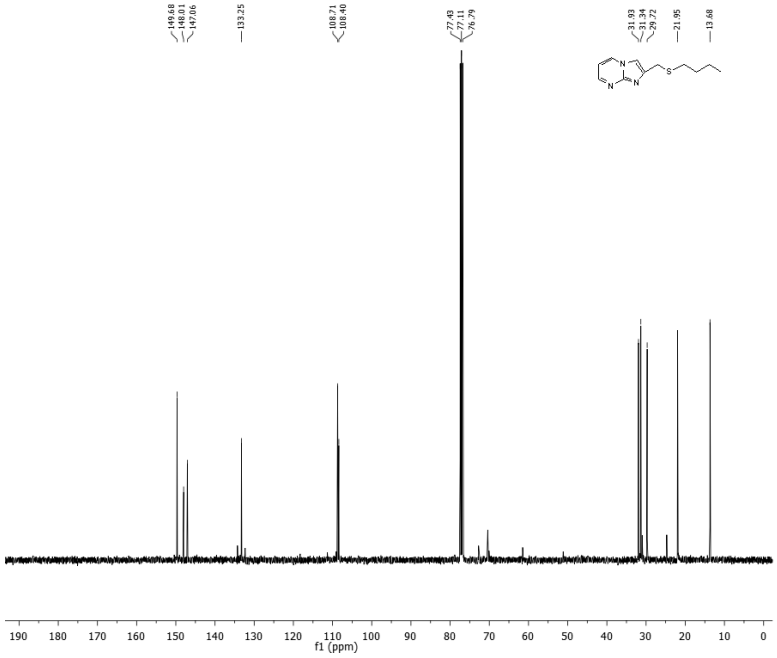
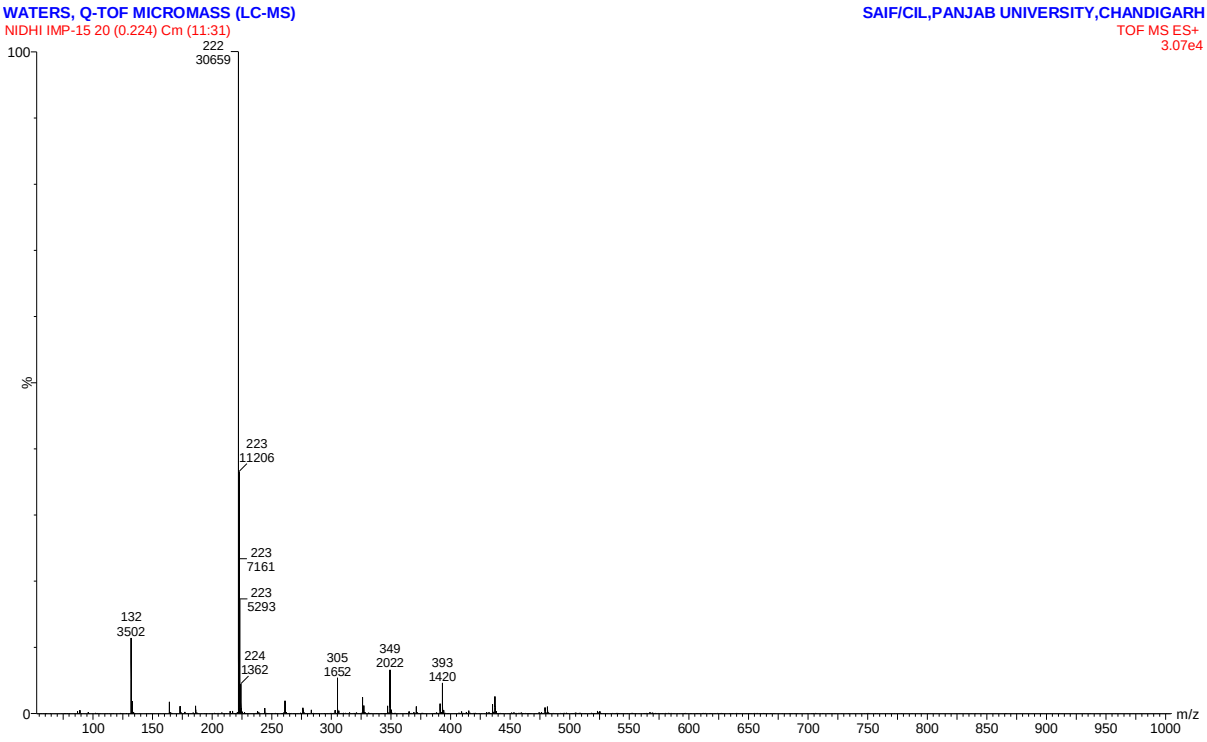
2-((Butylthio)methyl)imidazo[1,2-a]pyrimidine (4) ^{1}H, ^{13}C, Mass Spectra







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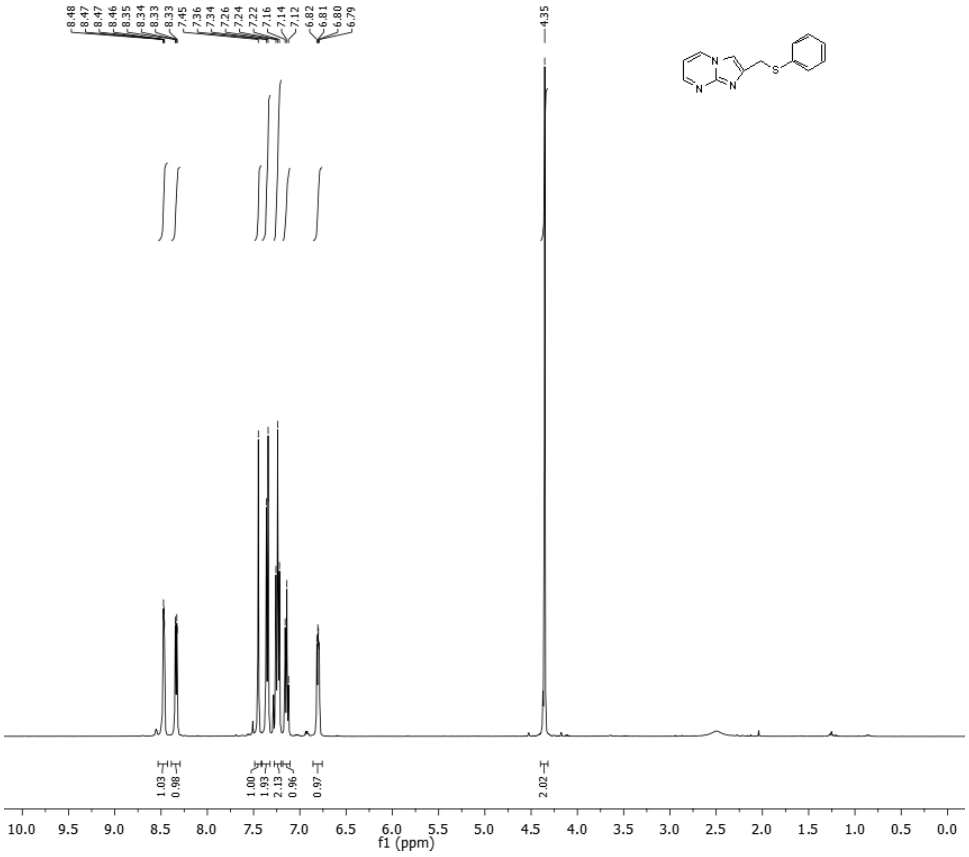

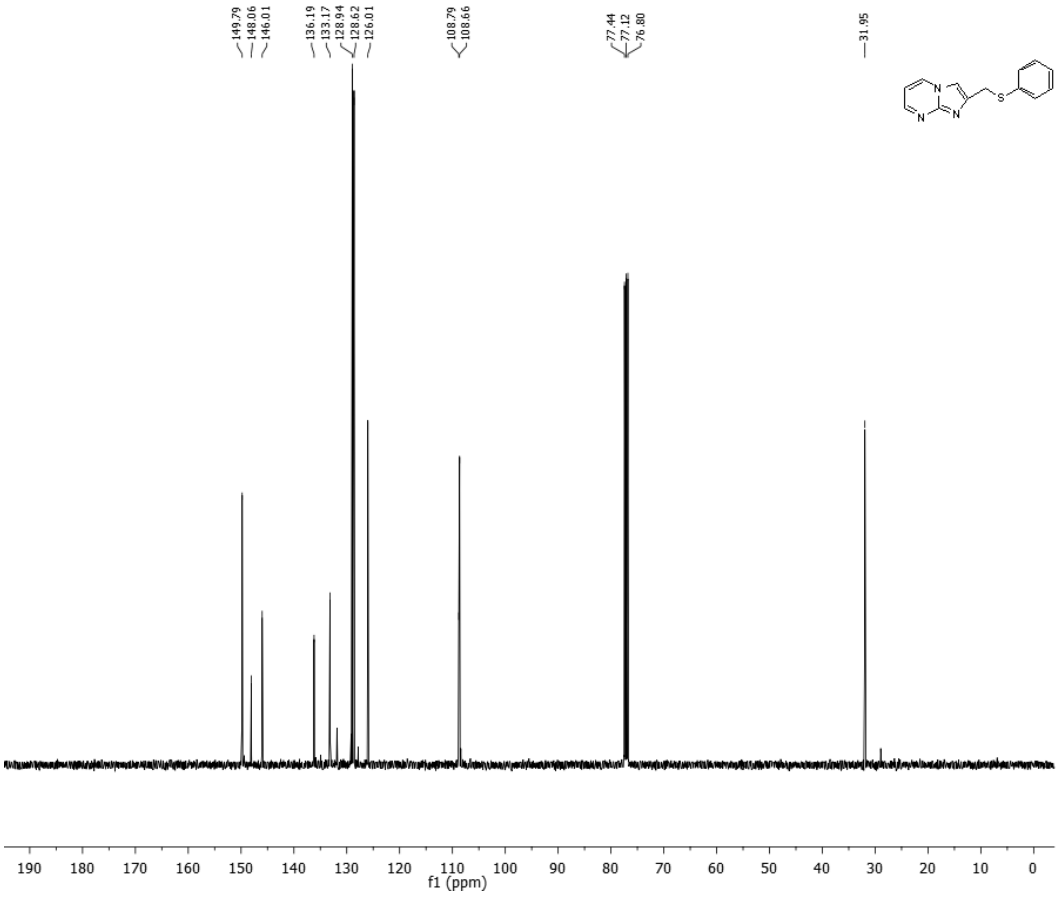

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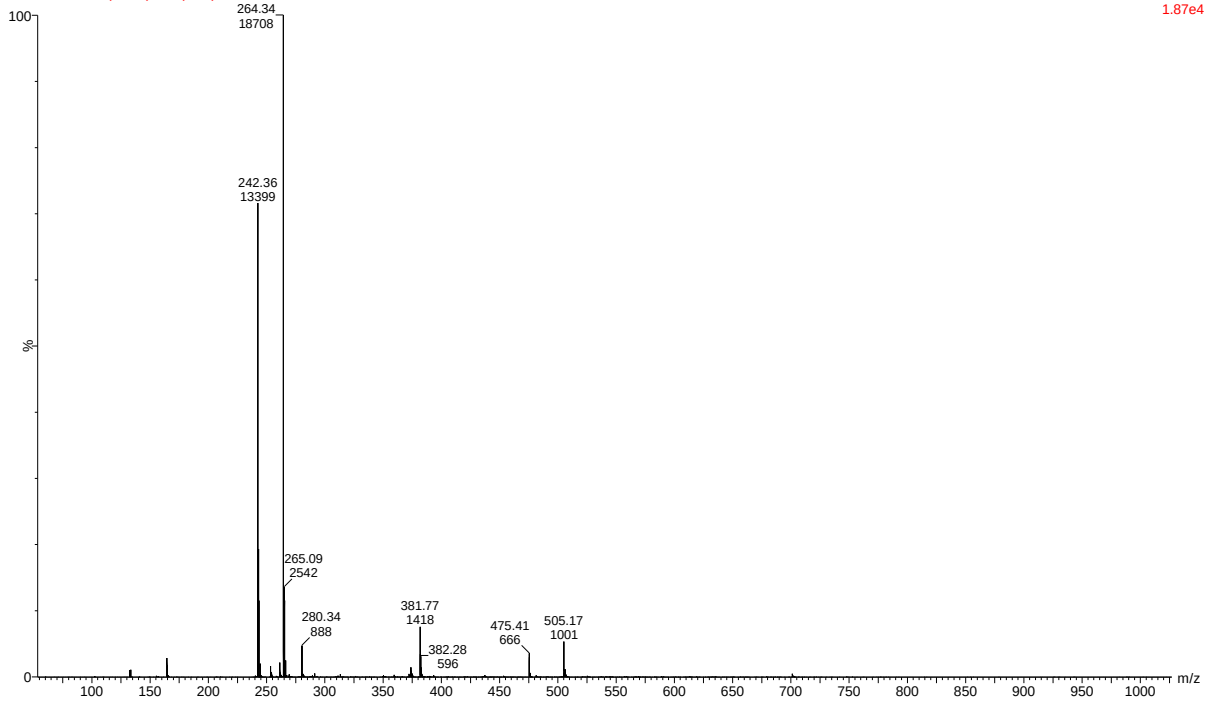
NIDHI IMP-16 8 (0.218) Cm (5:11)

SAIF/CIL,PANJAB UNIVERSITY,CHANDIGARH
TOF MS ES+
1.87e4



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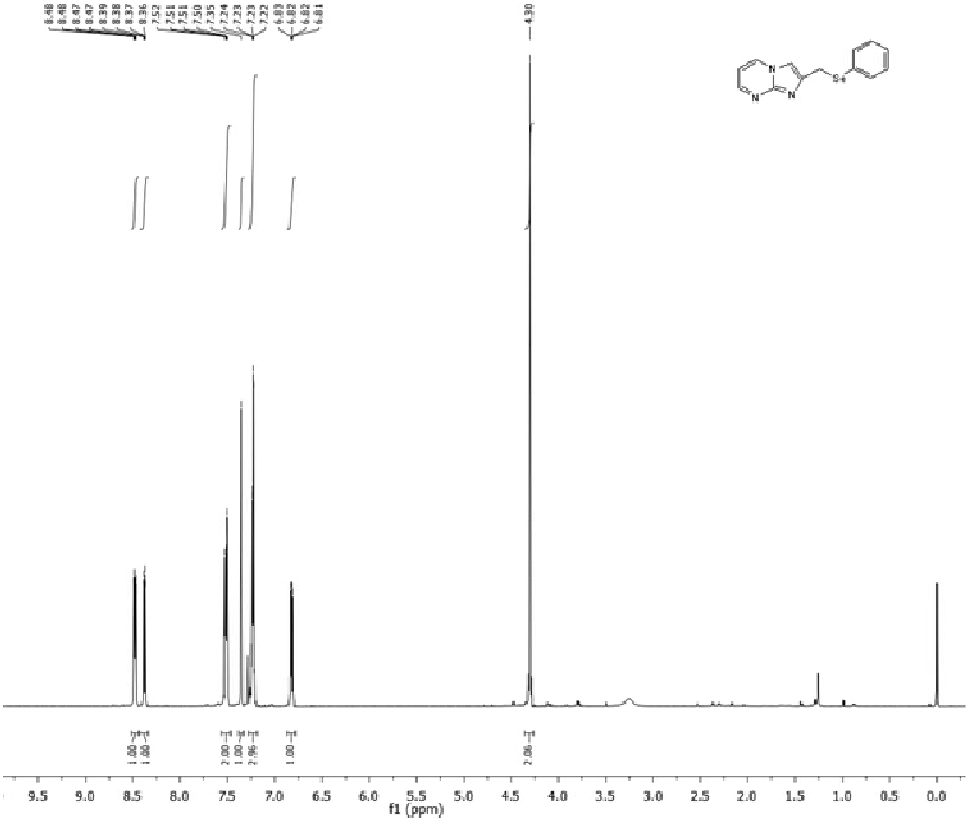

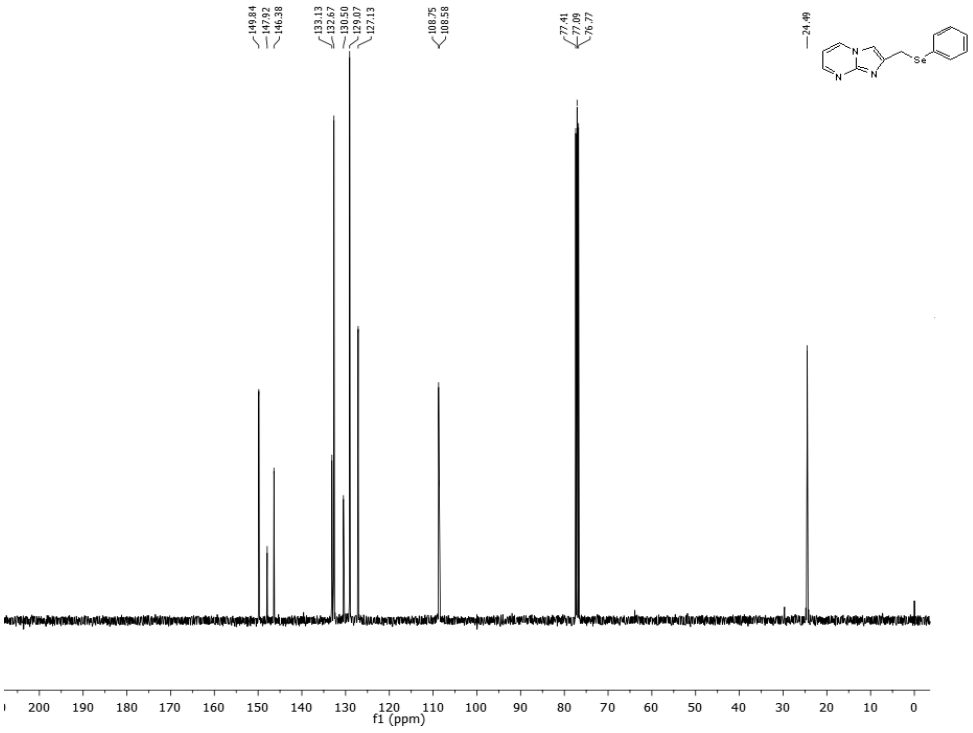

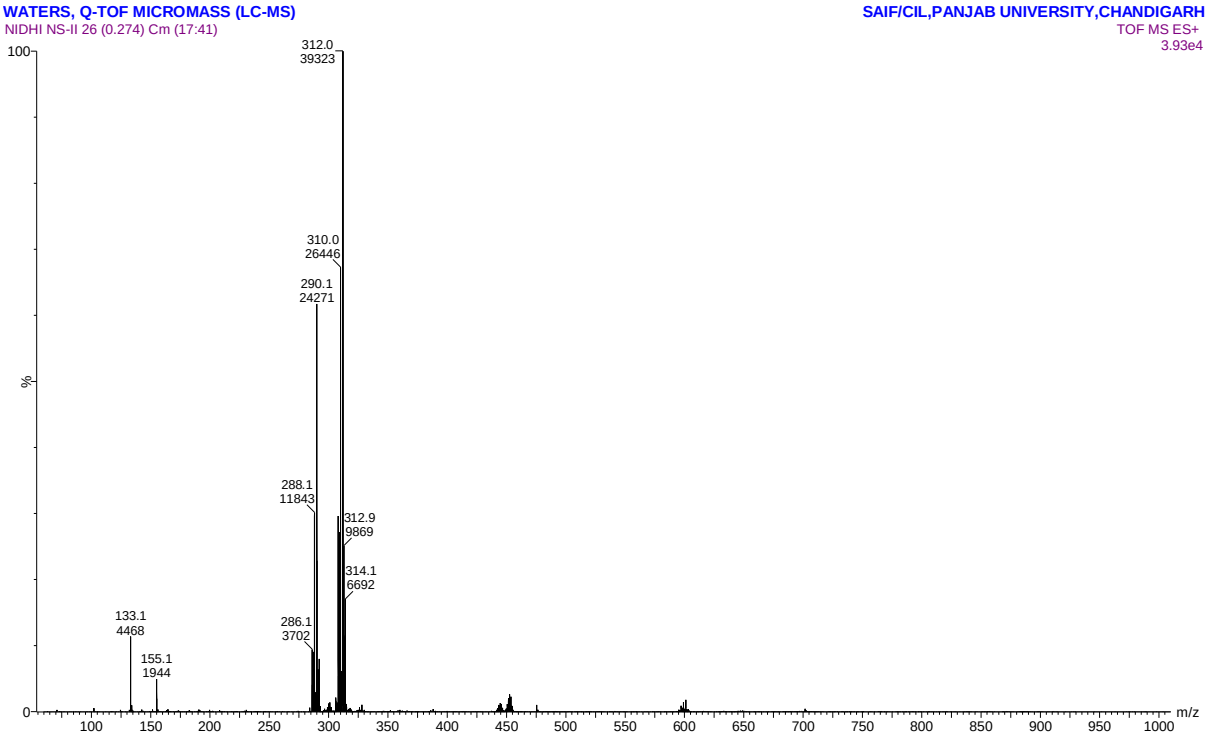

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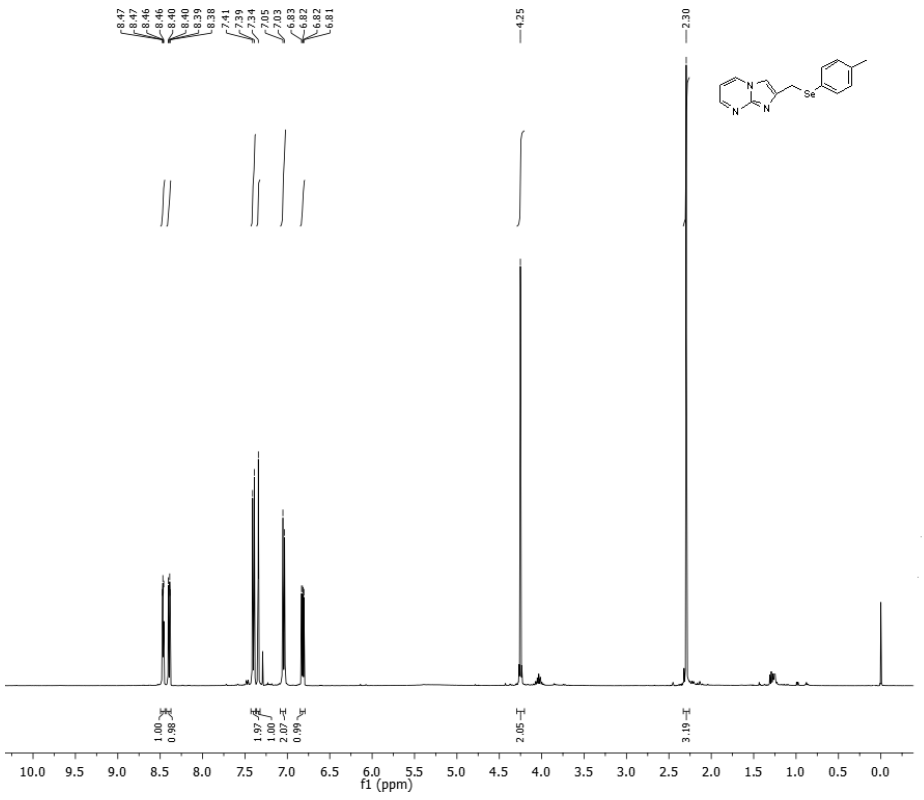

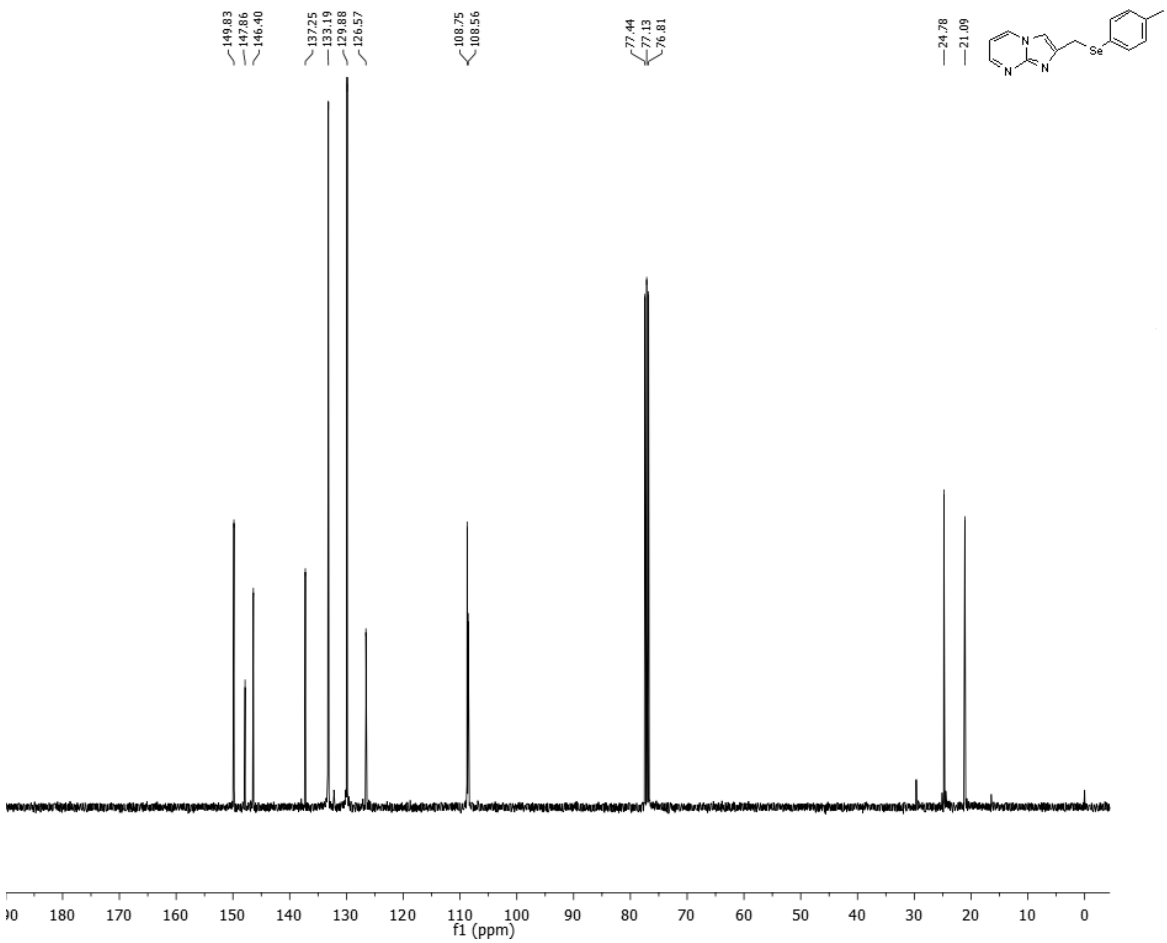

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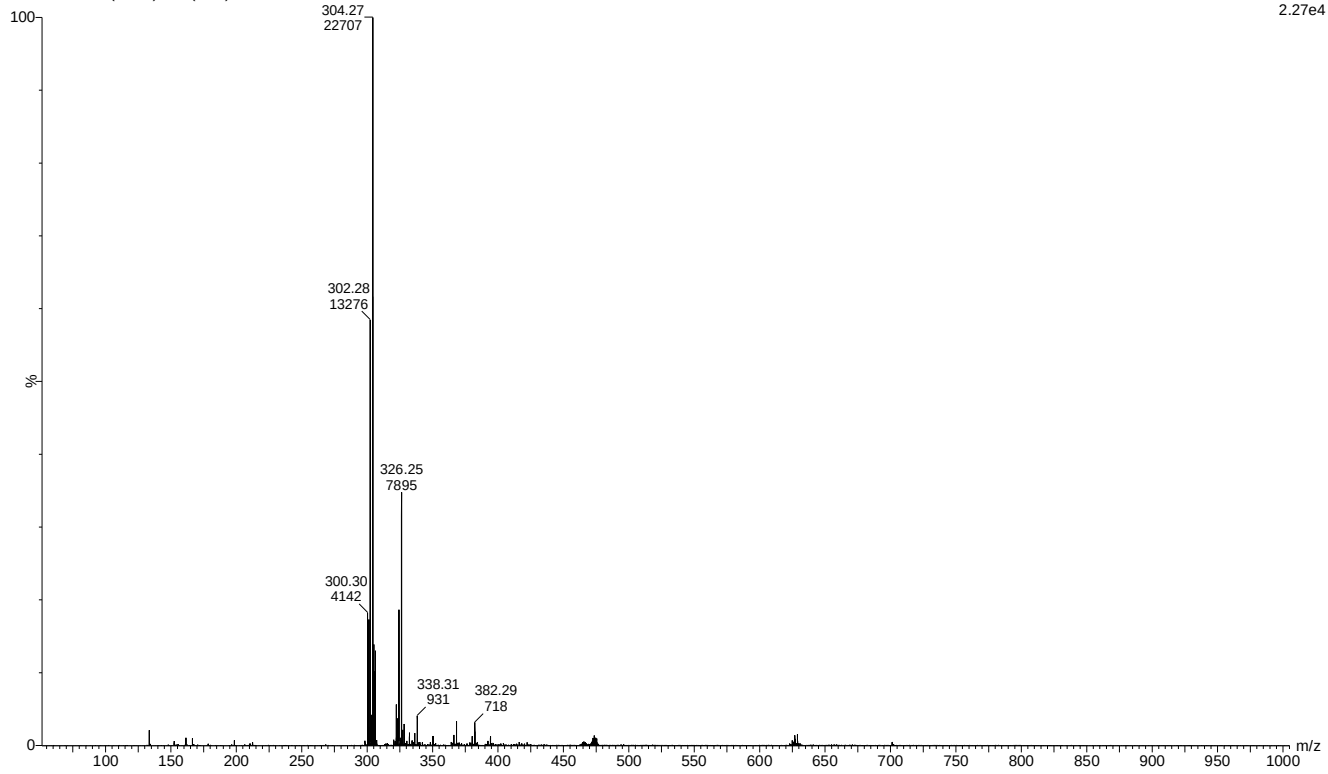
SAIF/CIL,PANJAB UNIVERSITY,CHANDIGARH

TOF MS ES+
2.27e4



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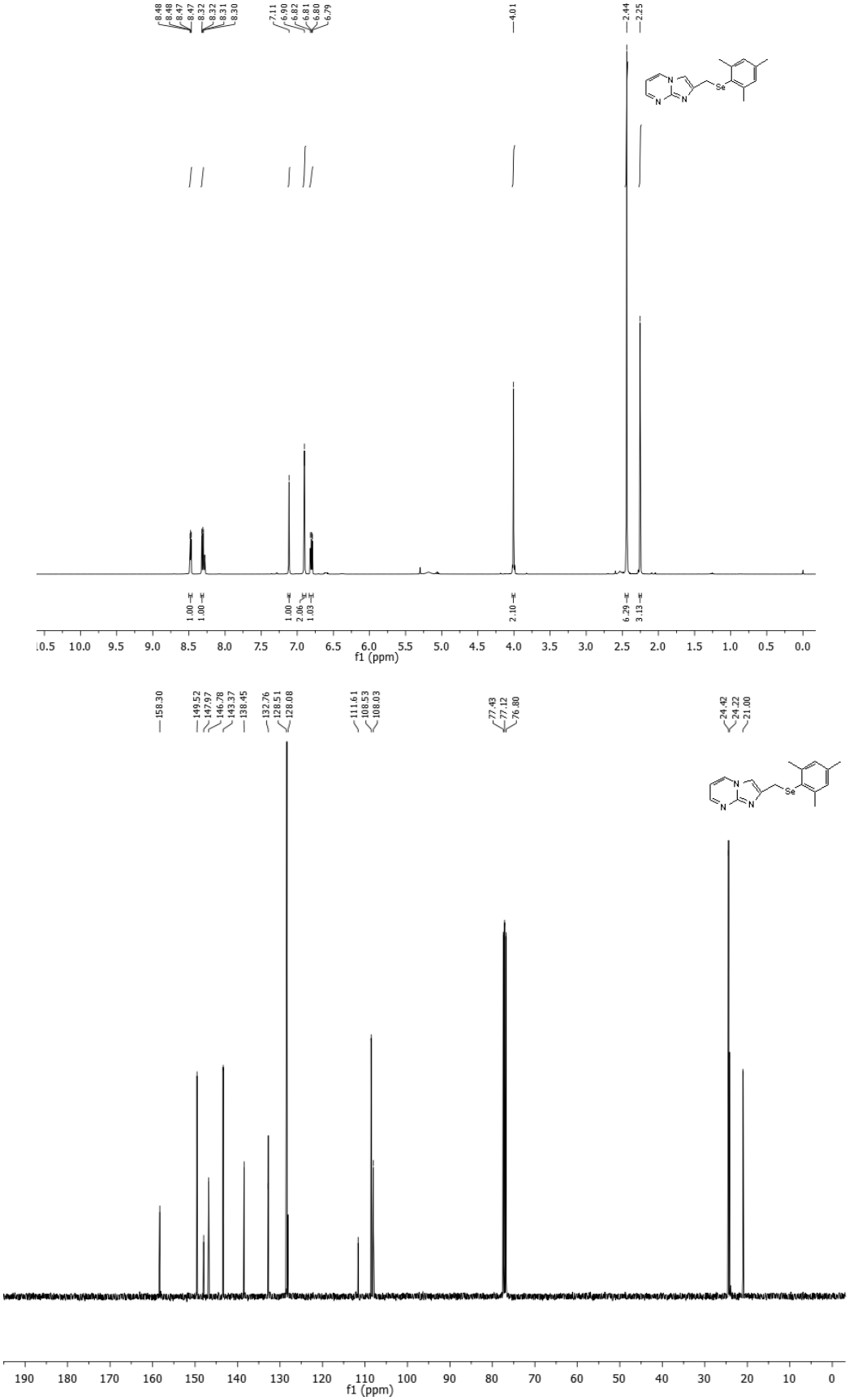

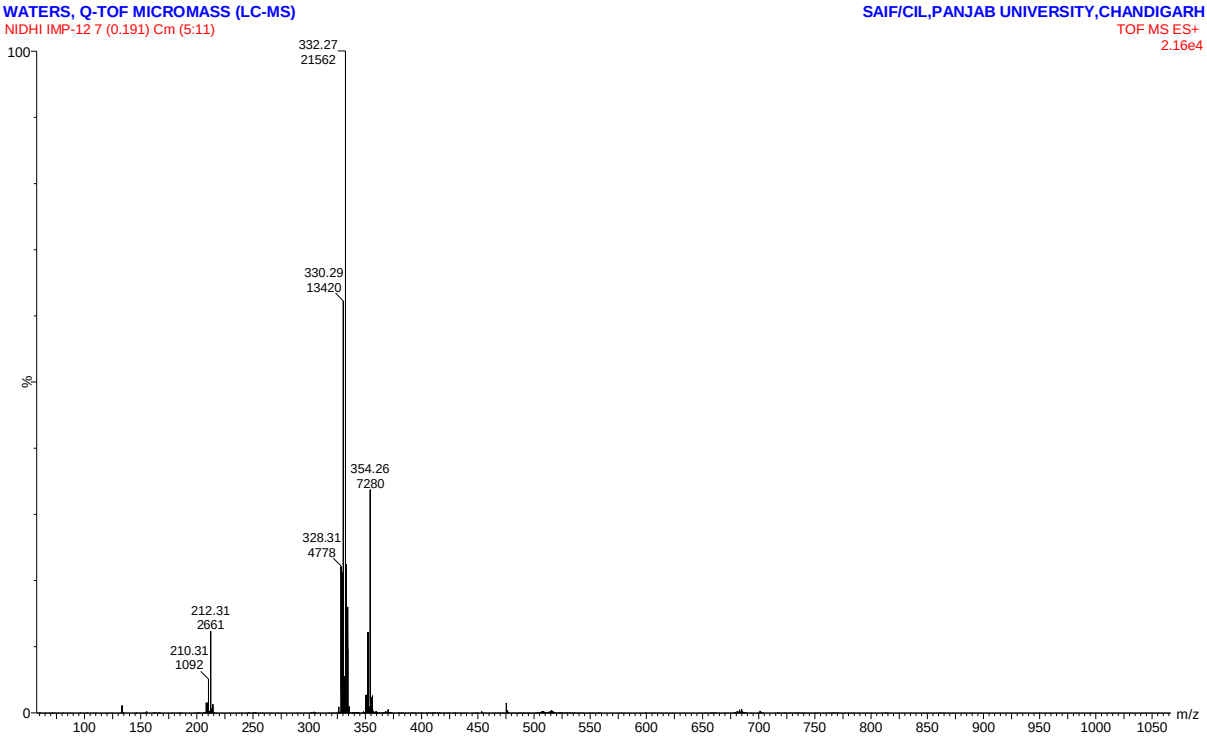

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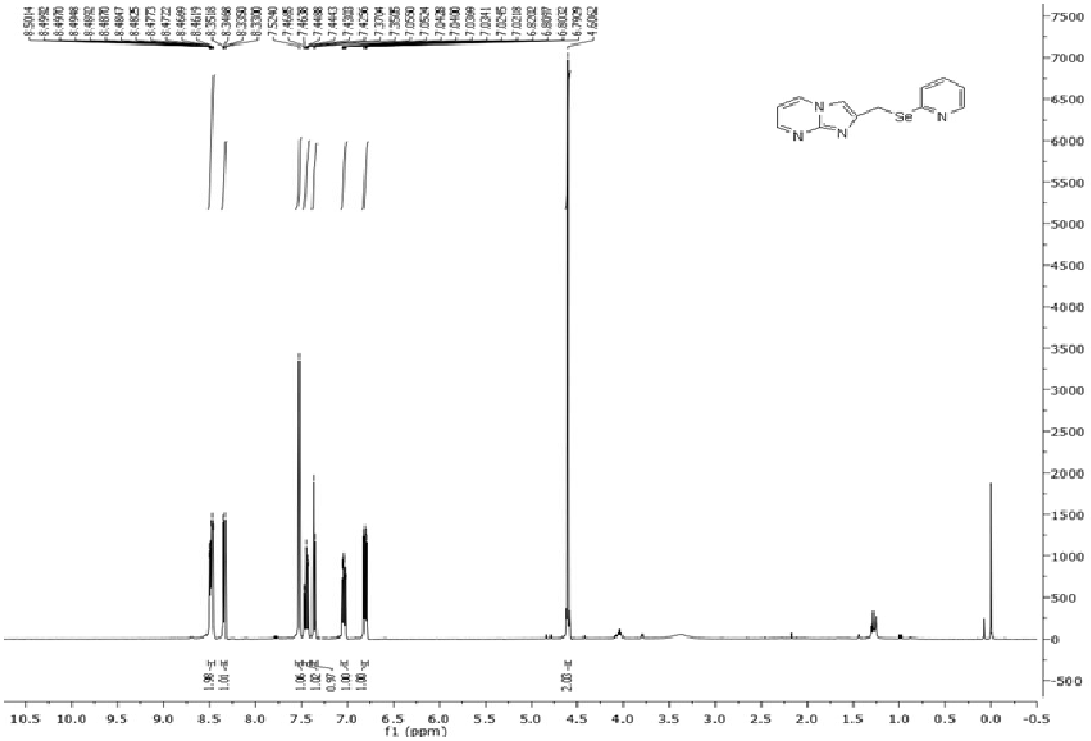

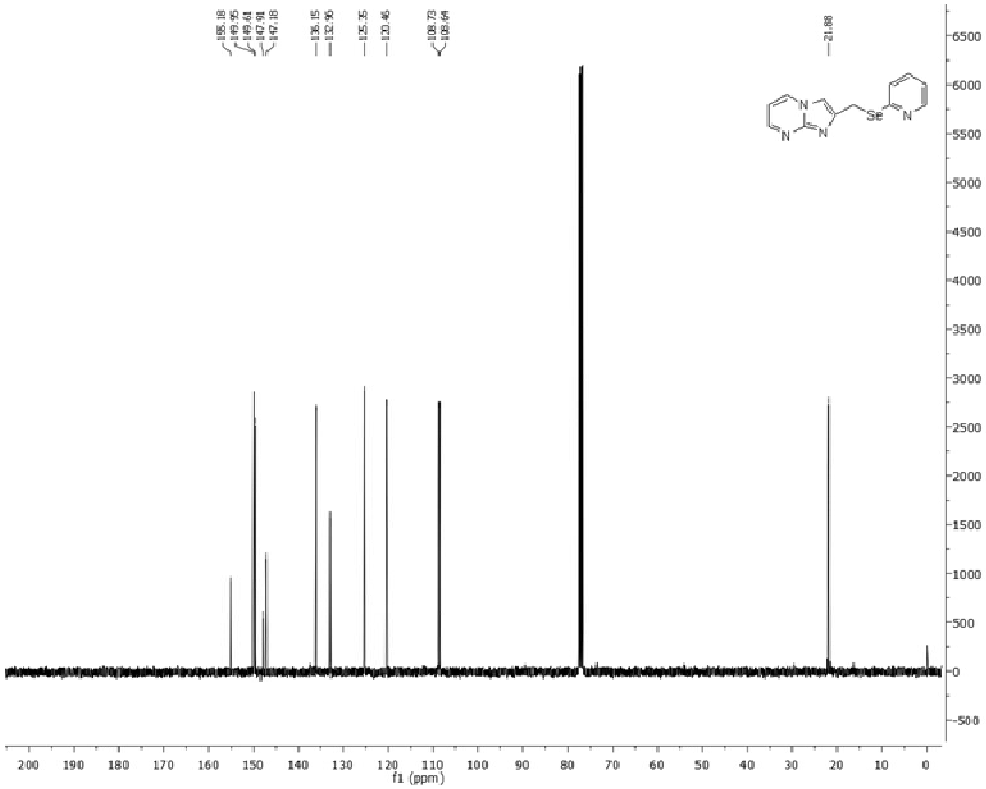

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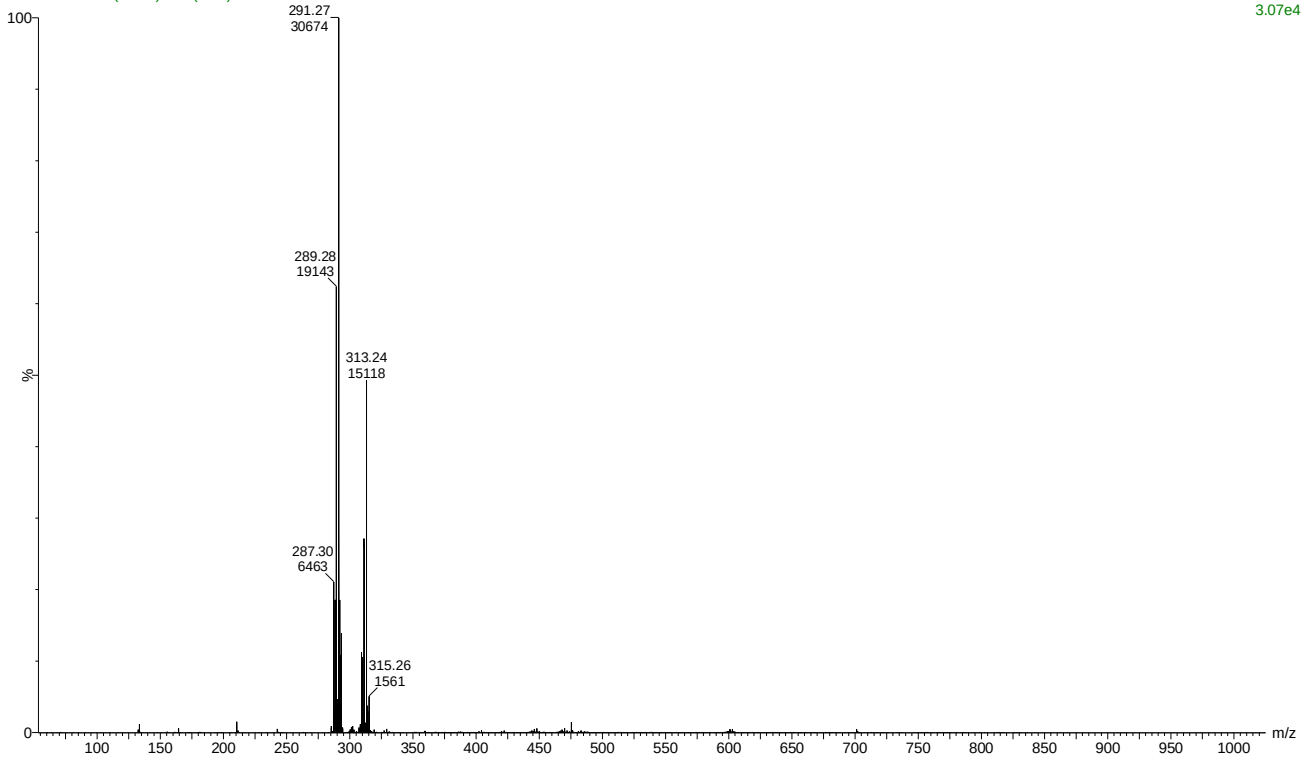
SAIF/CIL,PANJAB UNIVERSITY,CHANDIGARH
TOF MS ES+
3.07e4



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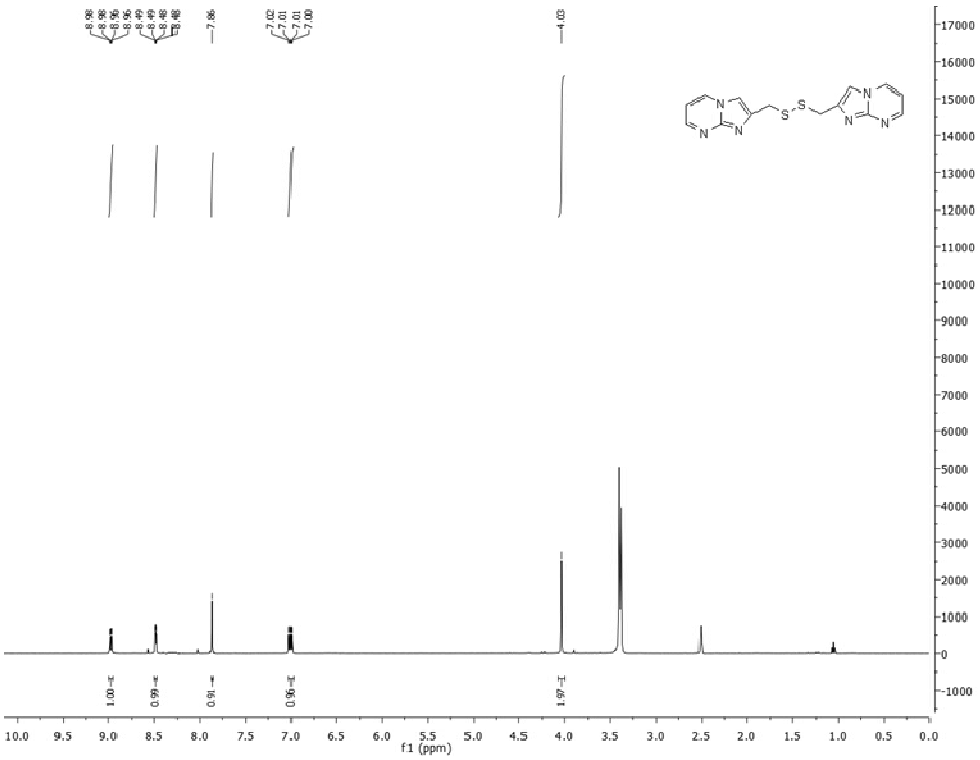
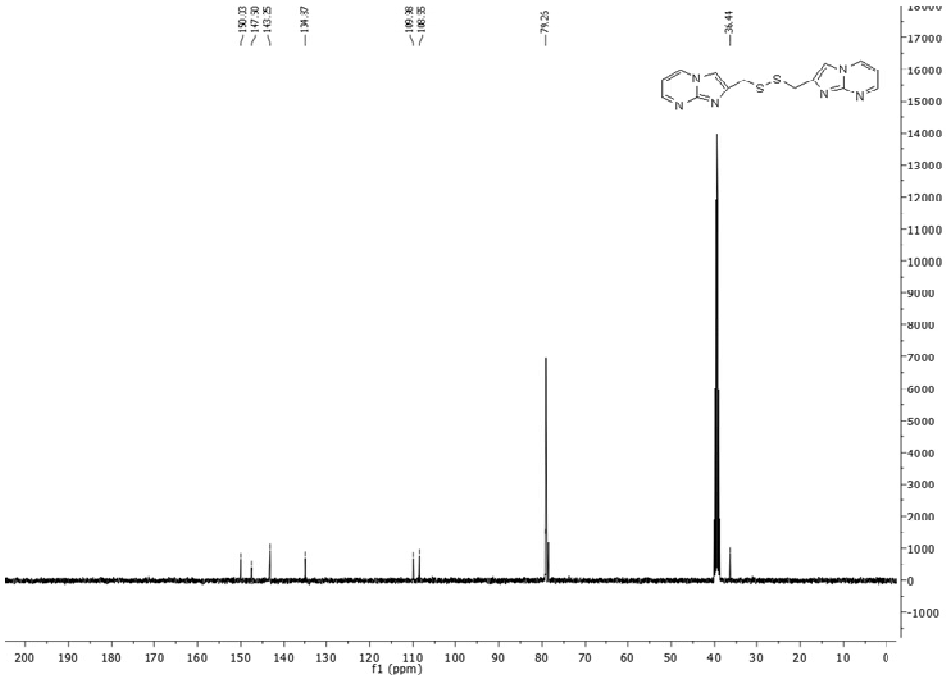
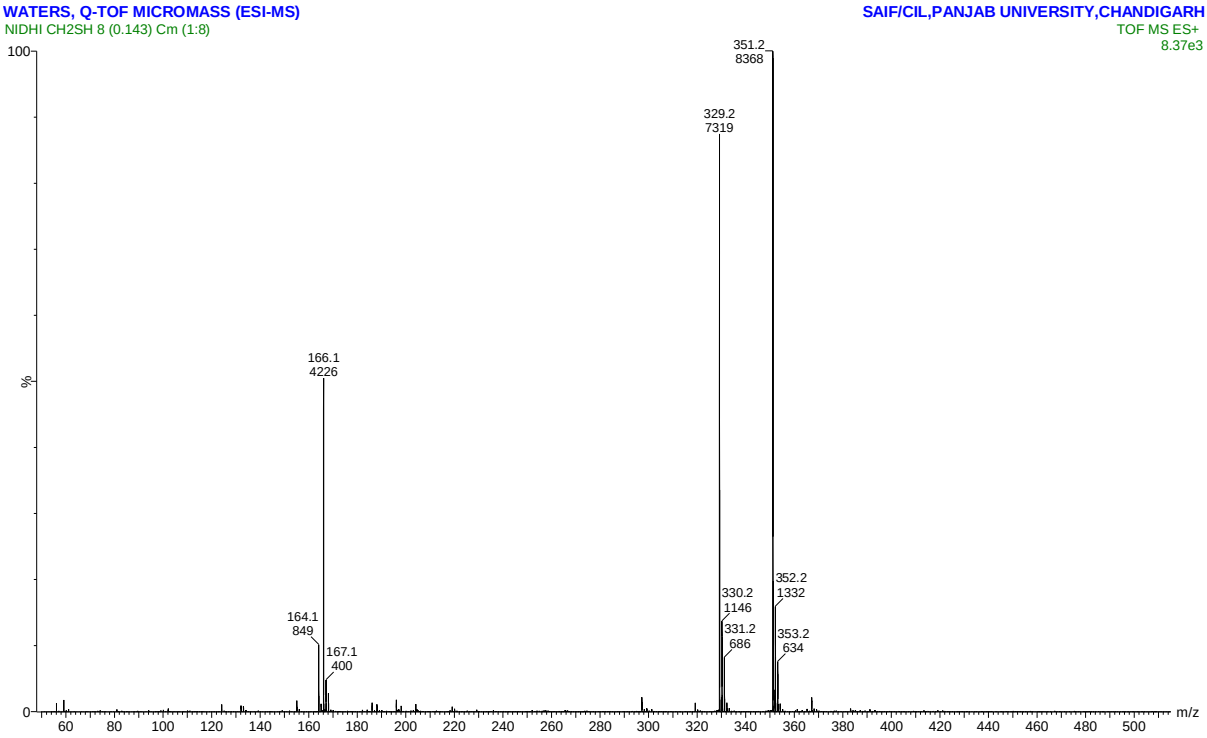
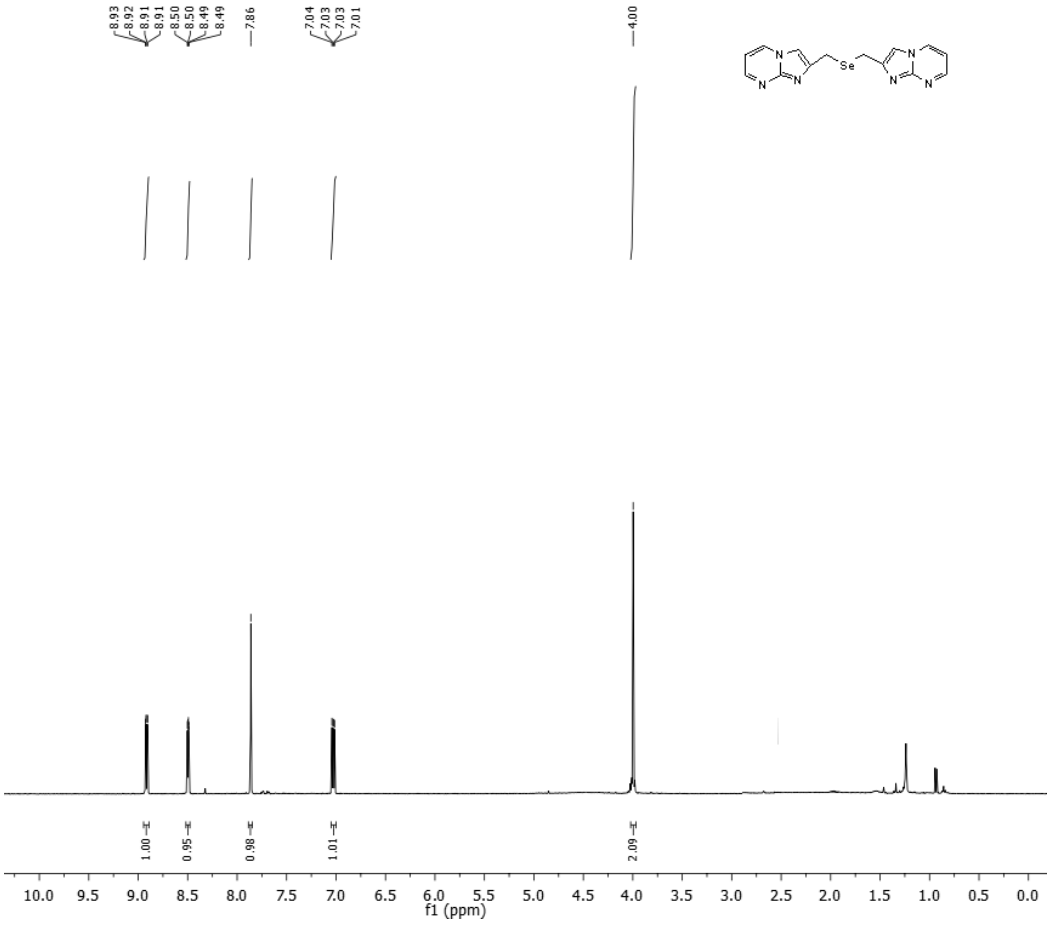
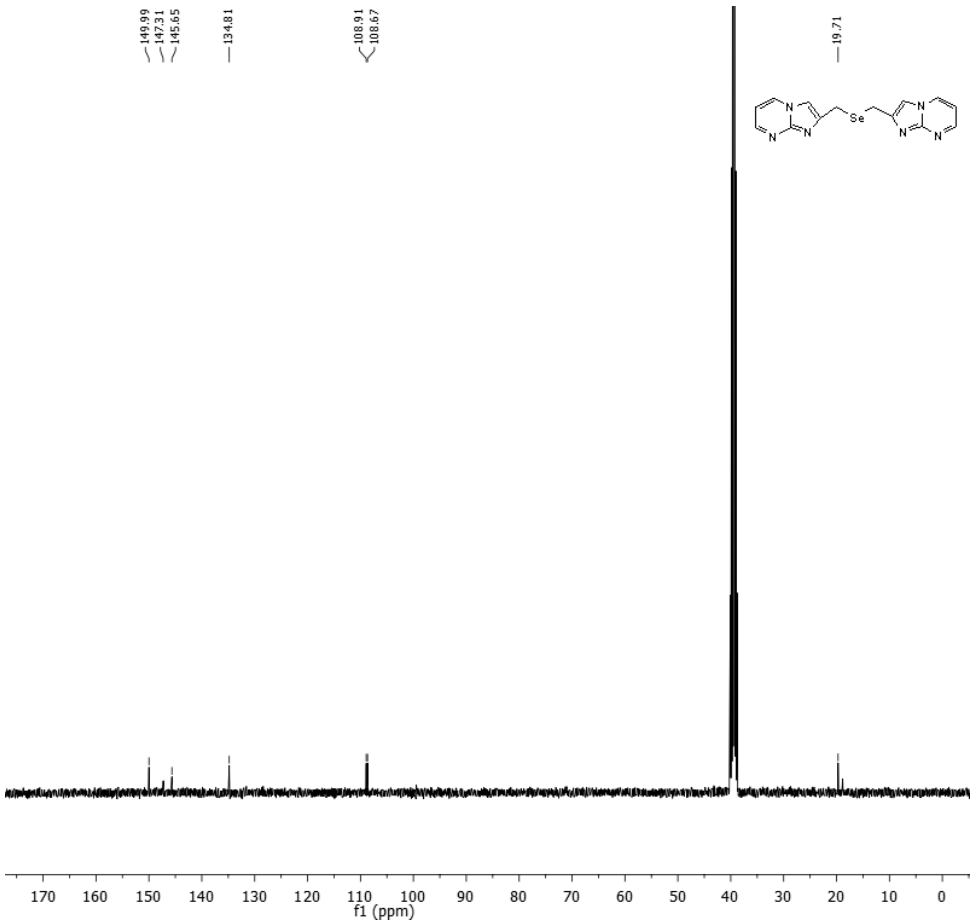






Bis(imidazo[1,2-a]pyrimidin-2-ylmethyl)selane (11) ^{1}H, ^{13}C, Mass Spectra



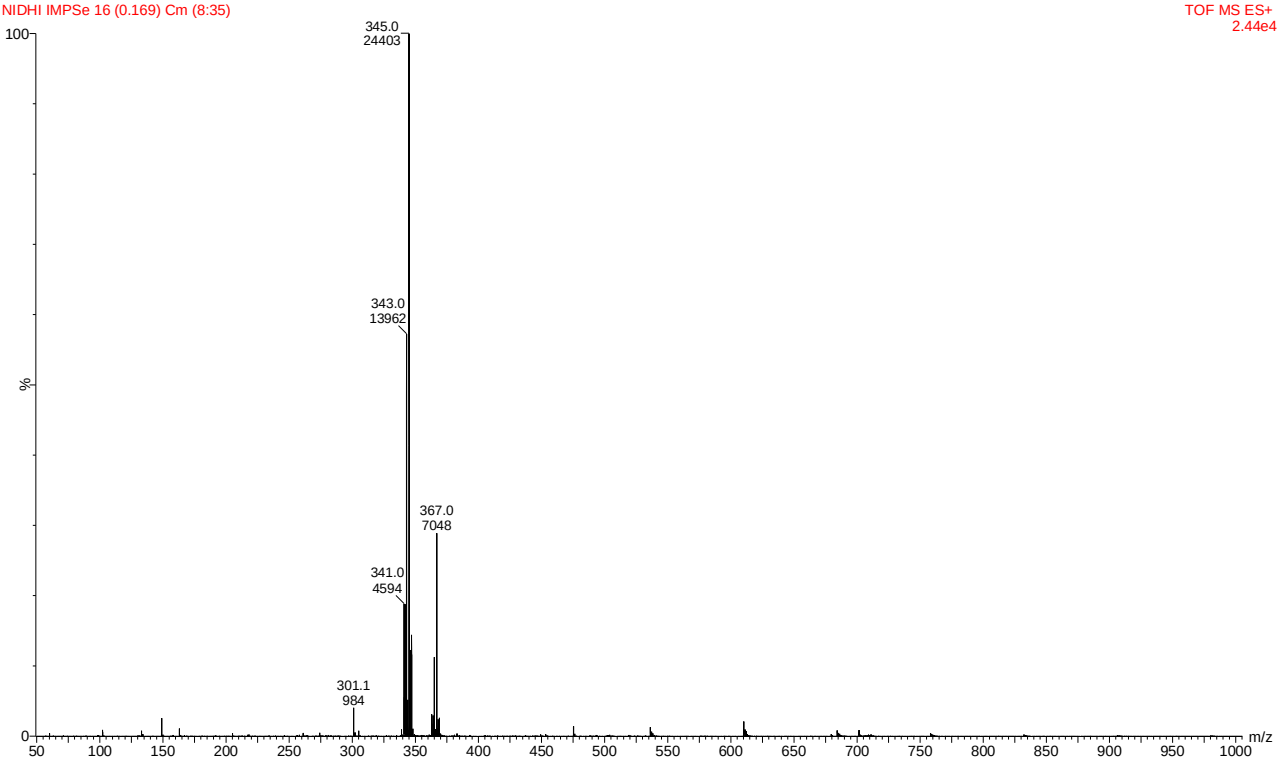


WATERS, Q-TOF MICROMASS (LC-MS)

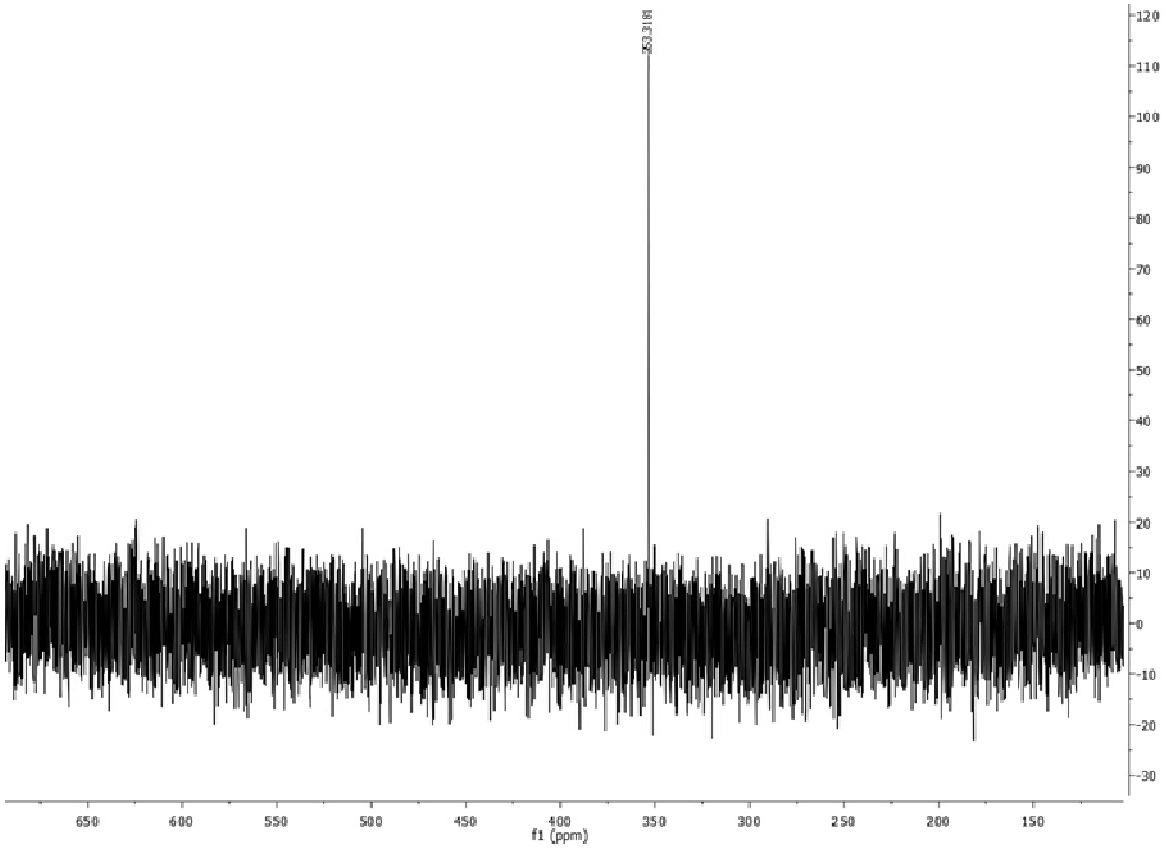
NIDHI IMPSe 16 (0.169) Cm (8:35)

SAIF/CIL,PANJAB UNIVERSITY,CHANDIGARH

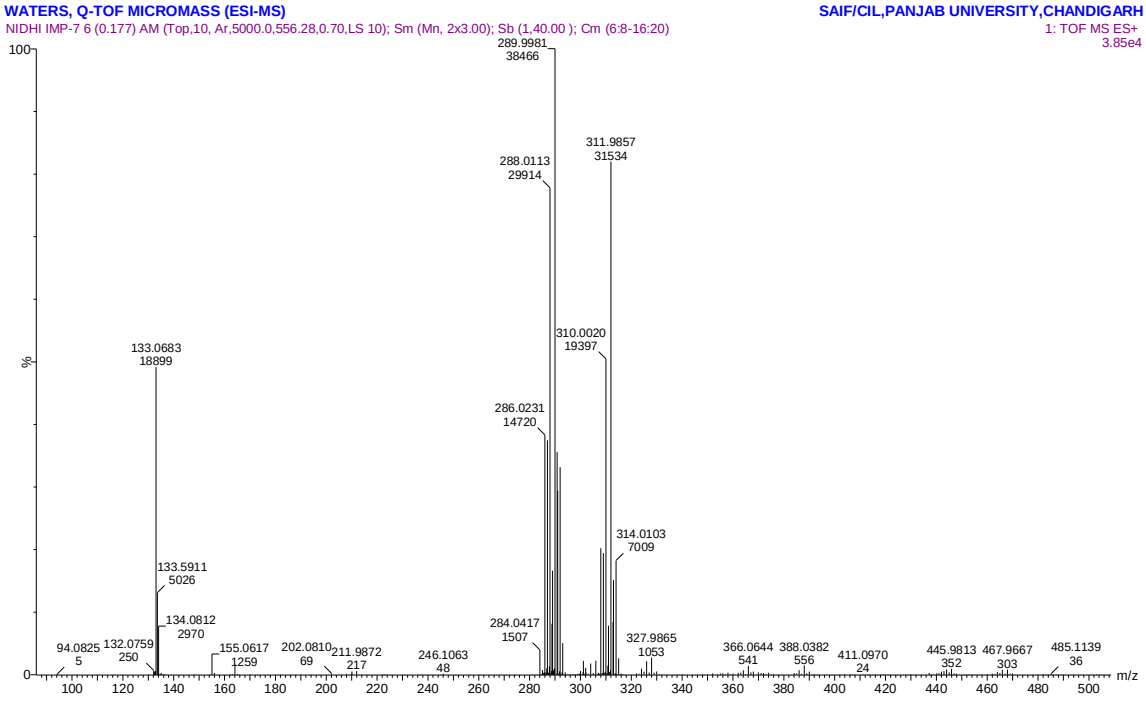
TOF MS ES+
2.44e4



2-((Phenylselanyl)methyl)imidazo[1,2-a]pyrimidine (6) ^{77}Se NMR



2-((Phenylselanyl)methyl)imidazo[1,2-a]pyrimidine (6) HRMS



2-((Tolylselanyl)methyl)imidazo[1,2-a]pyrimidine (7)

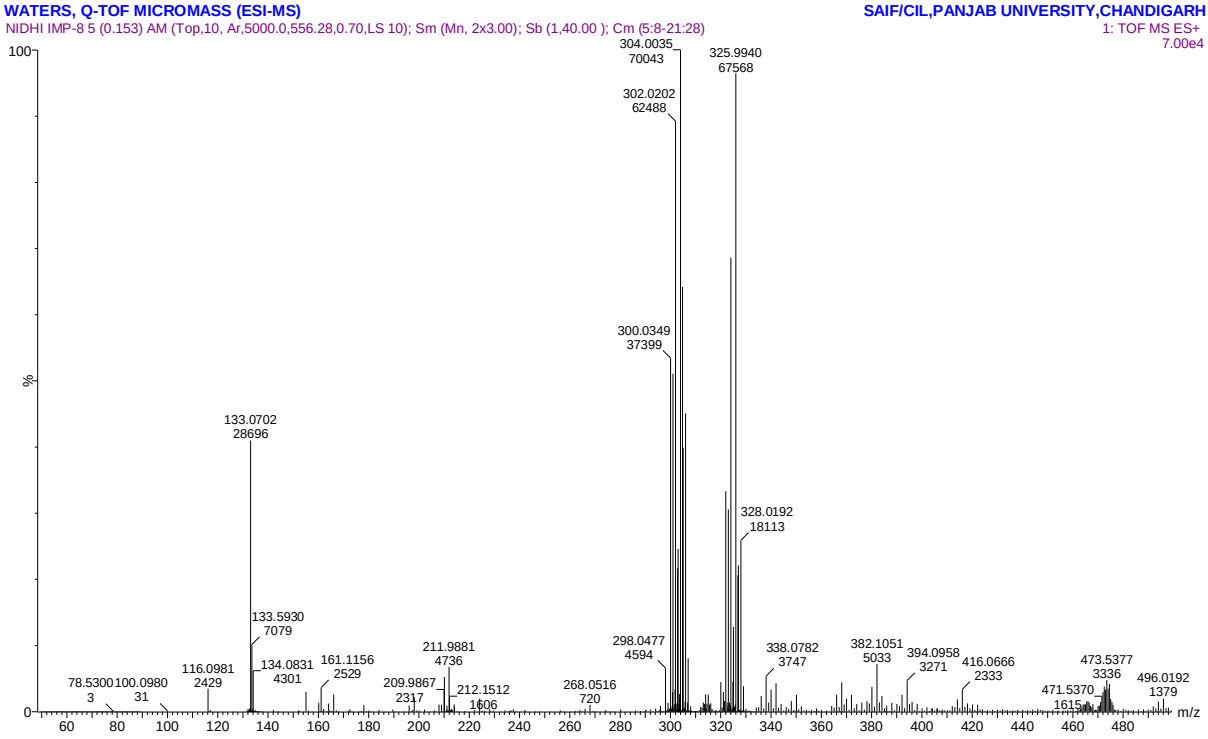


Table S1 Crystal data and structure refinement for **6**

Empirical formula	C13 H11 N3 Se
Formula weight	288.21
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal system	Trigonal
Space group	R -3
Unit cell dimensions	a = 31.935(2) Å, α= 90°
	b = 31.935(2) Å, β= 90°
	c = 6.3894(5) Å, γ = 120°
Volume	5643.3(9) $Å^3$
Z	18
Density (calculated)	1.526 g/cm^3
Absorption coefficient	2.974 mm^{-1}
F(000)	2592
Theta range for data collection	2.209 to 26.053°
Index ranges	-39<=h<=39, -39<=k<=39, -7<=l<=7
Reflections collected	27802
Independent reflections	2467 [R(int) = 0.0928]
Completeness to theta = 25.242°	99.5 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F2
Data / restraints / parameters	2467 / 0 / 154
Goodness-of-fit on F2	1.102
Final R indices [I>2sigma(I)]	R1 = 0.0442, wR2 = 0.1088
R indices (all data)	R1 = 0.0760, wR2 = 0.1186
Extinction coefficient	n/a
Largest diff. peak and hole	0.592 and -0.281 e $Å^{-3}$

Table S2 Selected bond lengths (Å), bond angles (^{0}) and torsional angles (^{0}) for compound **6**

Se1-C8	1.917	C8-C9	1.378
Se1-C1	1.966	C8-C13	1.383
N3-C3	1.371	C6-C5	1.402
N3-C4	1.372	C2-C1-Se1	113.100
N3-C7	1.391	C8-Se1-C1	101.280
N1-C7	1.316	C2-C3-H3	127.100
N1-C2	1.376	N3-C3-H3	127.100
N2-C6	1.318	C1-Se1-C8-C13	37.700
N2-C7	1.346	C1-Se1-C8-C9	-144.600
C2-C3	1.356	Se1-C8-C9-C10	-178.500
C5-C4	1.338	C8-Se1-C1-C2	68.500
C13-C12	1.368	N1-C2-C1-Se1	74.300
C9-C10	1.363	C3-C2-C1-Se1	-104.600
C12-C11	1.376	Se1-C8-C13-C12	178.700
C11-C10	1.384	C3-N3-C7-N1	-0.200
C2-C1	1.477	C3-N3-C7-N2	-179.100

Compound	Energy (a.u.)	Band gap (eV)	Se1/S1-C8 Bond length (Å)	Se1-C1 Bond length (Å)	C8-Se1-C1 Bond angle (^{0})	C8-Se1-C1-C2 Dihedral angle (^{0})
4	-990.6457	4.1676	1.840	1.850	100.53	-73.31
5	-1064.4399	3.9608	1.793	1.858	103.76	-99.03
6	-3065.6345	3.9197	1.920	2.000	99.70	-101.40
7	-3104.9527	3.8906	1.925	2.000	99.74	-101.13
8	-3183.5905	3.9017	1.930	2.000	99.63	-109.90
9	-3081.6726	4.2019	1.920	1.972	101.30	-70.19
10	-3268.5440	3.5740	1.940	1.940	109.40	-60.00
11	-1665.5157	3.5541	1.780	1.780	-	-

Table S3 Calculations of theoretical parameters using density functional theory (DFT)

Table S4 Optimized structures of compounds **4**-**11** with DFT

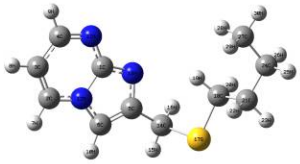
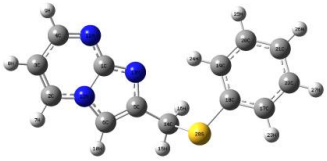
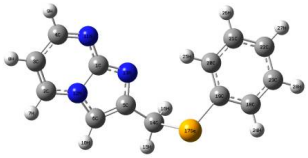
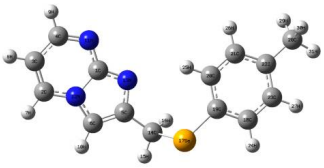
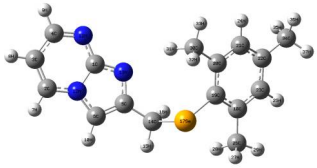
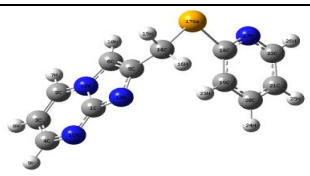
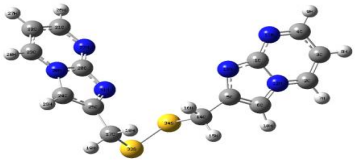
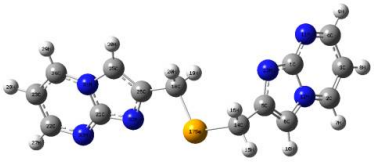
Compound	Optimized structure
4	
5	
6	
7	
8	
9	
10	
11	

Fig. S1 HOMO-LUMO diagrams of compounds **4**-**11**

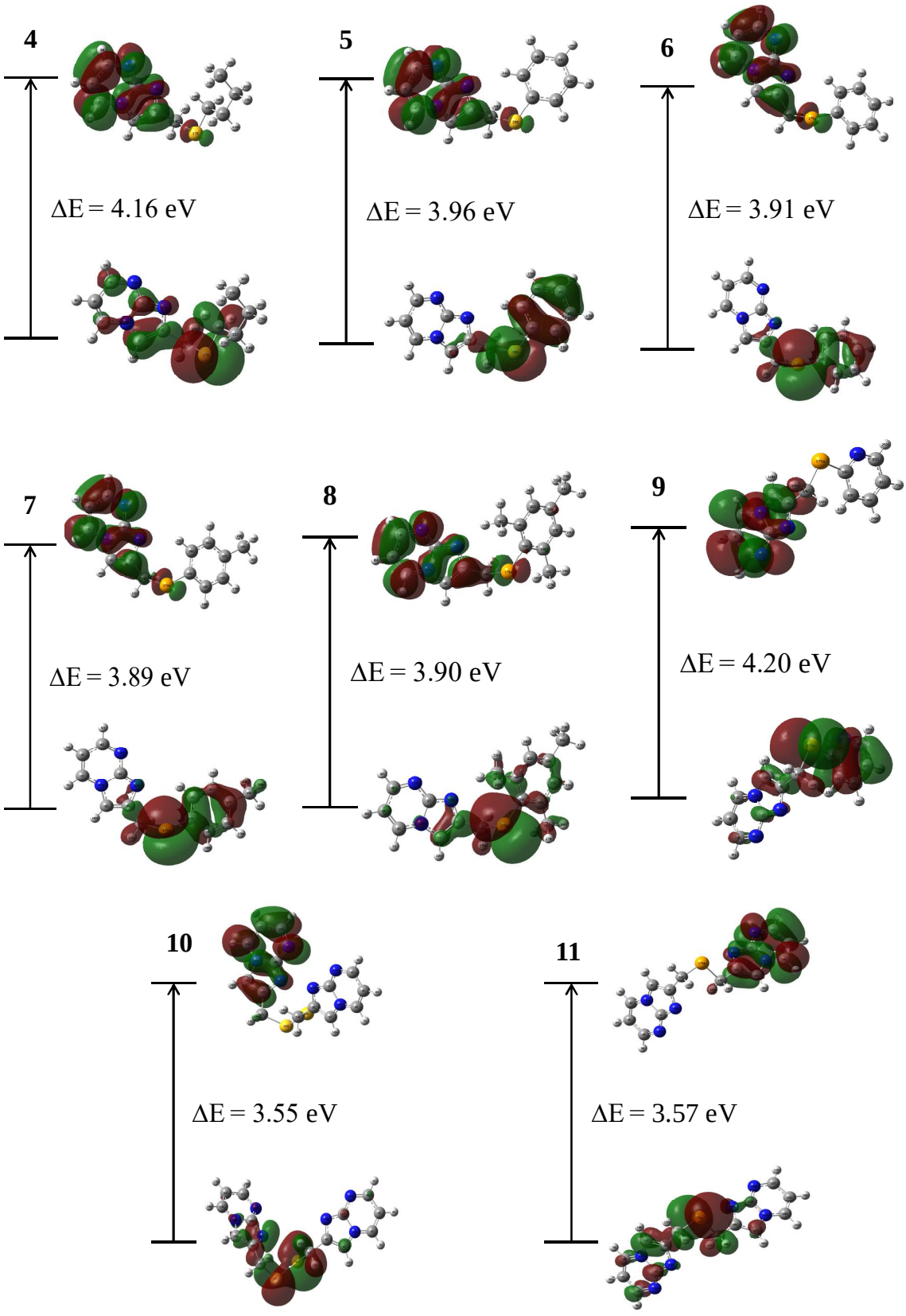


Table S5 MIC values of compounds **4**-**11** and standard antifungal agent (Amp B) against various fungal stains (in ug/ml)[a]

Compound	*Candida albicans*	*Candida glabrata*	*Candida tropicals*	*Candida krusei*	*Candida parapsolisis*	*Candida kyfer*	*Cryptococcus neoformans*	*Aspergillus niger*	*Neurospora crassa*
4	>27.62	>27.62	>27.62	>27.62	>27.62	>27.62	>27.62	NT	NT
5	>30.12	>30.12	>30.12	>30.12	>30.12	>30.12	>30.12	NT	NT
6	**36.00**	>36.00	>36.00	>36.00	>36.00	>36.00	>36.00	>36.00	**18**
7	>37.75	>37.75	>37.75	>37.75	>37.75	**18.87**	>37.75	**37.75**	**18.87**
8	>41.25	NT	NT	NT	NT	>41.25	>41.25	>41.25	**20.62**
9	>36.12	NT	NT	NT	NT	>36.12	>36.12	>36.12	**18.06**
10	>42.87	NT	NT	NT	NT	>42.87	>42.87	>42.87	>42.87
11	NT	NT	NT	NT	NT	NT	NT	NT	NT
Amp B	0.78	-	-	-	-	12.50	0.20	0.39	0.39

[a]NT = Not Tested

Table S6 MIC values of compounds **4**-**11** and standard antibacterial agent (RIF) against various bacterial strains (in µg/ml)

Compounds	*Escherichia coli*	*Staphylococcus aureus*	*Vibrio cholera*	*Enterococcus faecalis*	*Listeria monocytogens*
4	>27.62	>27.62	>27.62	>27.62	>27.62
5	>30.12	>30.12	>30.12	>30.12	>30.12
6	>36.00	>36.00	>36.00	>36.00	>36.00
7	**18.87**	>37.75	>37.75	**37.75**	>37.75
8	>41.25	>41.25	>41.25	>41.25	>41.25
9	>36.12	>36.12	>36.12	>36.12	>36.12
10	>42.87	>42.87	>42.87	>42.87	42.87
11	NT	NT	NT	NT	NT
RIF	4.00	-	-	12.50	78.80