Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting information

Thioester-appended organosilatranes: Synthetic investigations and application in the modification of magnetic silica surface

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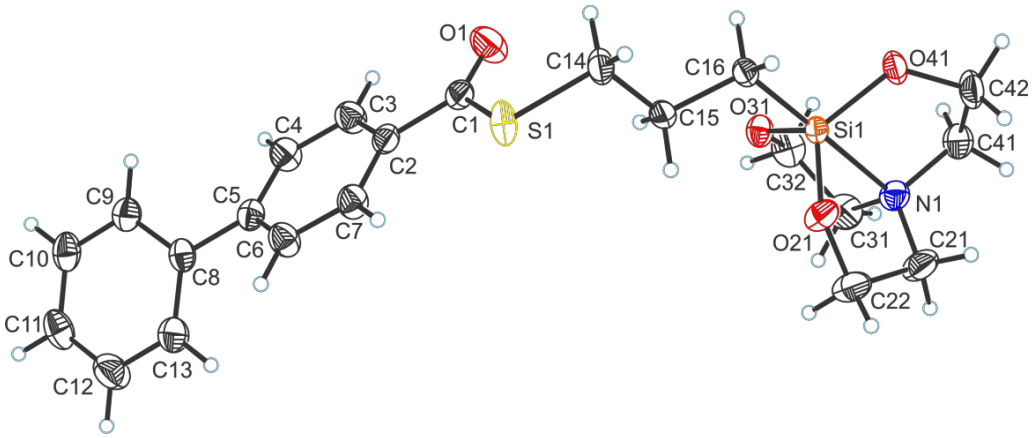


Fig. S1 ORTEP showing the crystal structure of ***3c*** with displacement ellipsoids drawn at the 20% probability level, selected atoms are labeled.

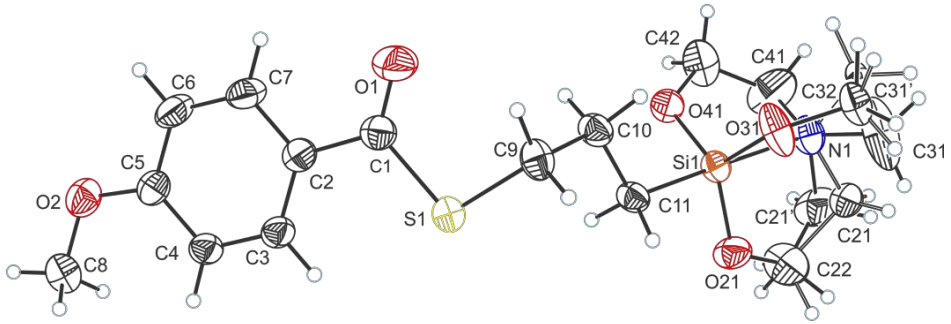


Fig. S2 ORTEP showing the crystal structure of ***3f*** with displacement ellipsoids drawn at the 30% probability level, selected atoms are labeled.

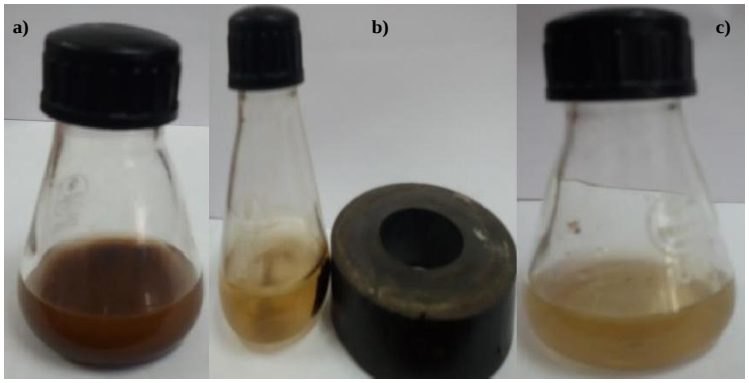


Fig. S3 Digital photographs of aqueous dispersions of hybrid nanoparticles (a); in the presence of external magnet (b); after magnetic separation (c)

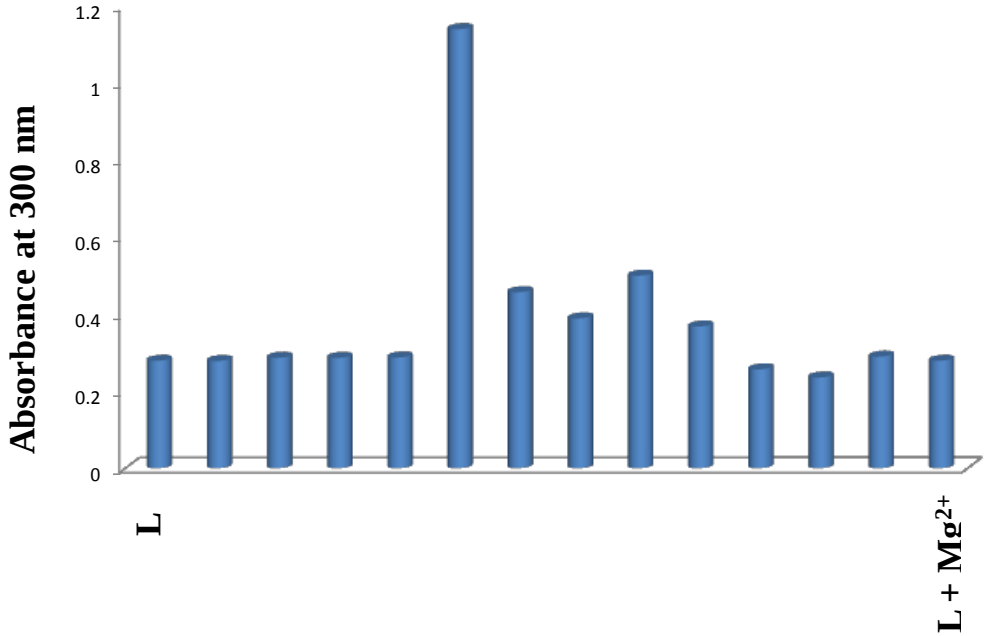


Fig. S4 Chemosensing activity of probe Fe_3O_4@SiO_2@silatrane (L) towards different cationic species (20 equiv.) in acetonitrile

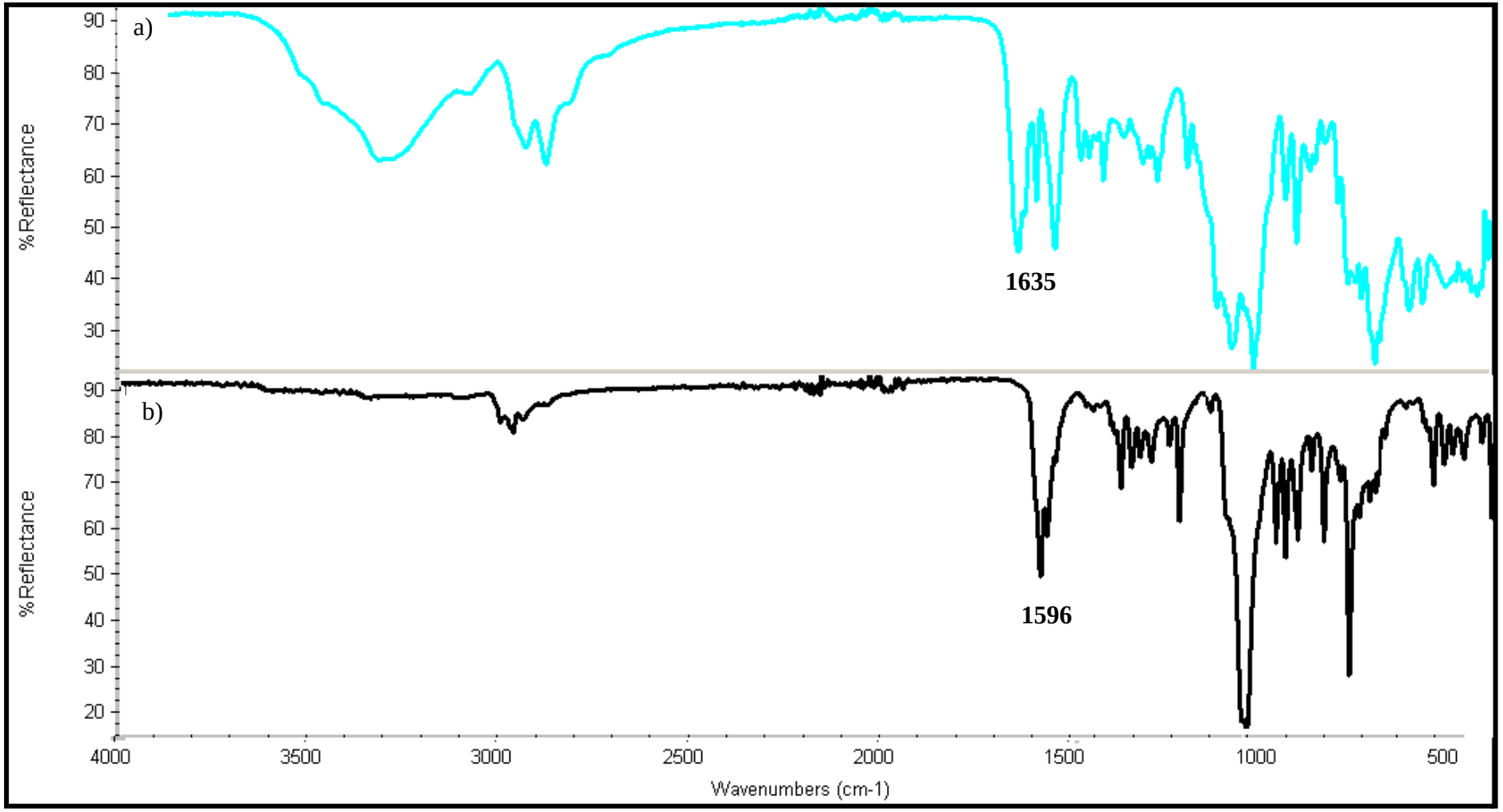


Fig. S5 IR spectra of **3g** (a) and **3g** + Cu^{2+} (b)

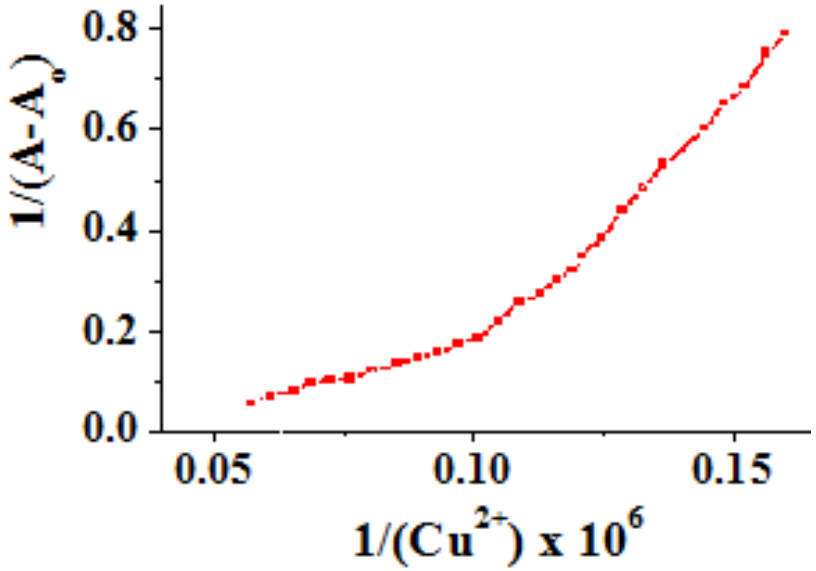


Fig. S6 B-H plot for 1:1 complexation between hybrid nanomaterial and Cu^{2+} at 300 nm

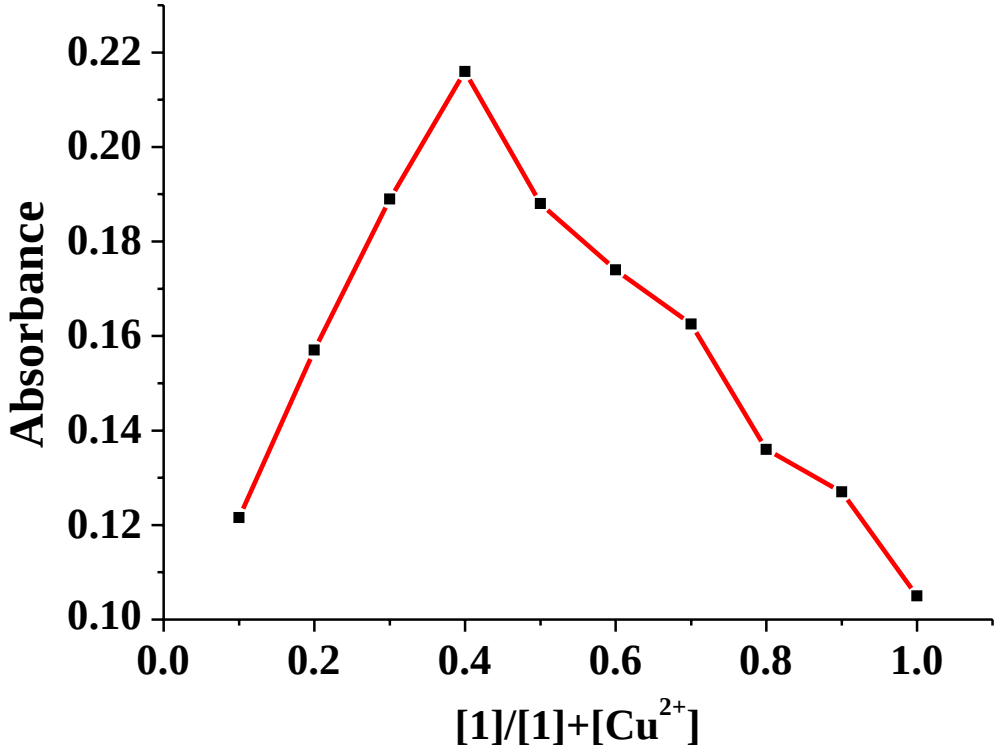


Fig. S7 Job's Plot for the determination of stoichiometry of complexes of the hybrid nanomaterial (1) with Cu^{2+}

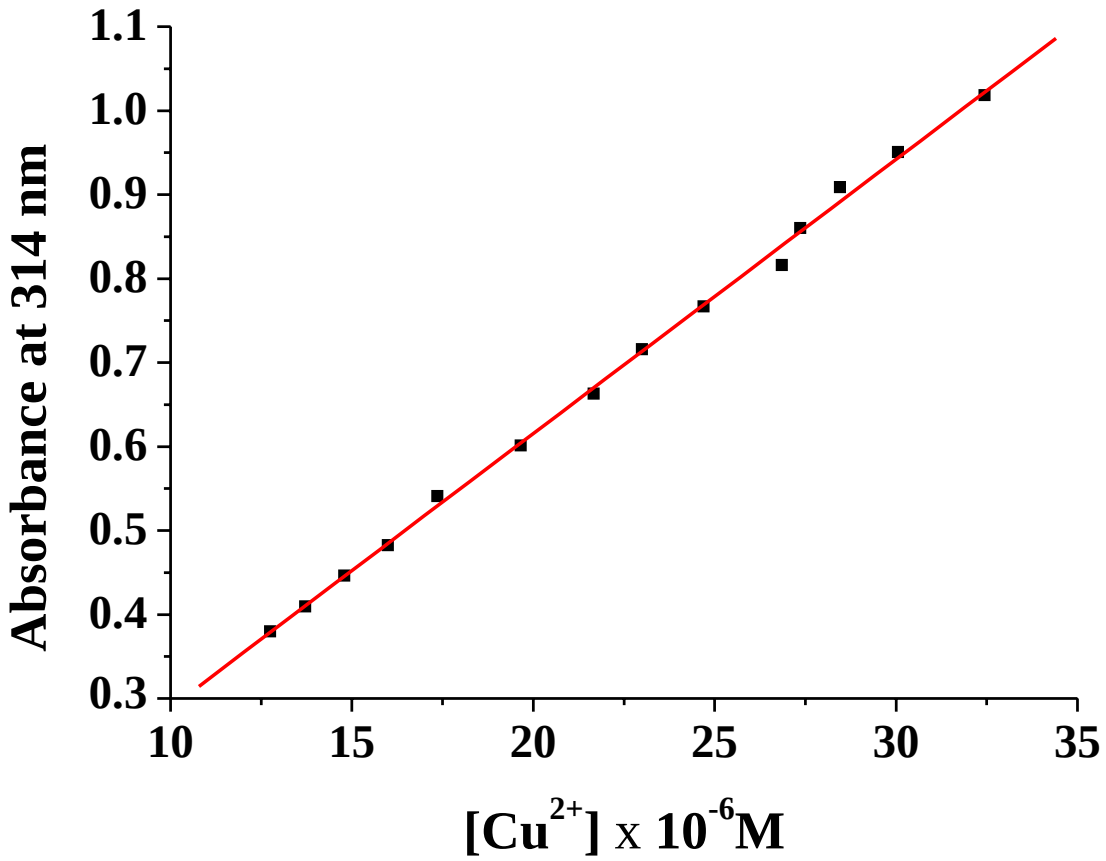


Fig. S8 Variation of absorbance with increase in Cu (II) concentration

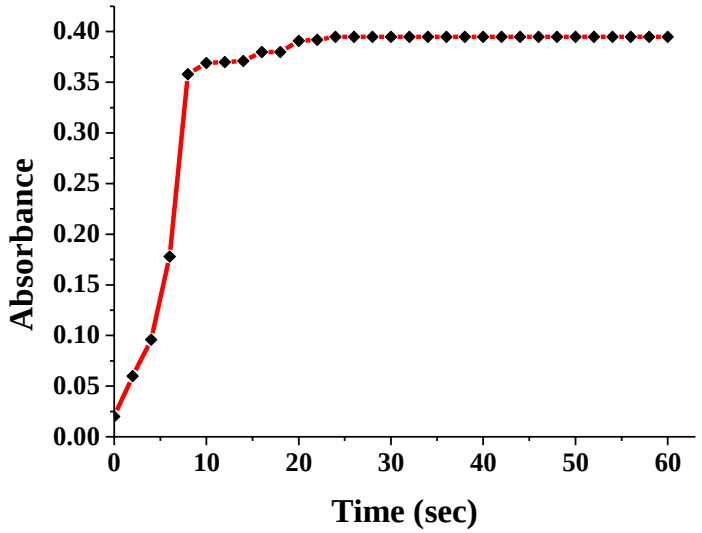


Fig. S9 Reaction-time profile of hybrid nanomaterial with Cu^{2+}

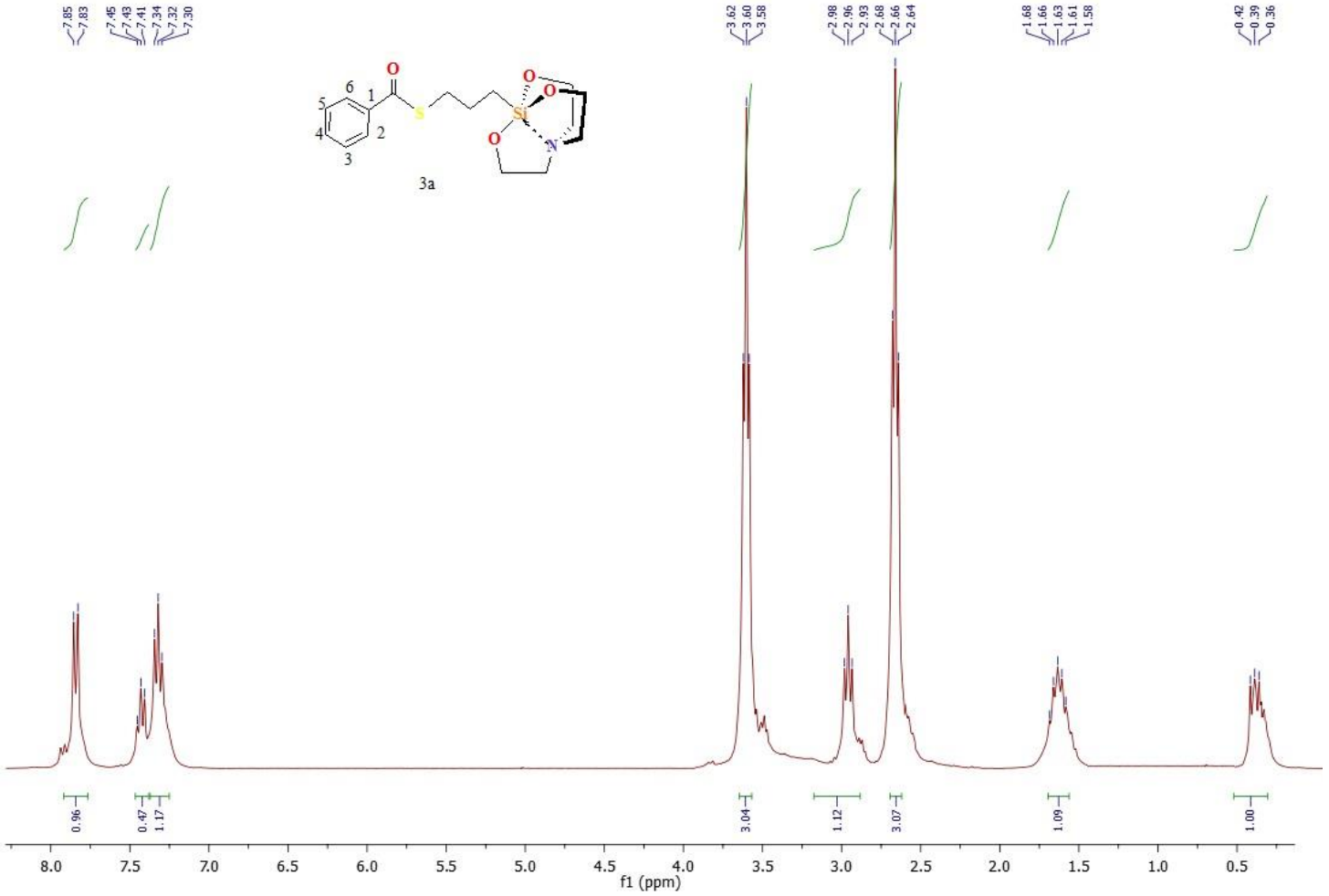


Fig. S10 ^{1}H NMR spectrum of **3a**

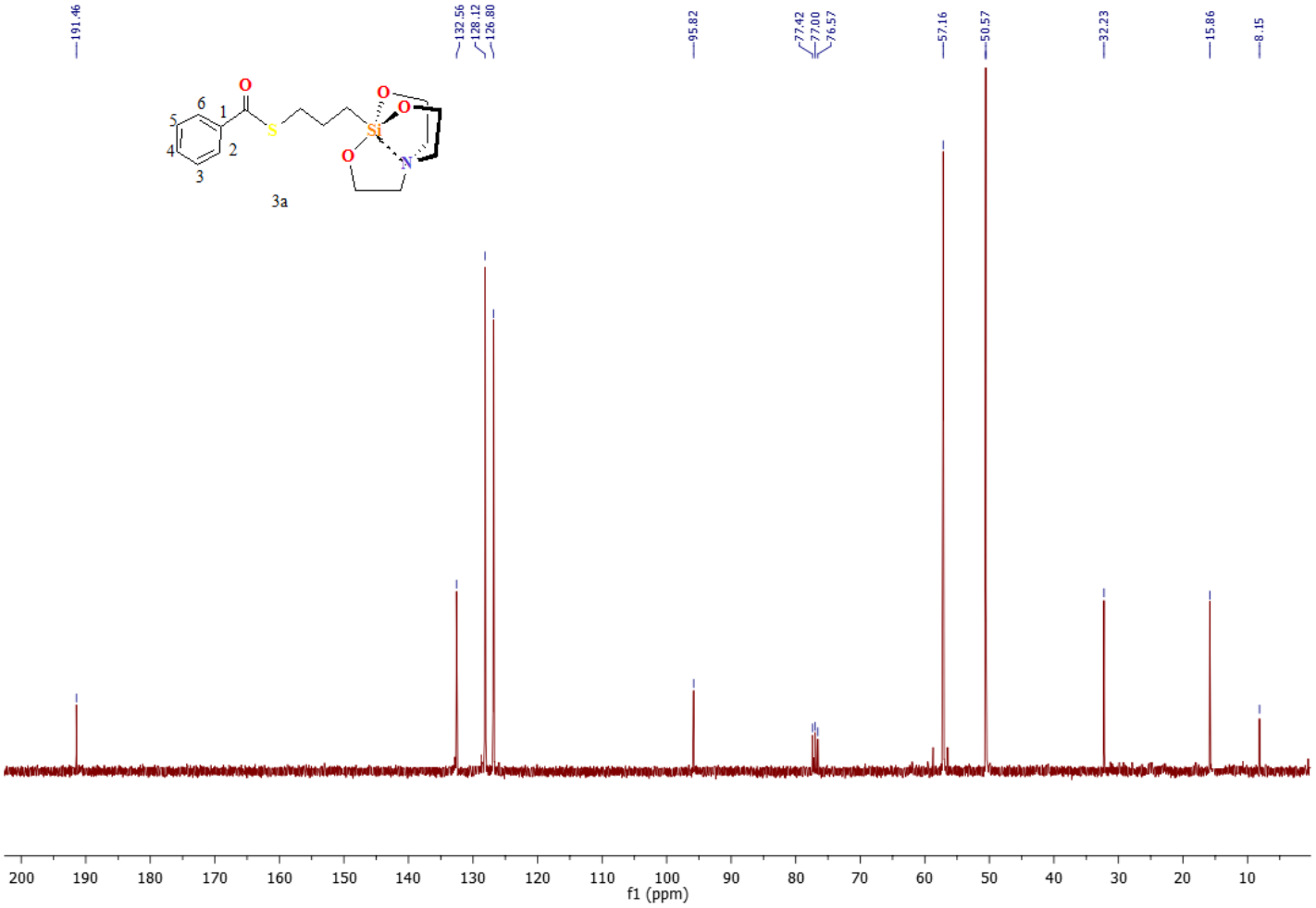


Fig. S11 ^{13}C NMR spectrum of **3a**

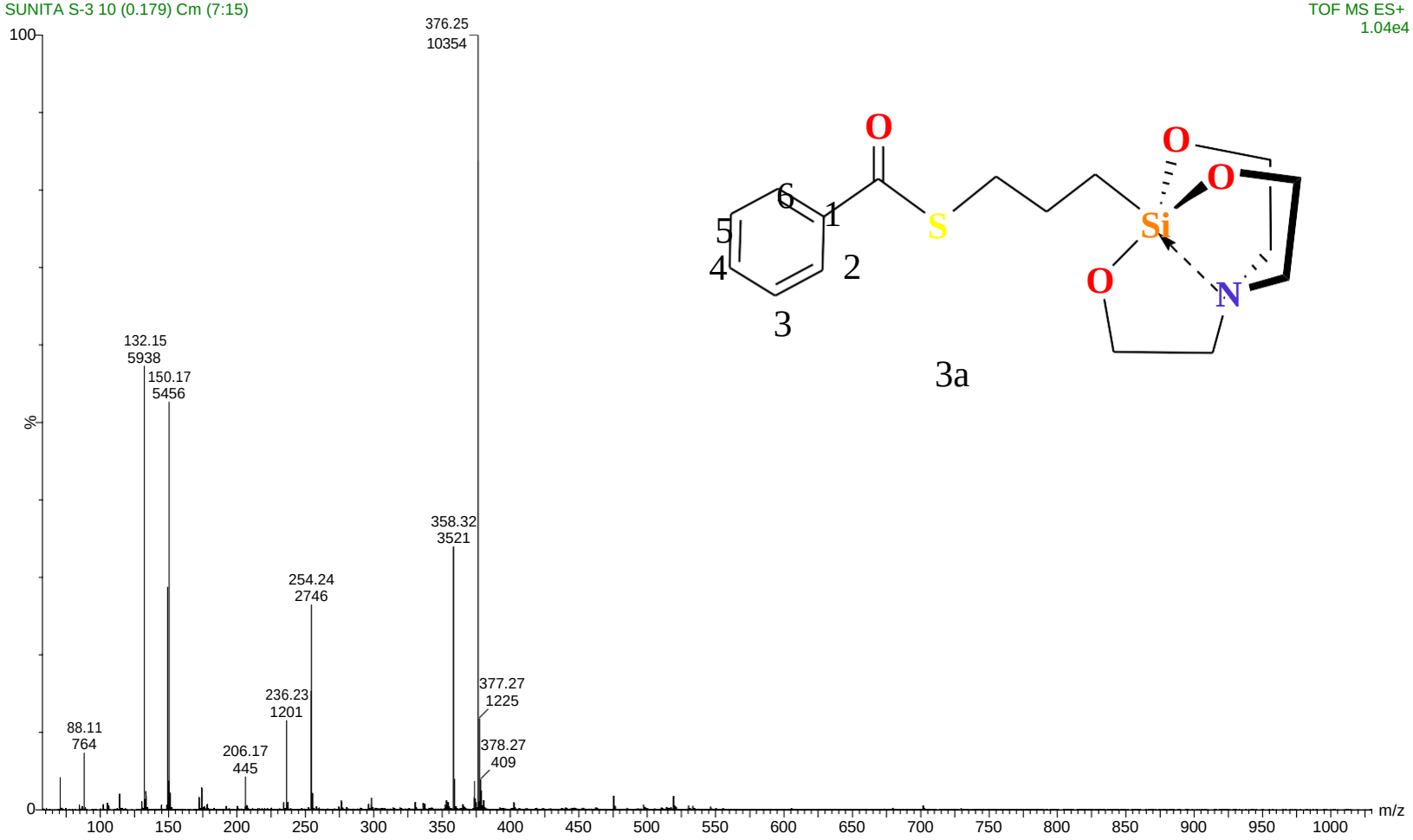


Fig. S12 Mass spectrum of **3a**

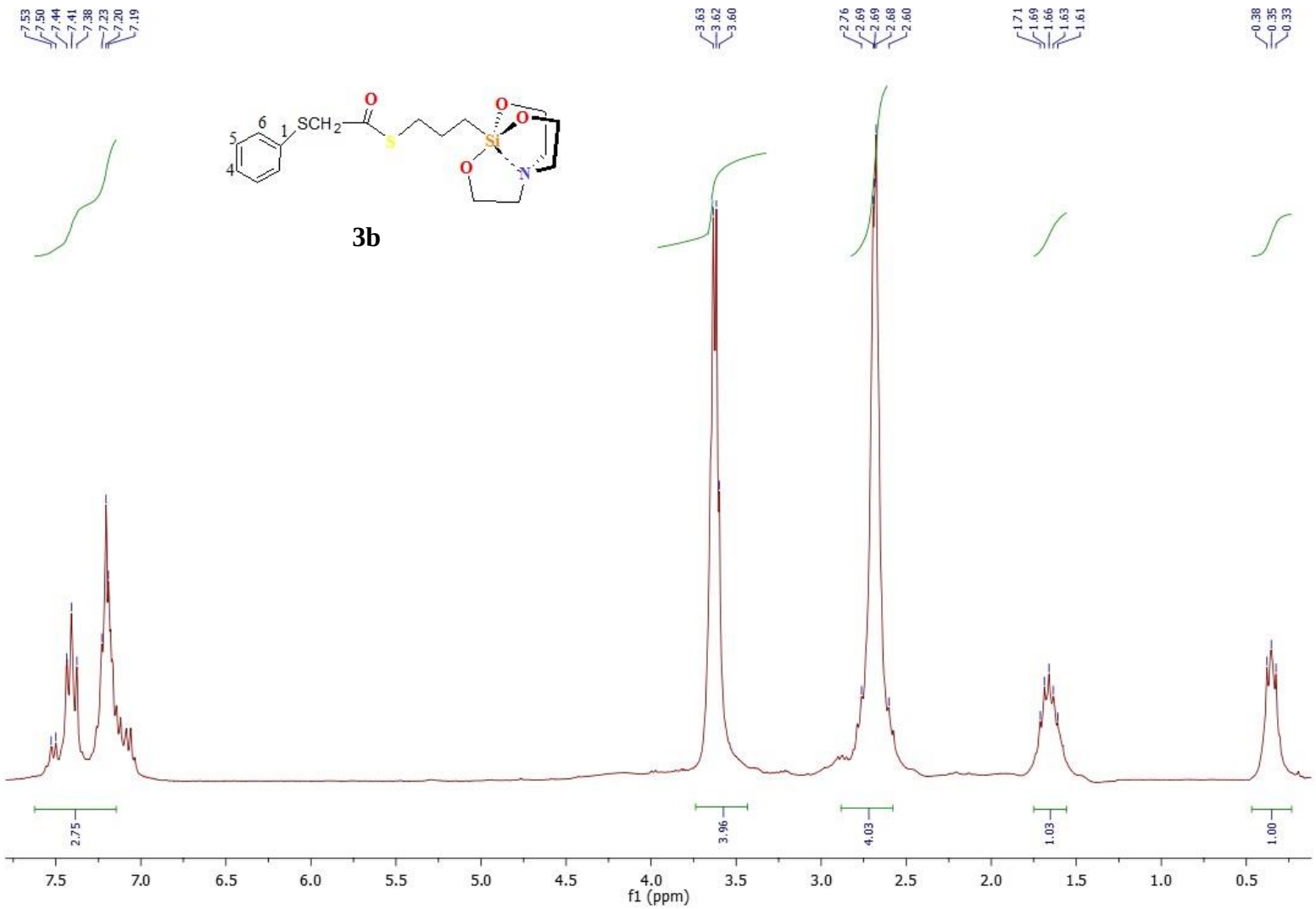


Fig. S13 ^{1}H NMR spectrum of **3b**

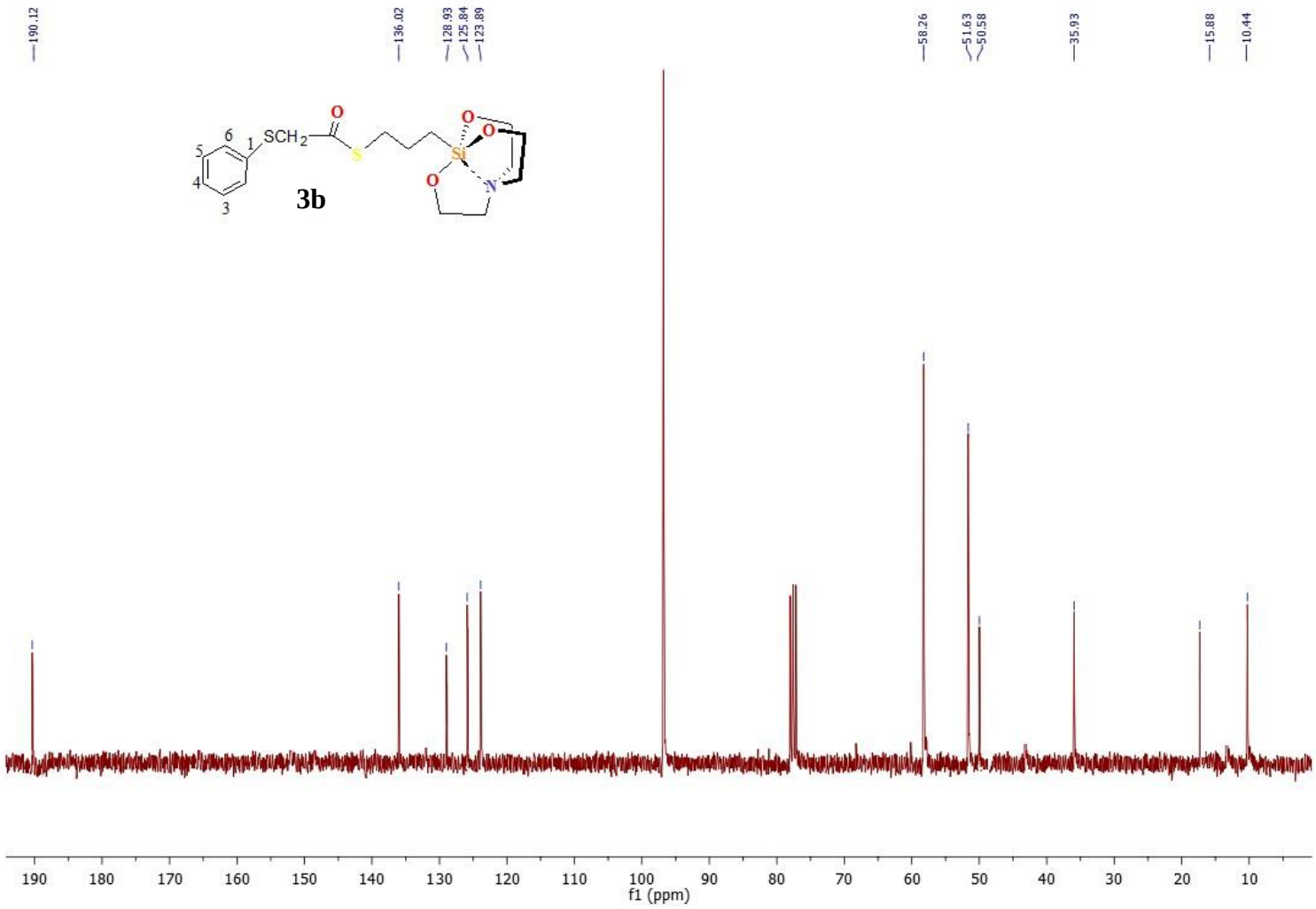


Fig. S14 ^{13}C NMR spectrum of **3b**

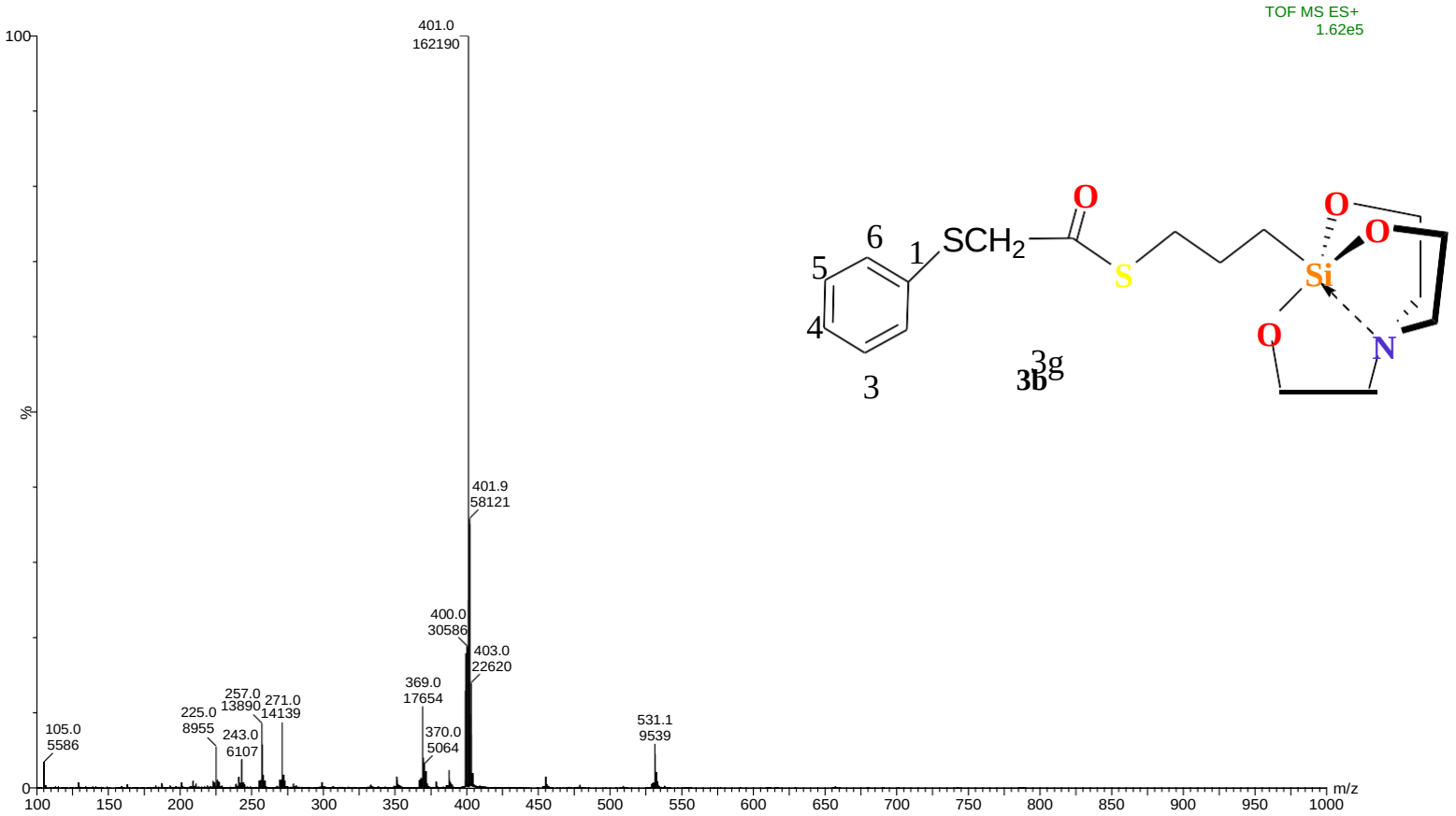


Fig. S15 Mass spectrum of **3b**

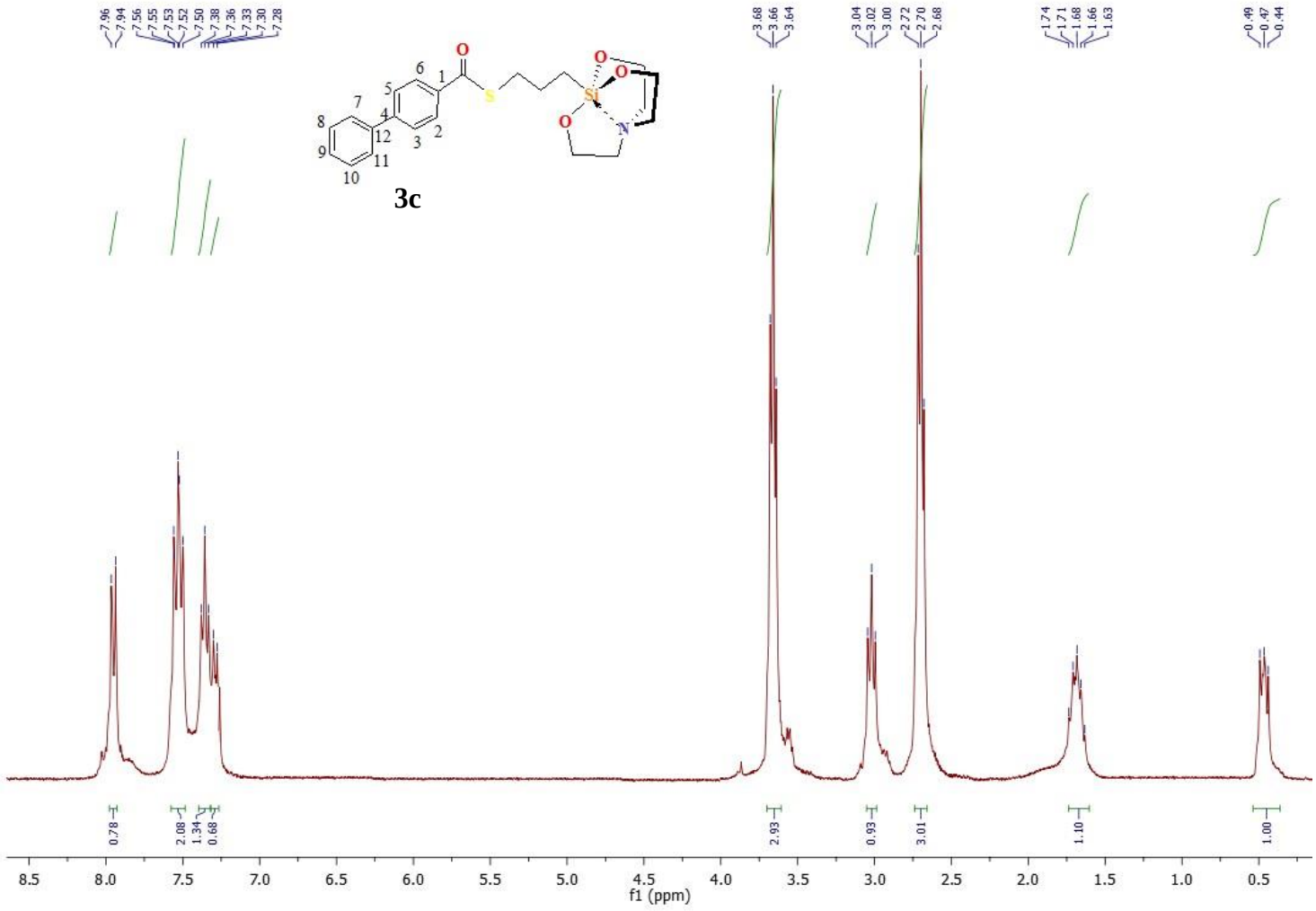


Fig. S16 ^{1}H NMR spectrum of **3c**

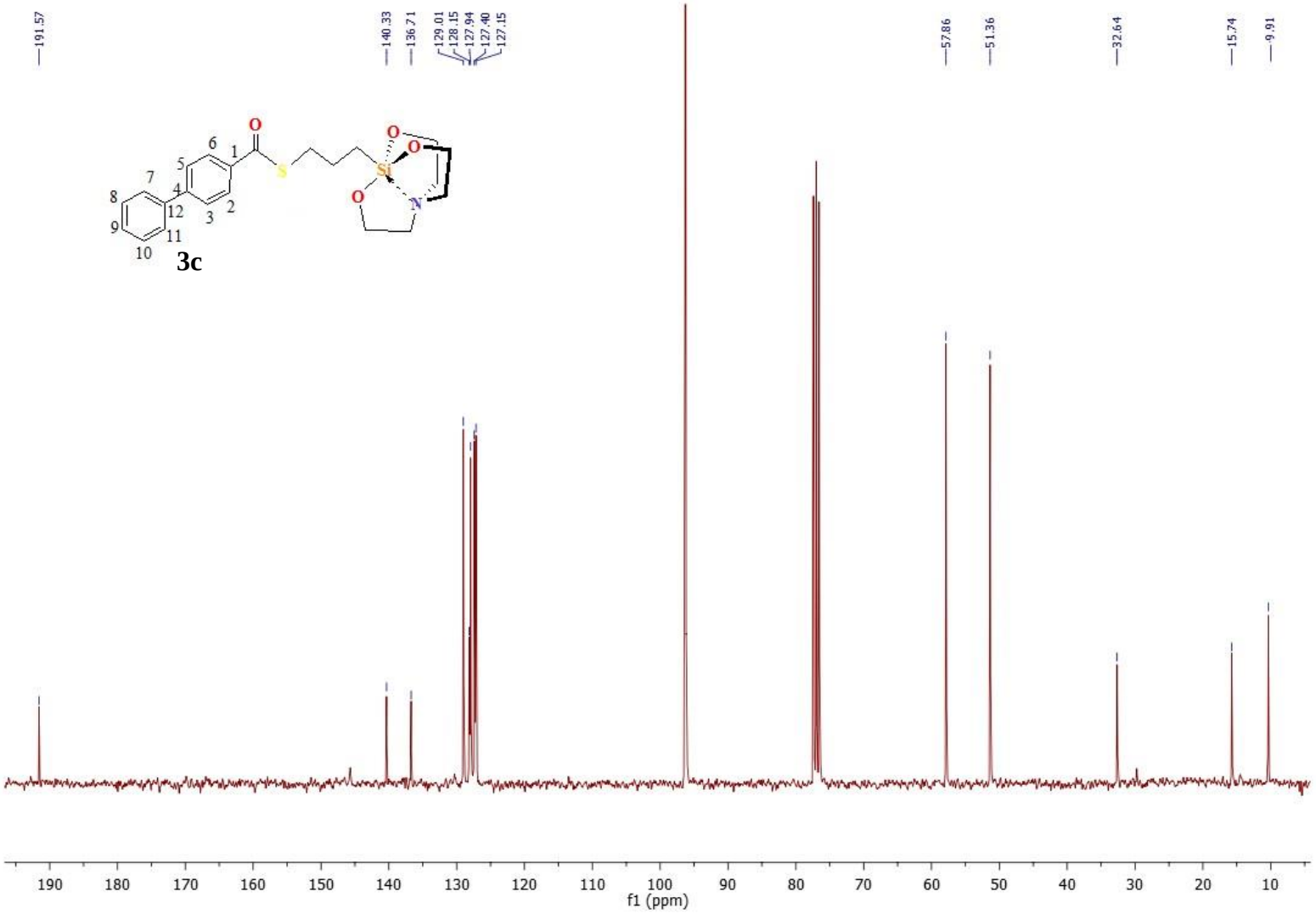


Fig. S17 ^{13}C NMR spectrum of **3c**

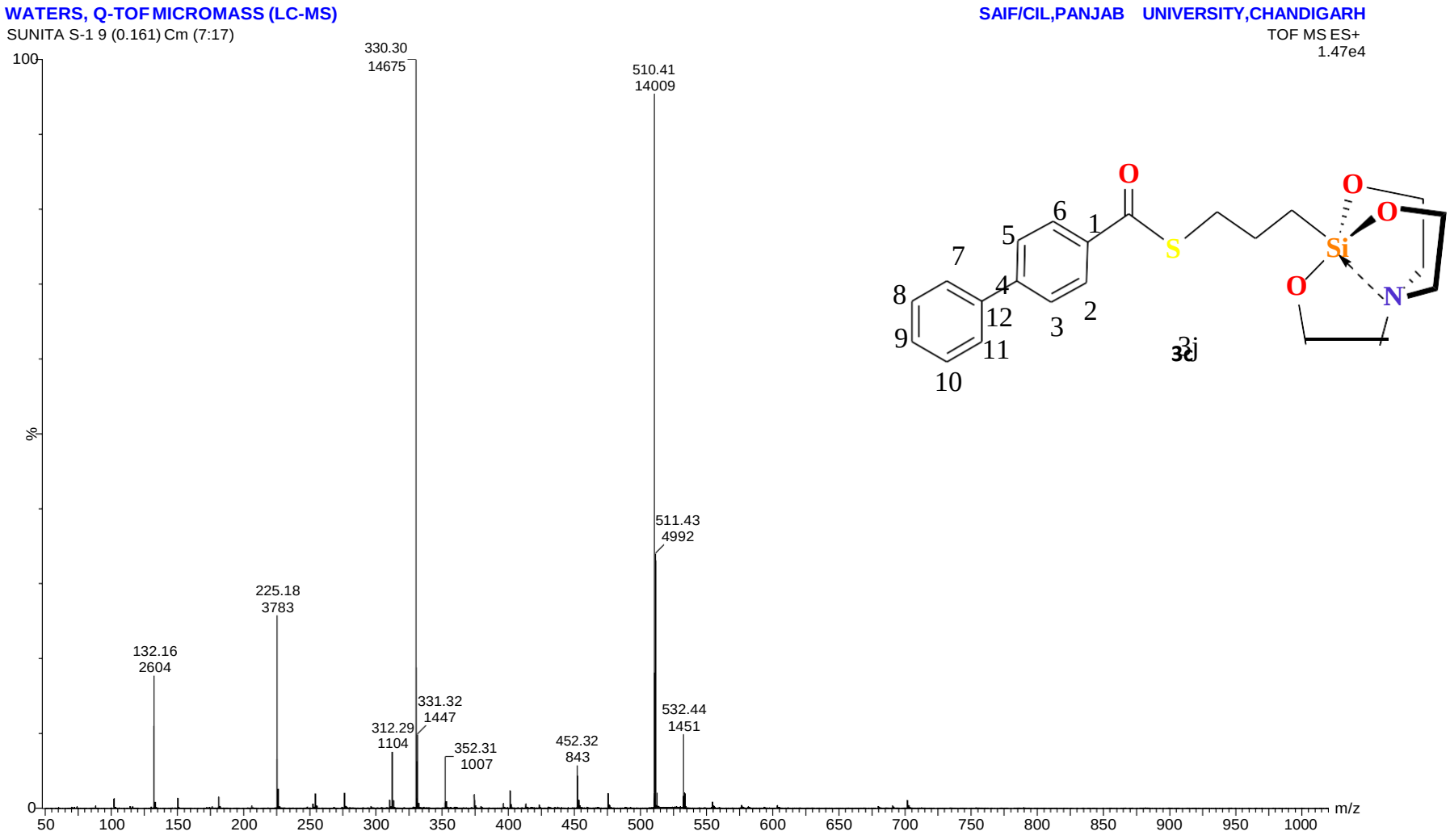


Fig. S18 Mass spectrum of **3c**

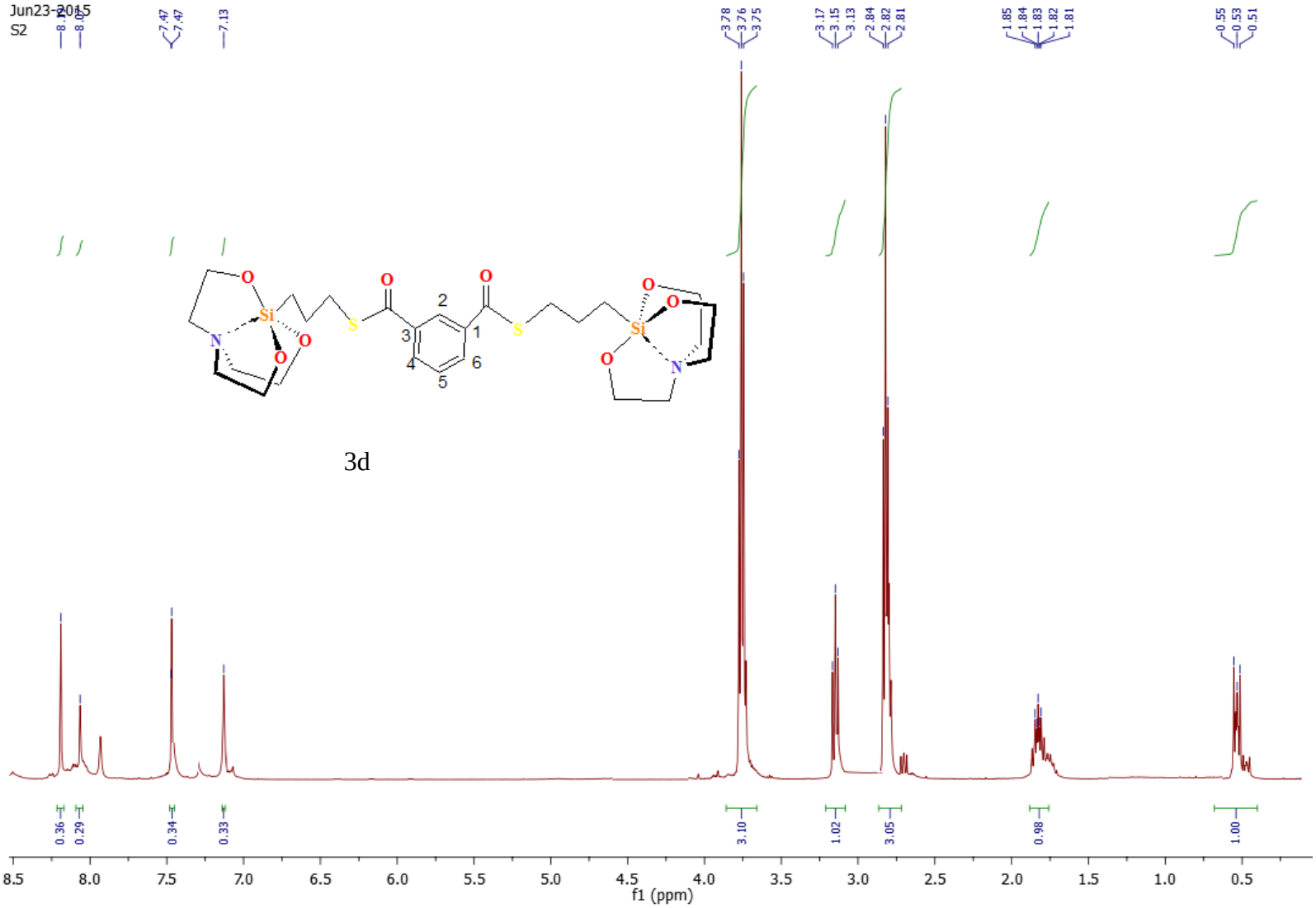


Fig. S19 ^{1}H NMR spectrum of **3d**

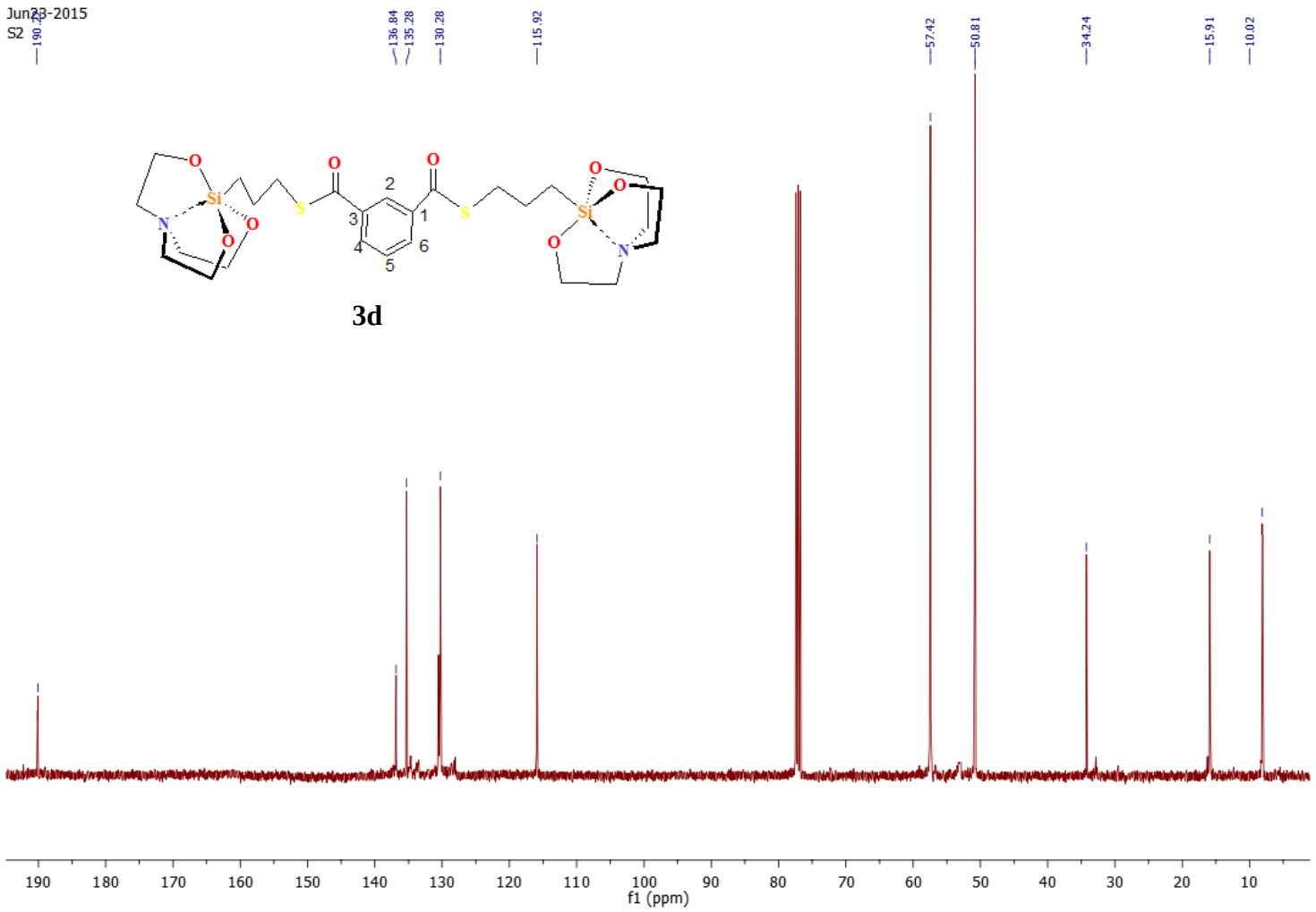


Fig. S20 ^{13}C NMR spectrum of **3d**

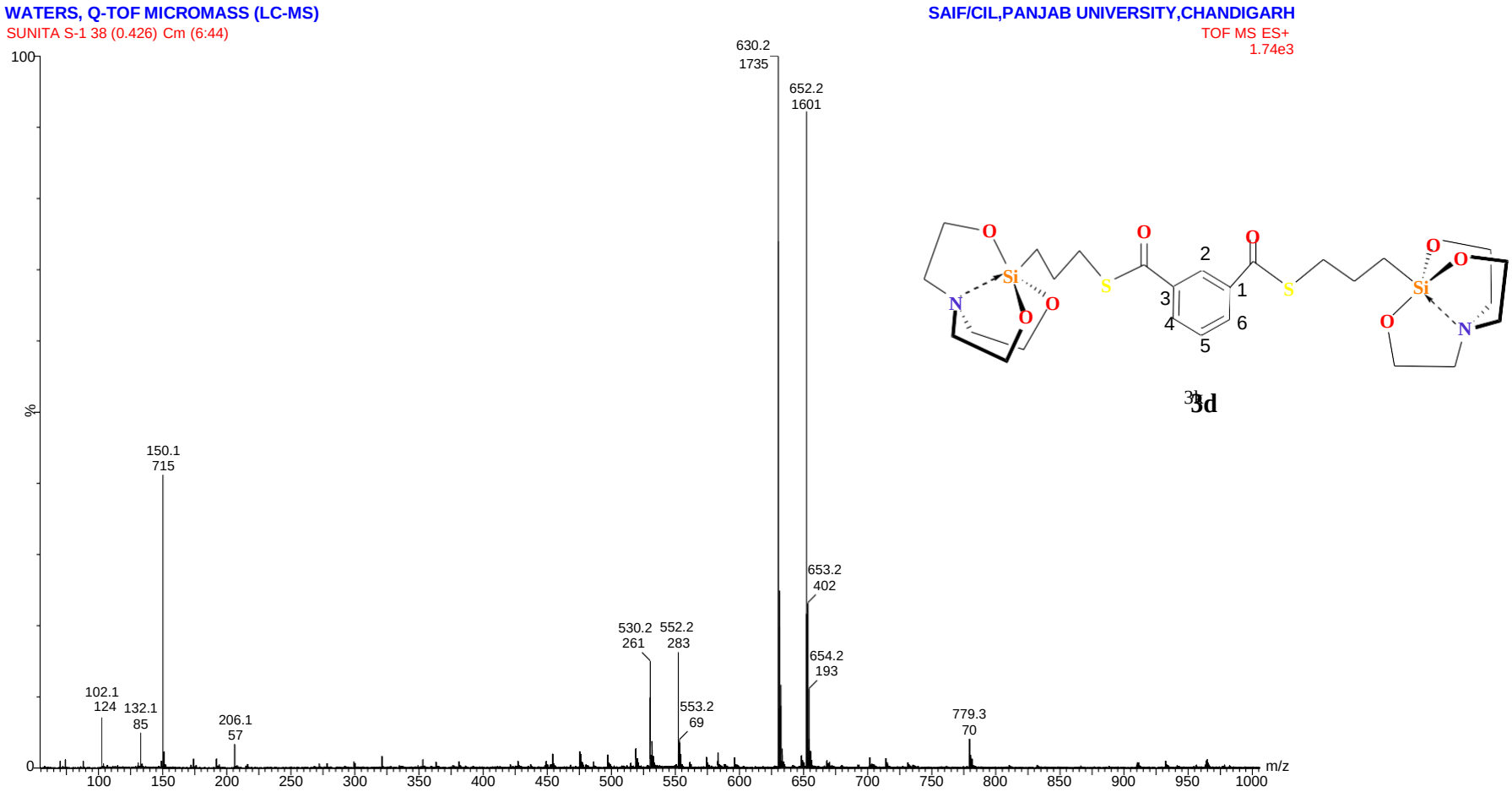


Fig. S21 Mass spectrum of **3d**

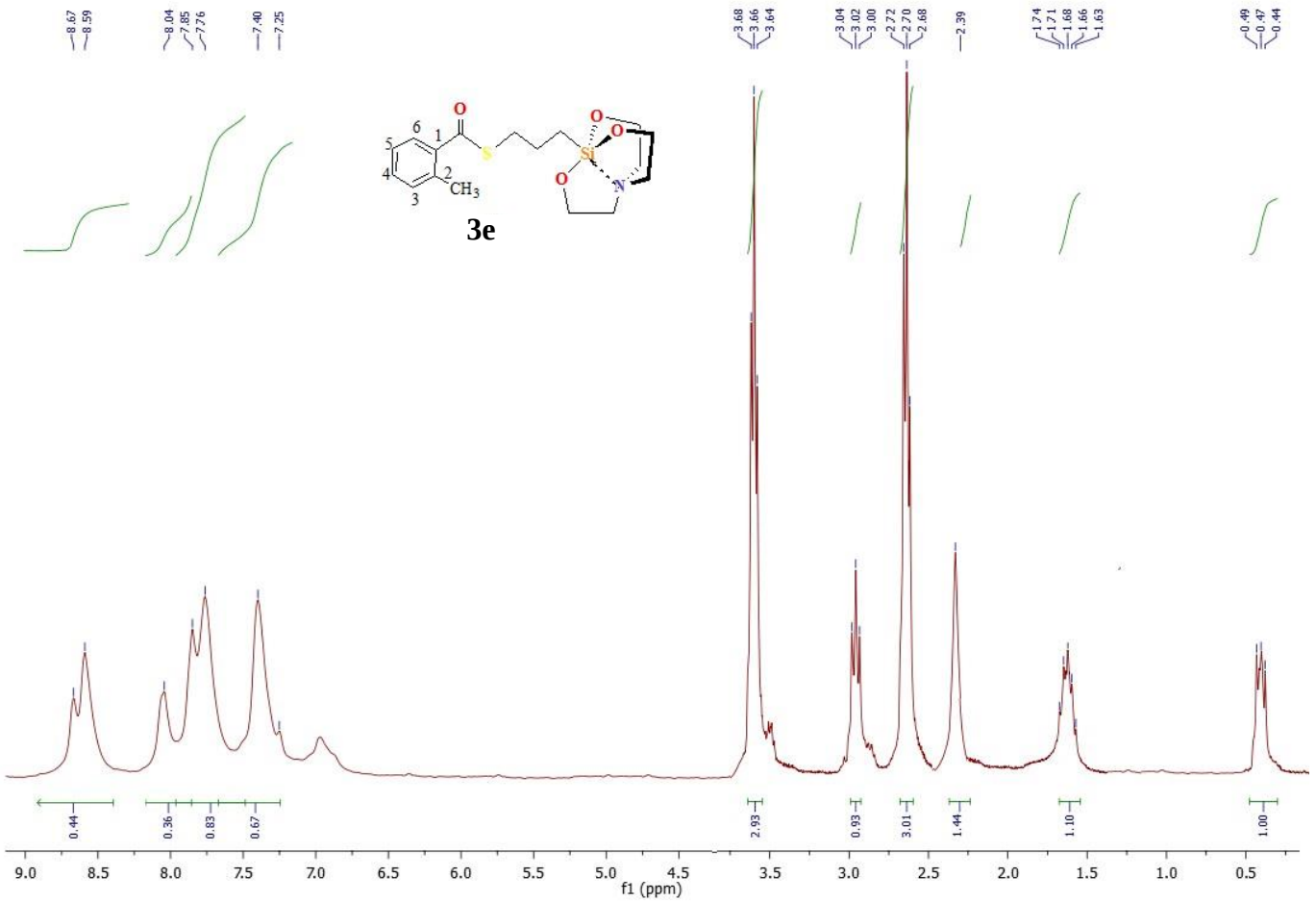


Fig. S22 ^{1}H NMR spectrum of **3e**

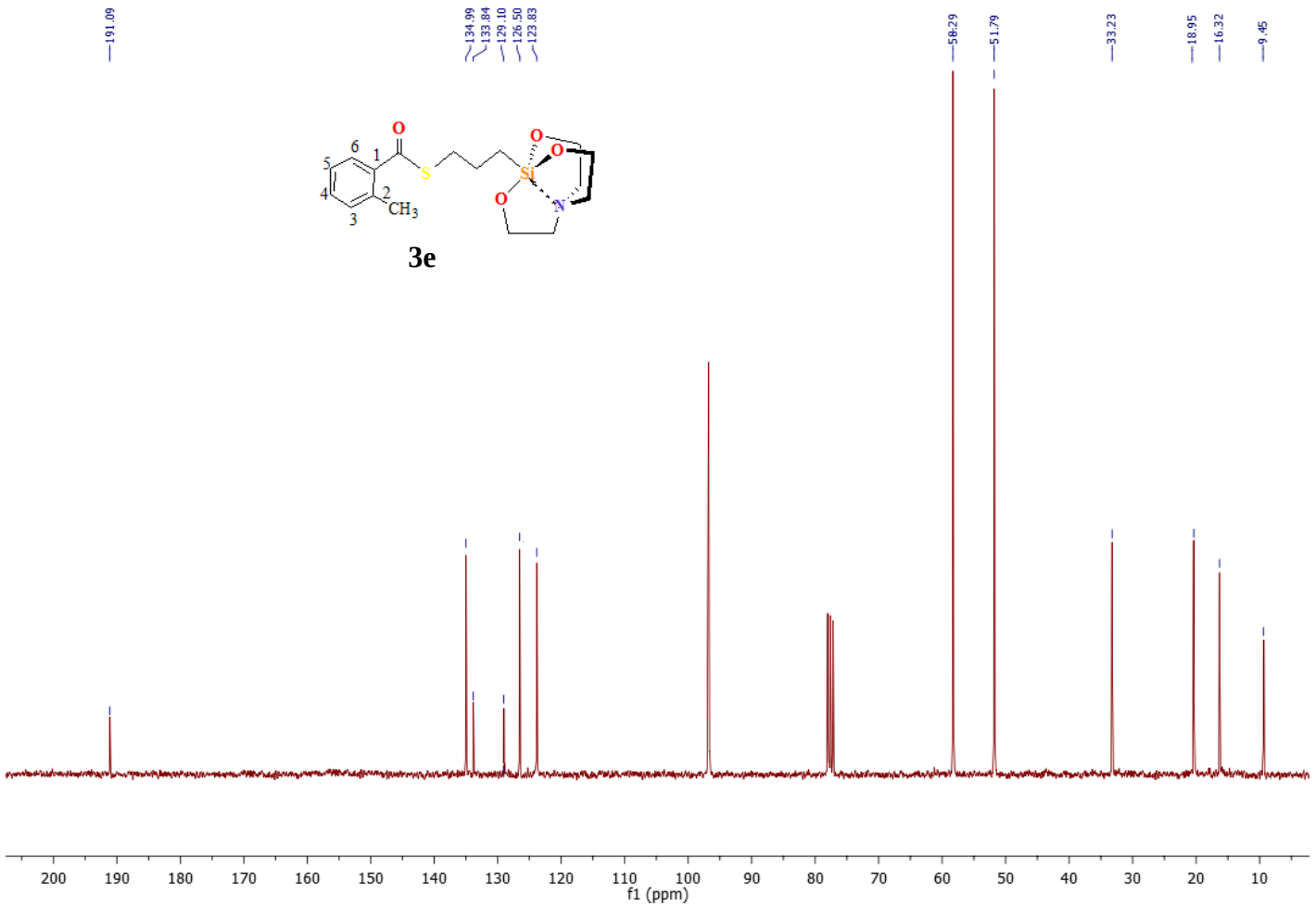


Fig. S23 ^{13}C NMR spectrum of **3e**

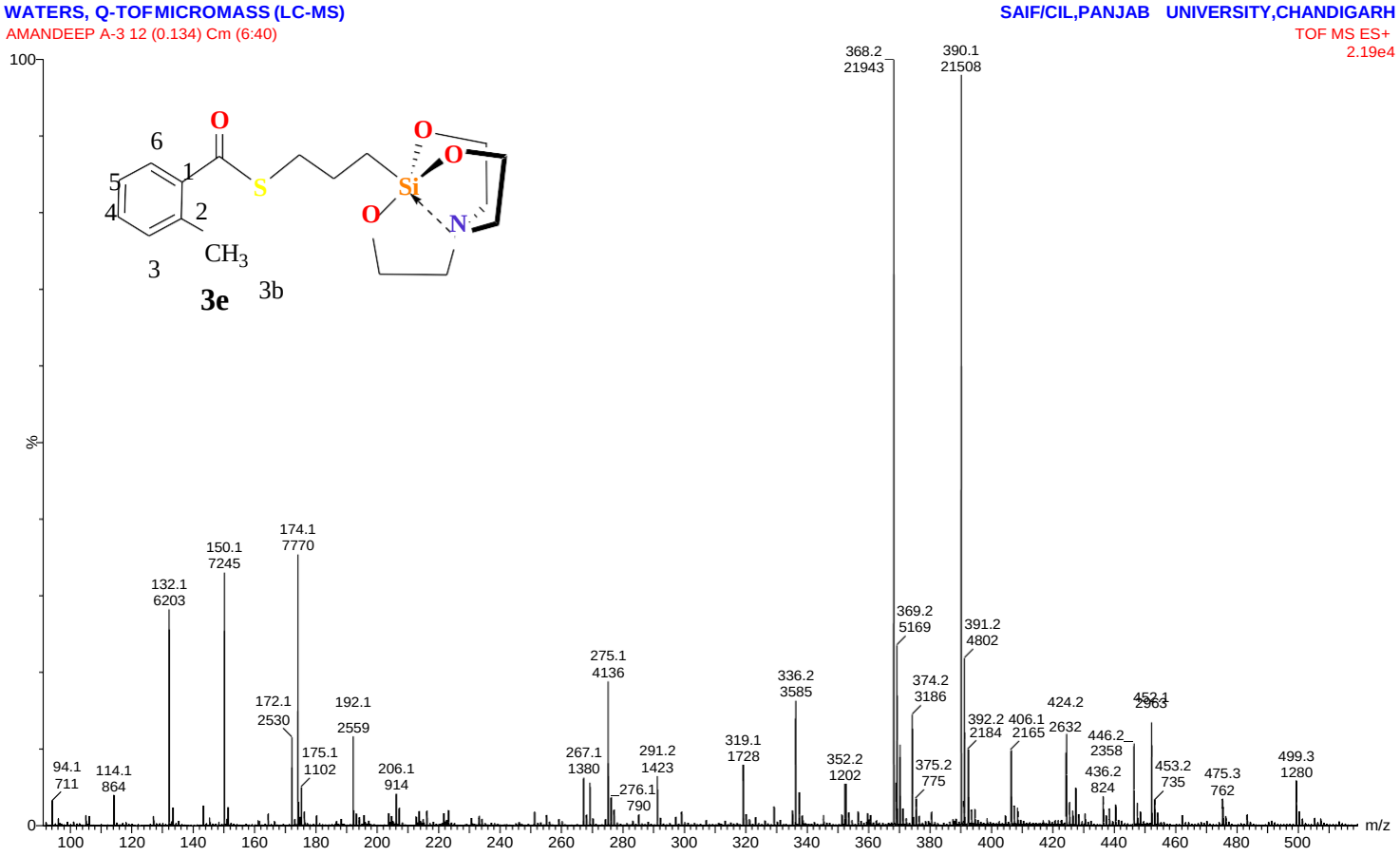


Fig. S24 Mass spectrum of **3e**

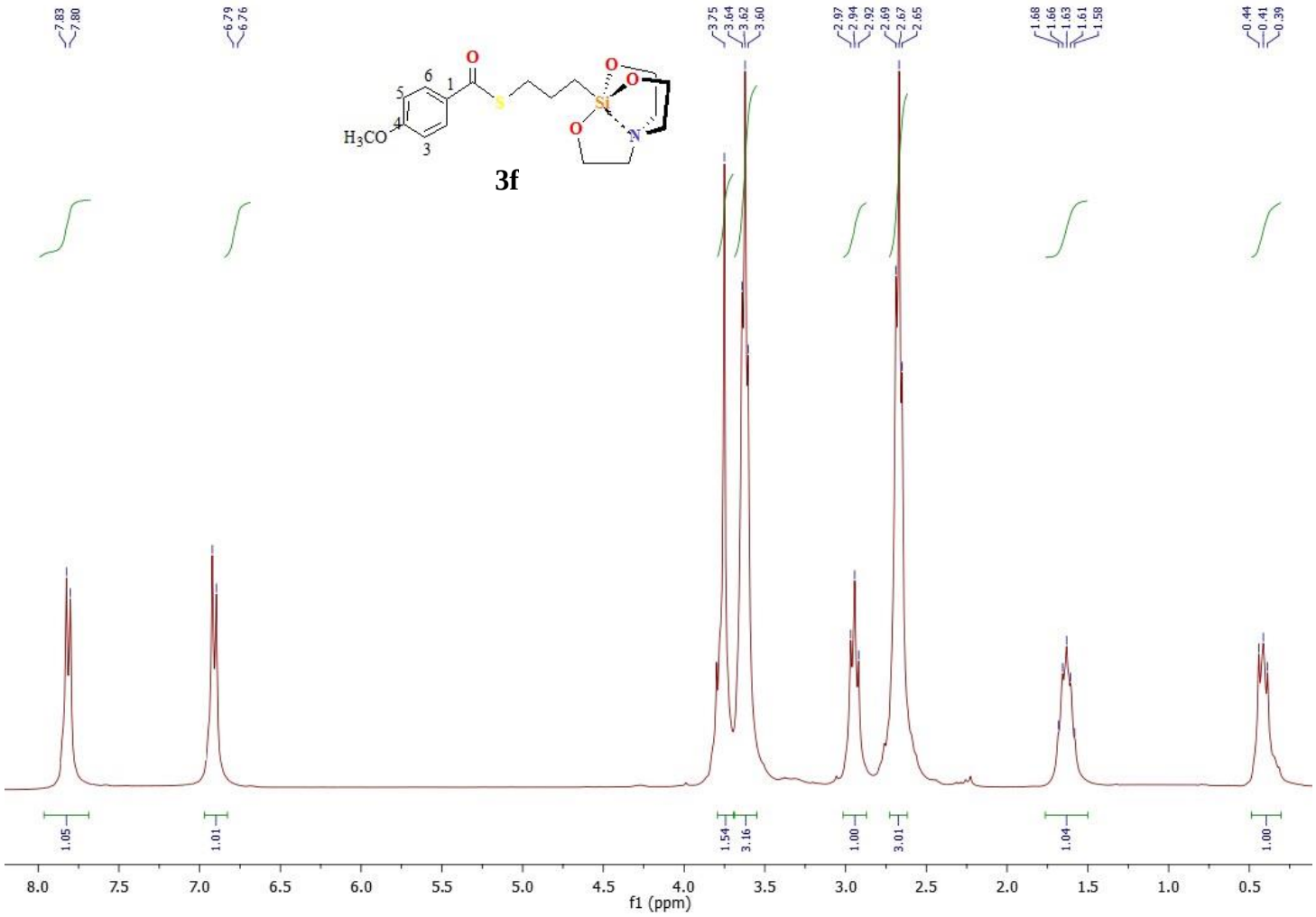


Fig. S25 ^{1}H NMR spectrum of **3f**

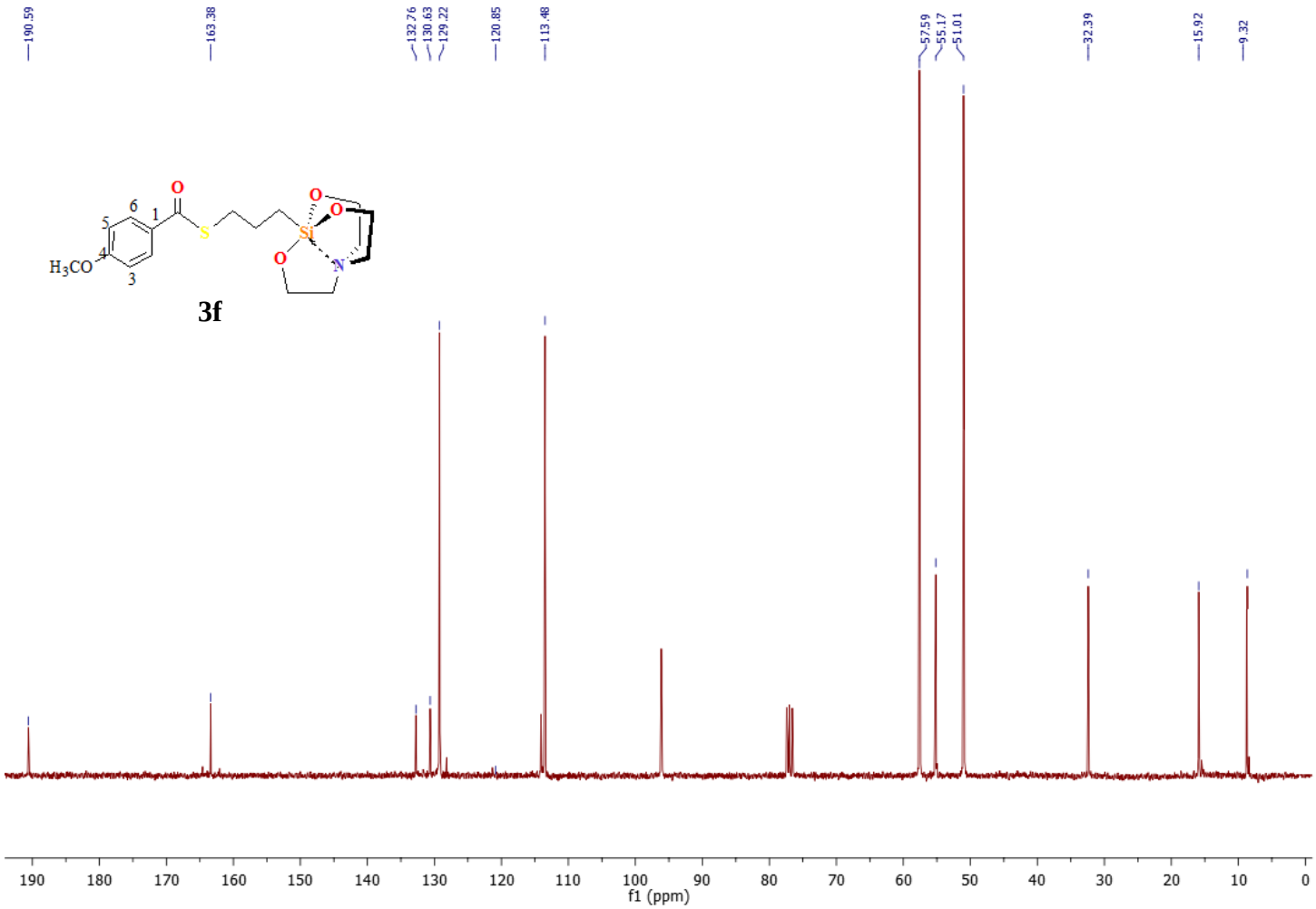


Fig. S26 ^{13}C NMR spectrum of **3f**

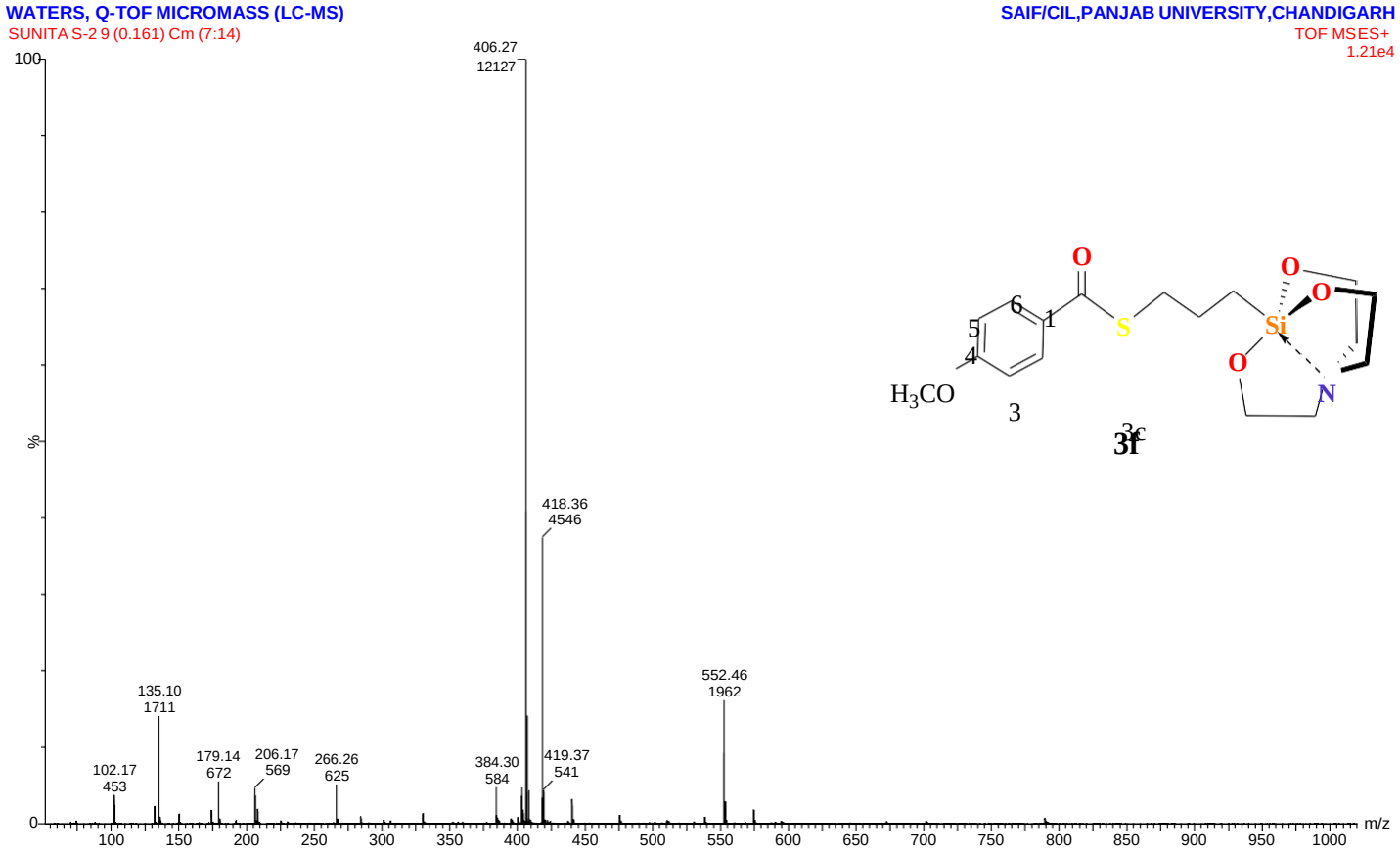


Fig. S27 Mass spectrum of **3f**

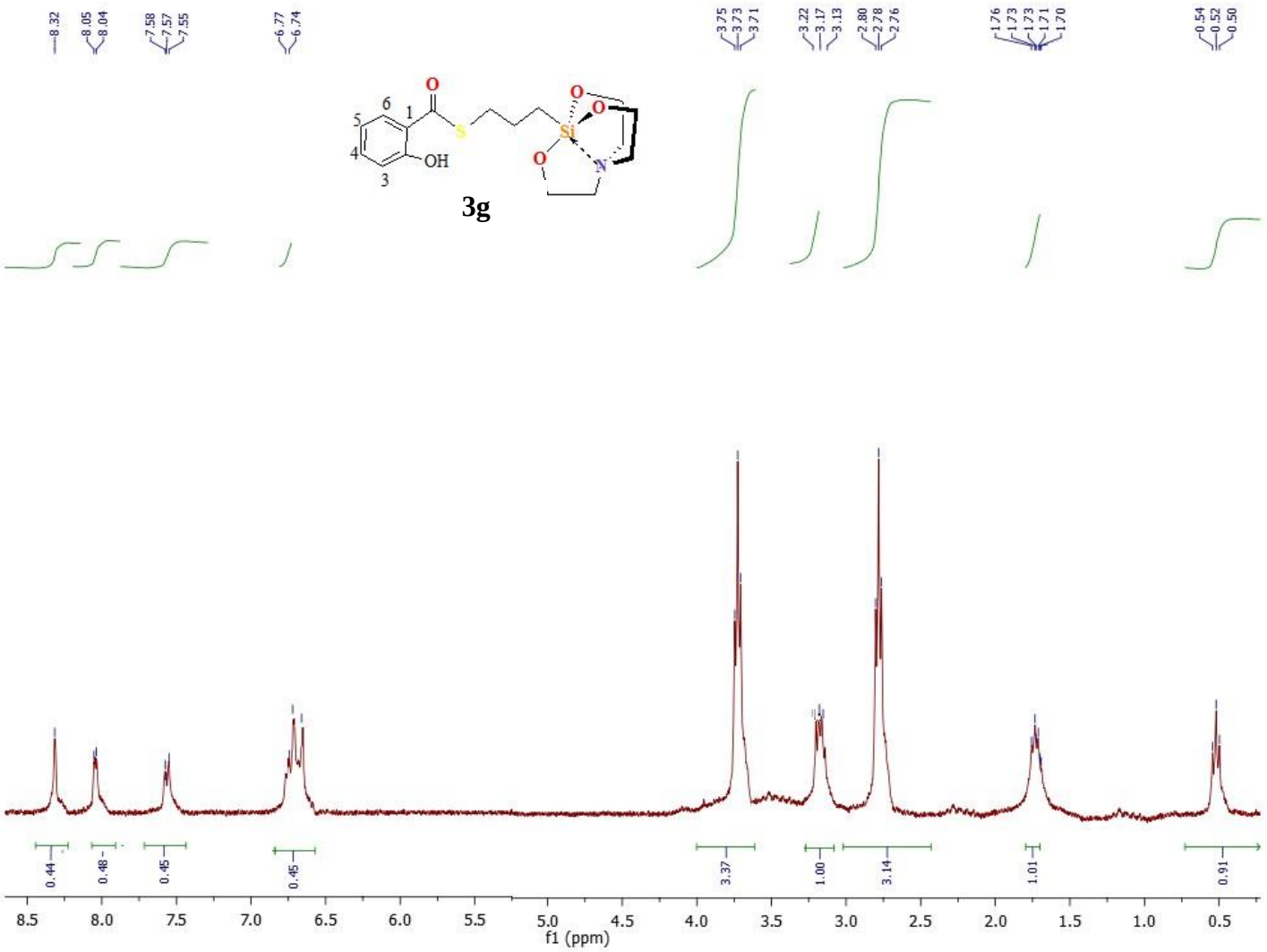


Fig. S28 ^{1}H NMR spectrum of **3g**

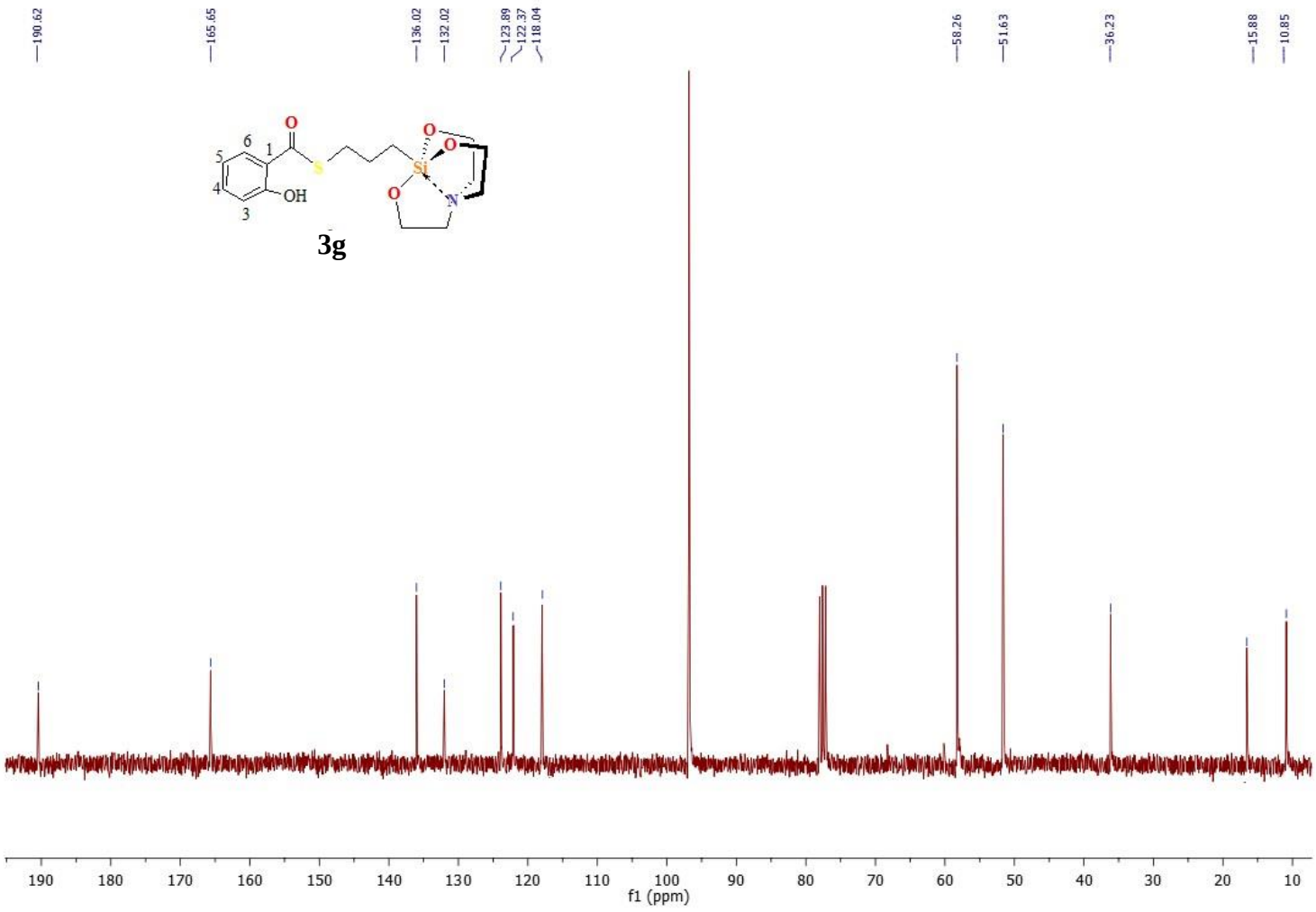


Fig. S29 ^{13}C NMR spectrum of **3g**

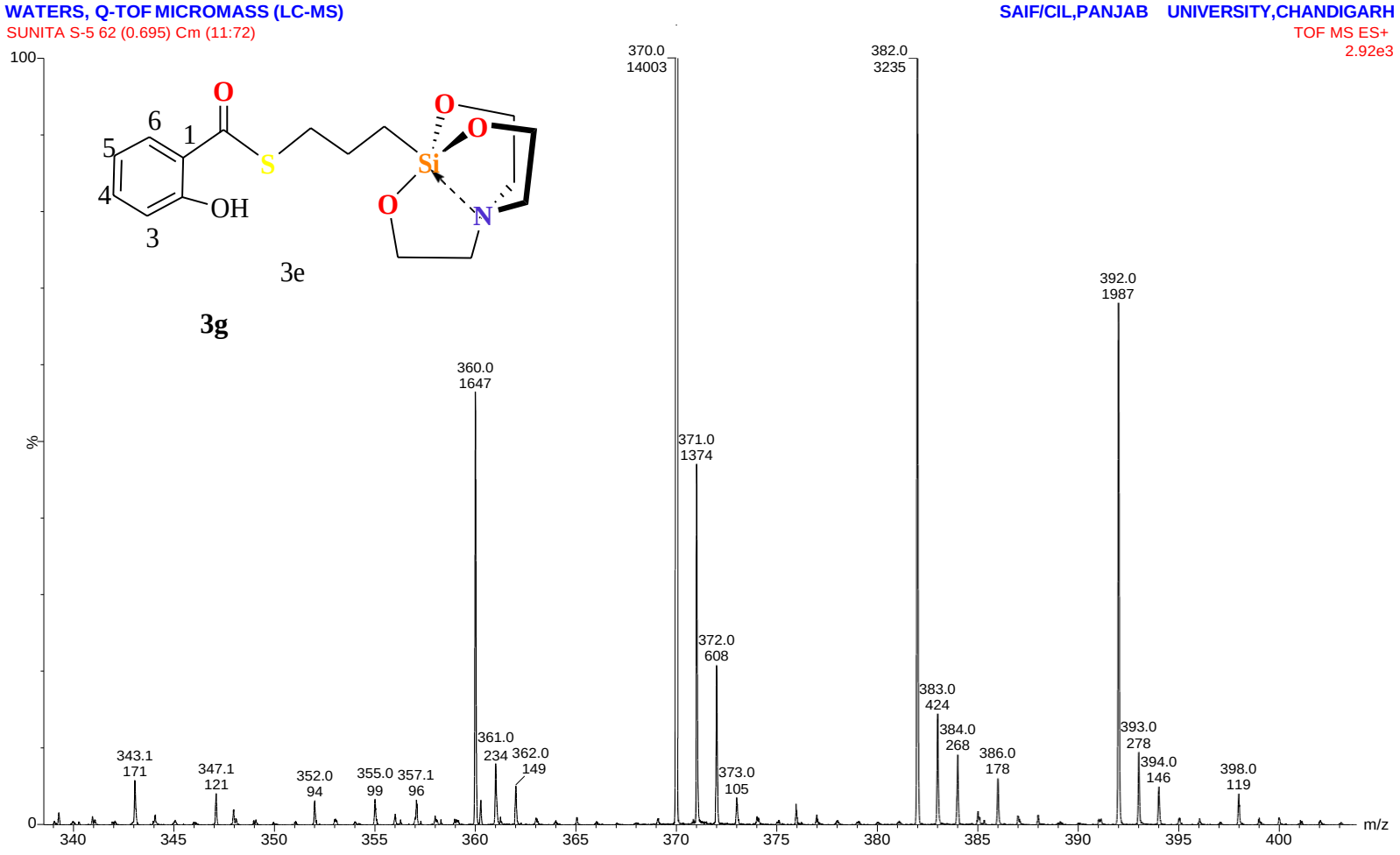


Fig. S30 Mass spectrum of **3g**

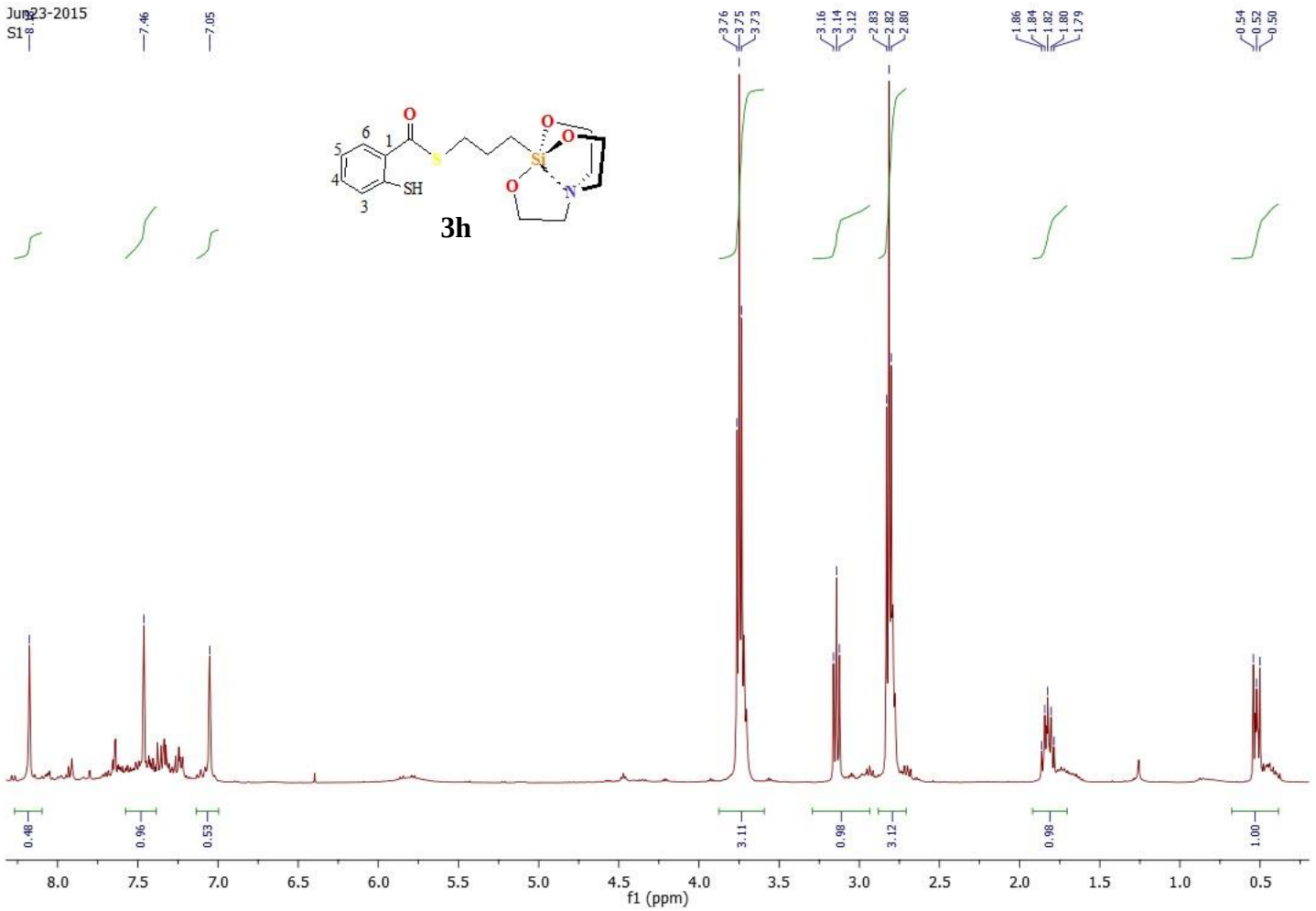


Fig. S31 ^{1}H NMR spectrum of **3h**

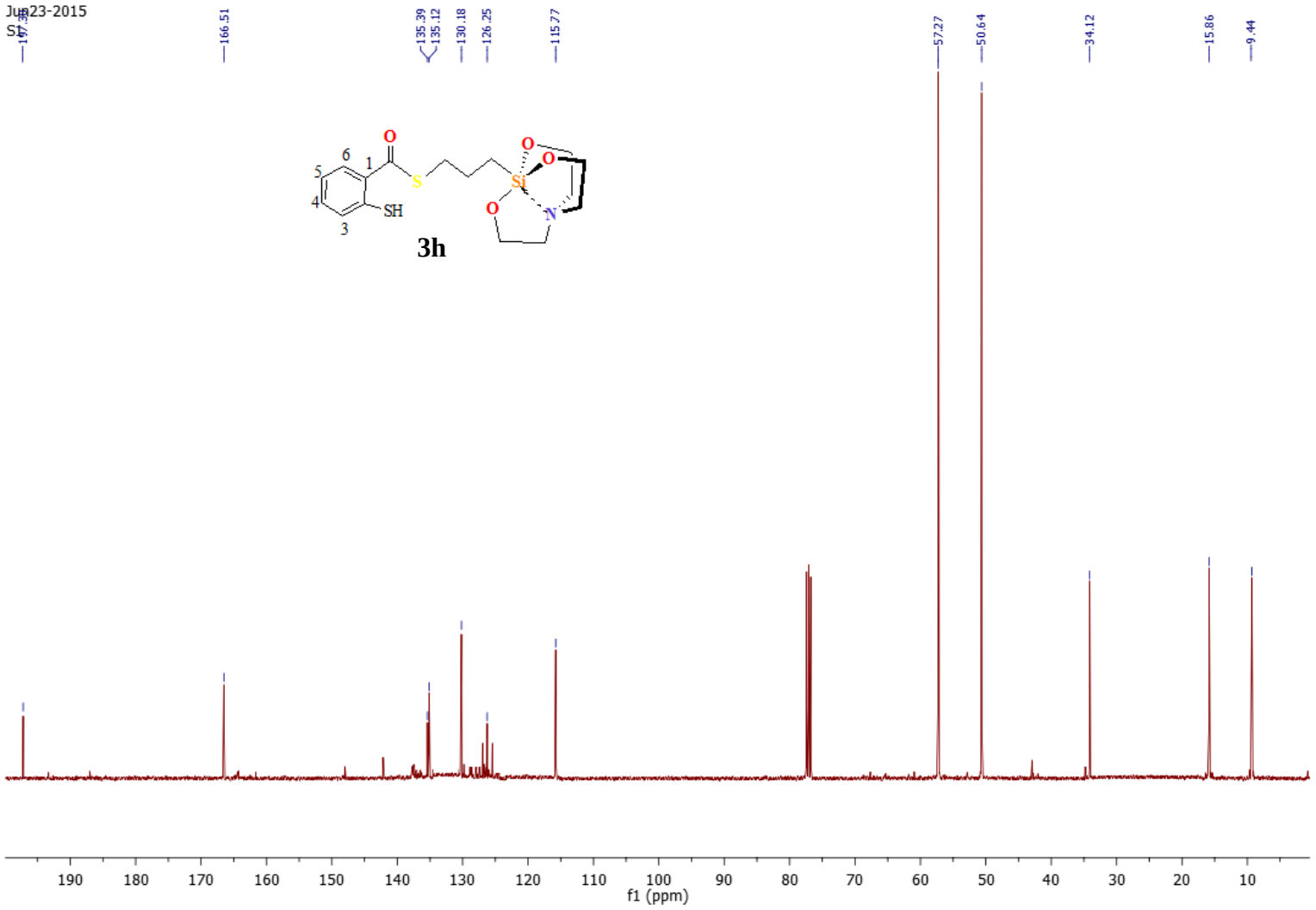


Fig. S32 ^{13}C NMR spectrum of **3h**

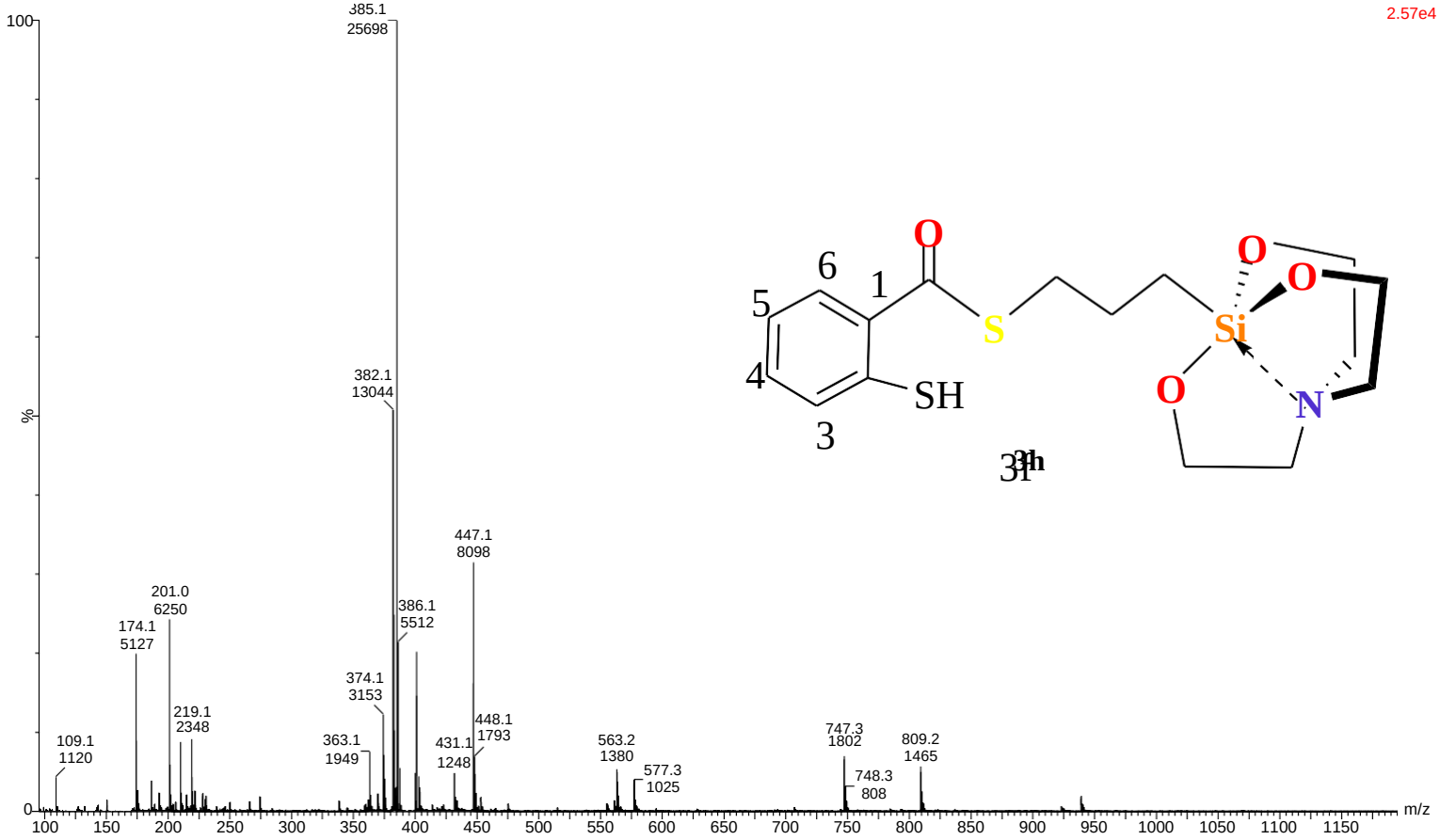


Fig. S33 Mass spectrum of **3h**

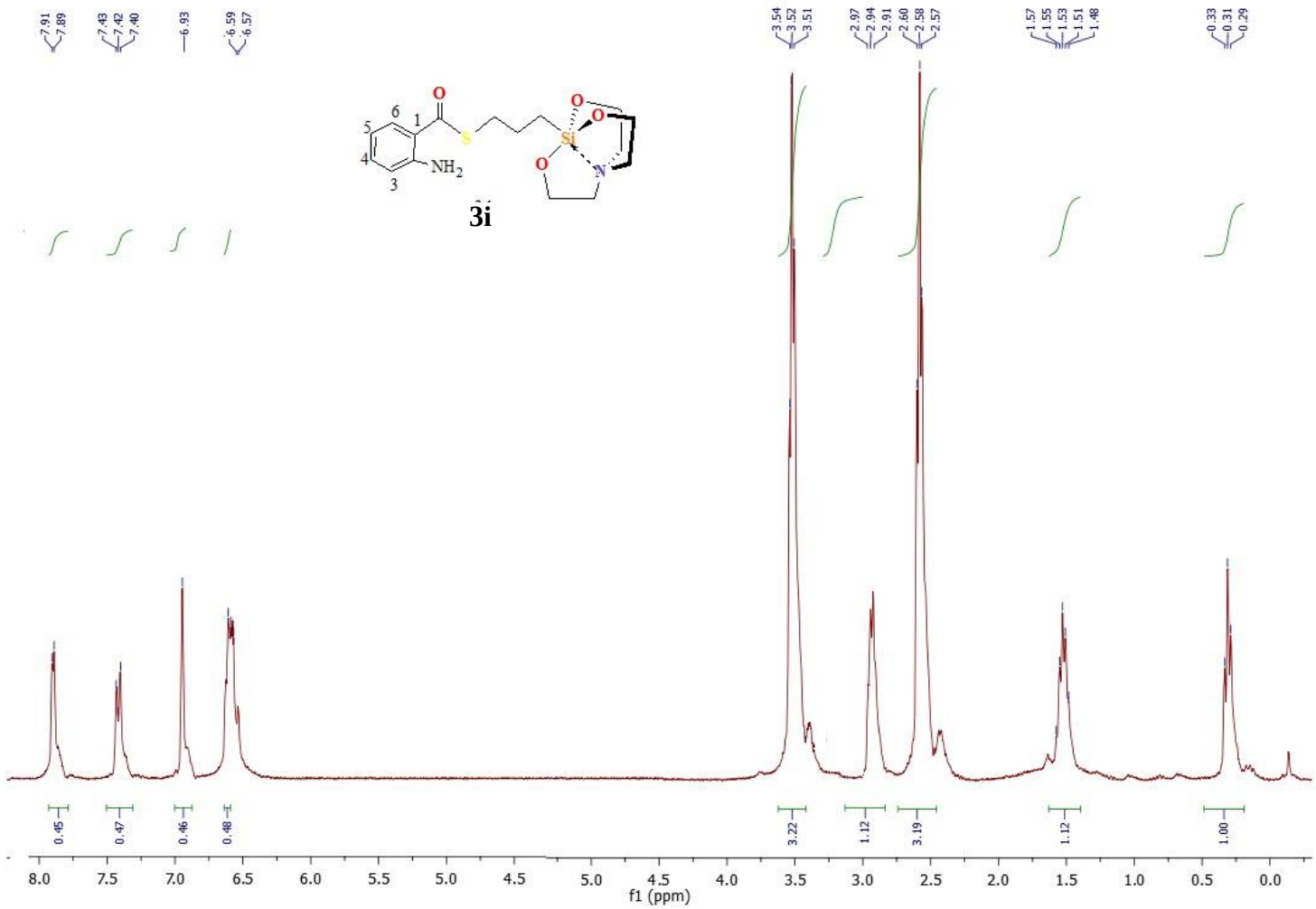


Fig. S34 ^{1}H NMR spectrum of **3i**

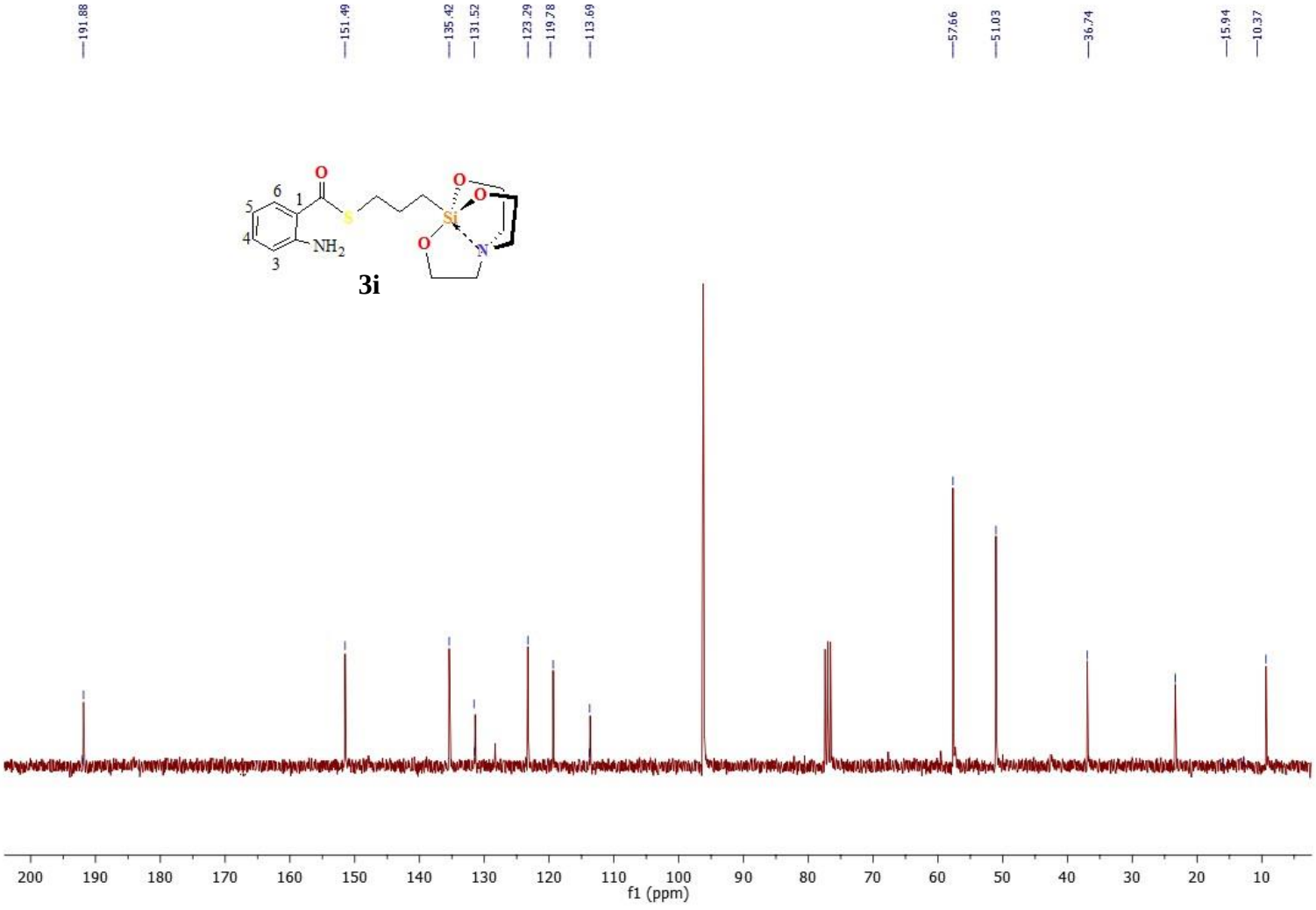
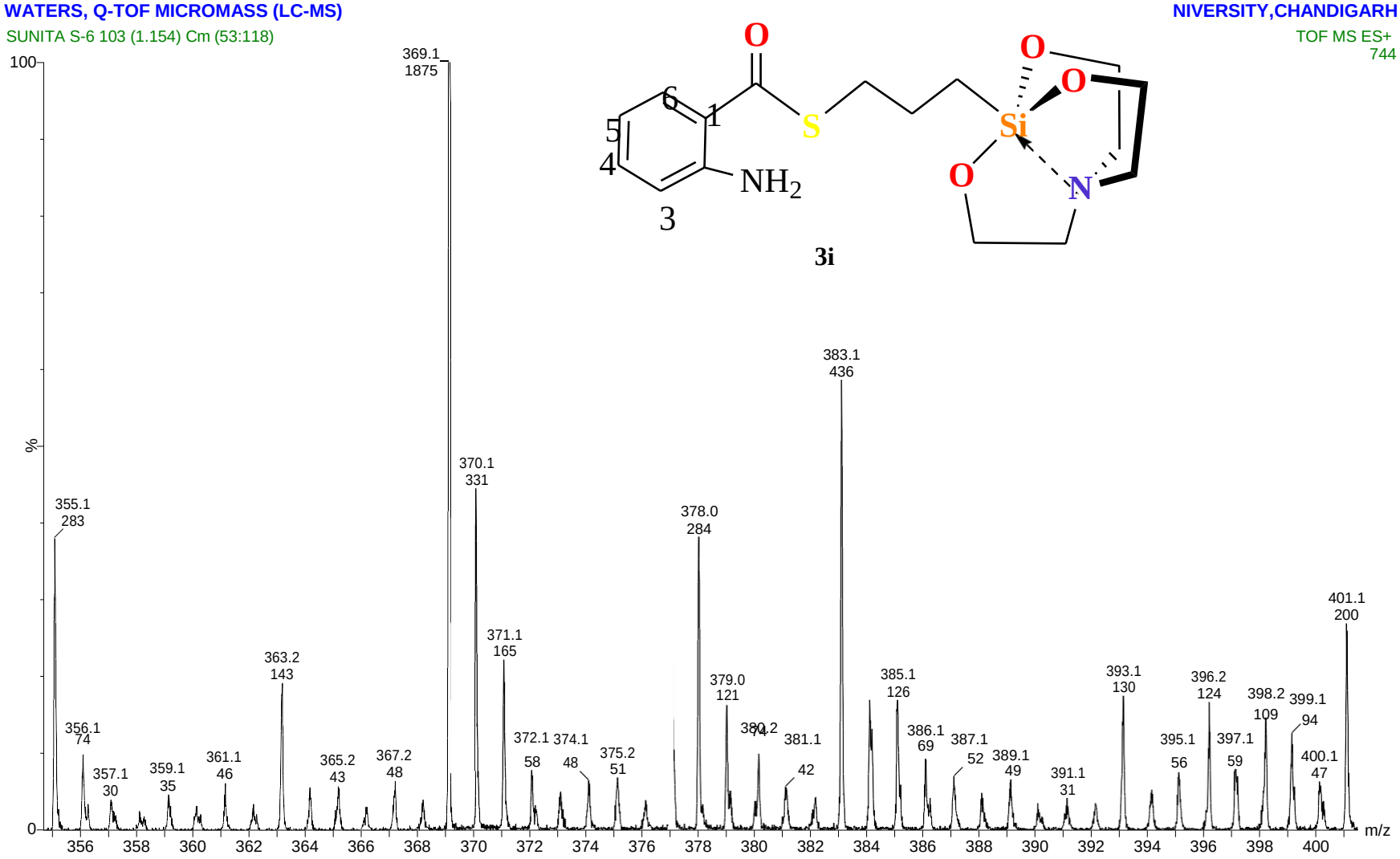


Fig. S35 ^{13}C NMR spectrum of **3i**



3i

Fig. S36 Mass spectrum of **3i**

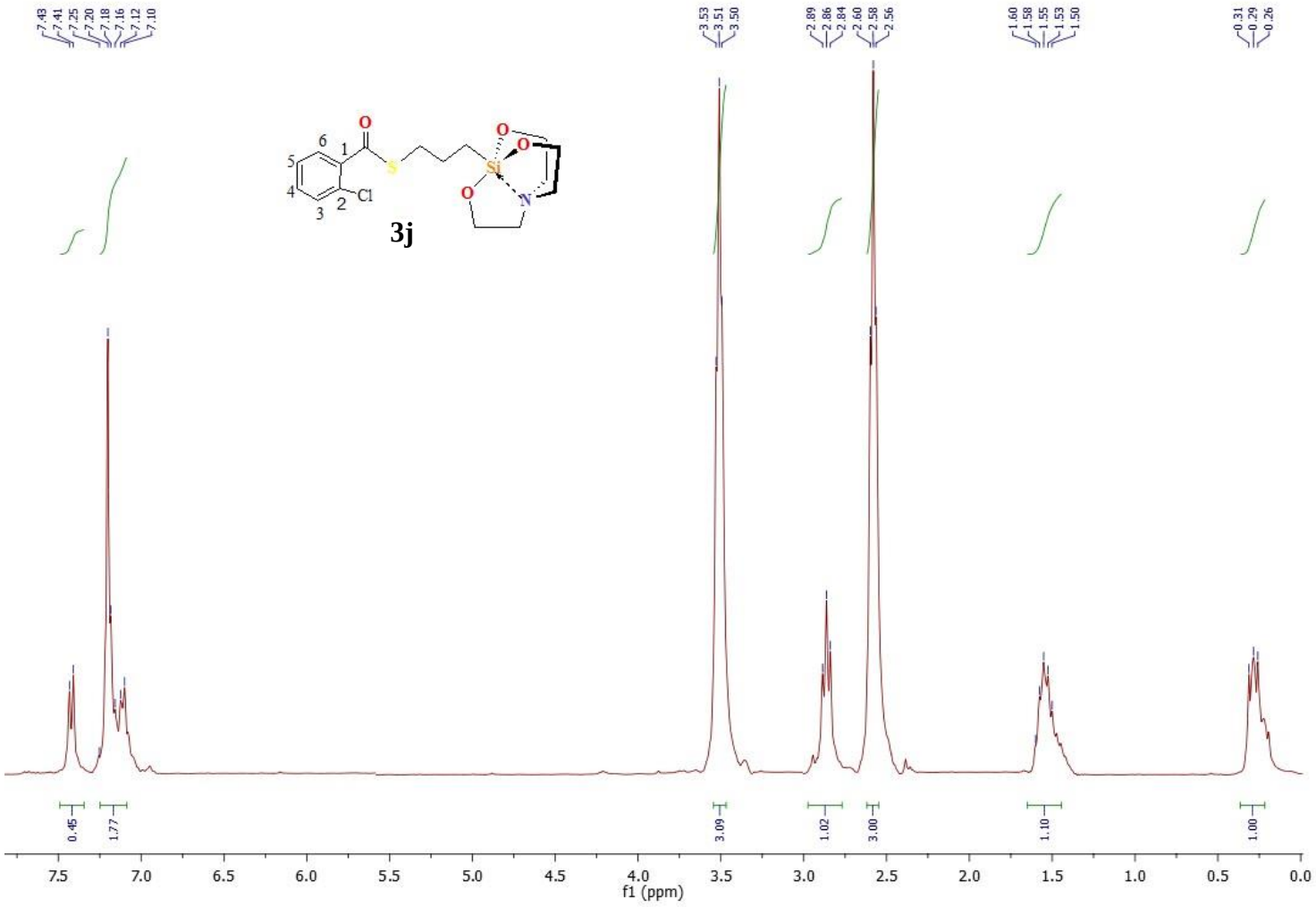


Fig. S37 ^{1}H spectrum of **3j**

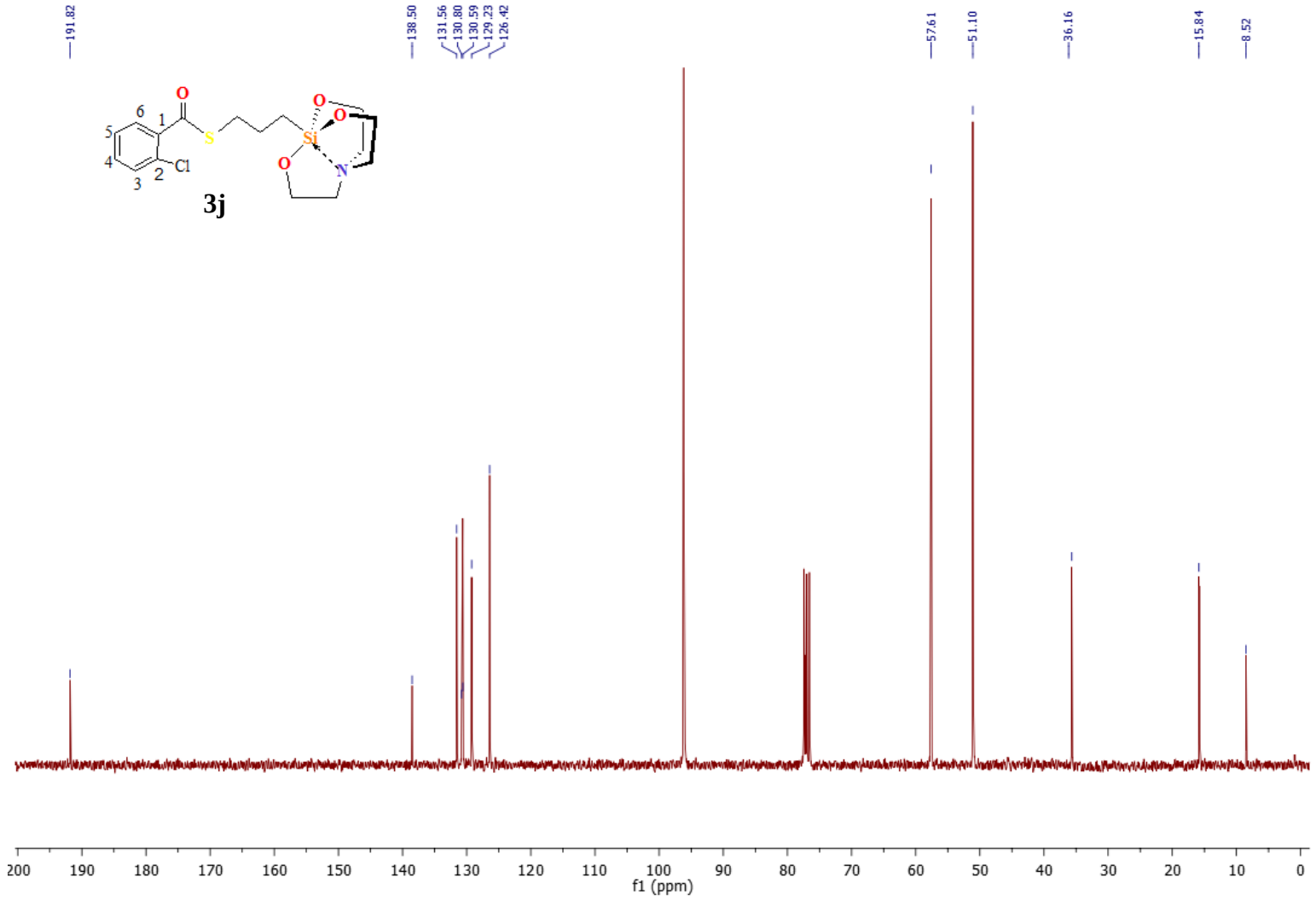


Fig. S38 ^{13}C spectrum of **3j**

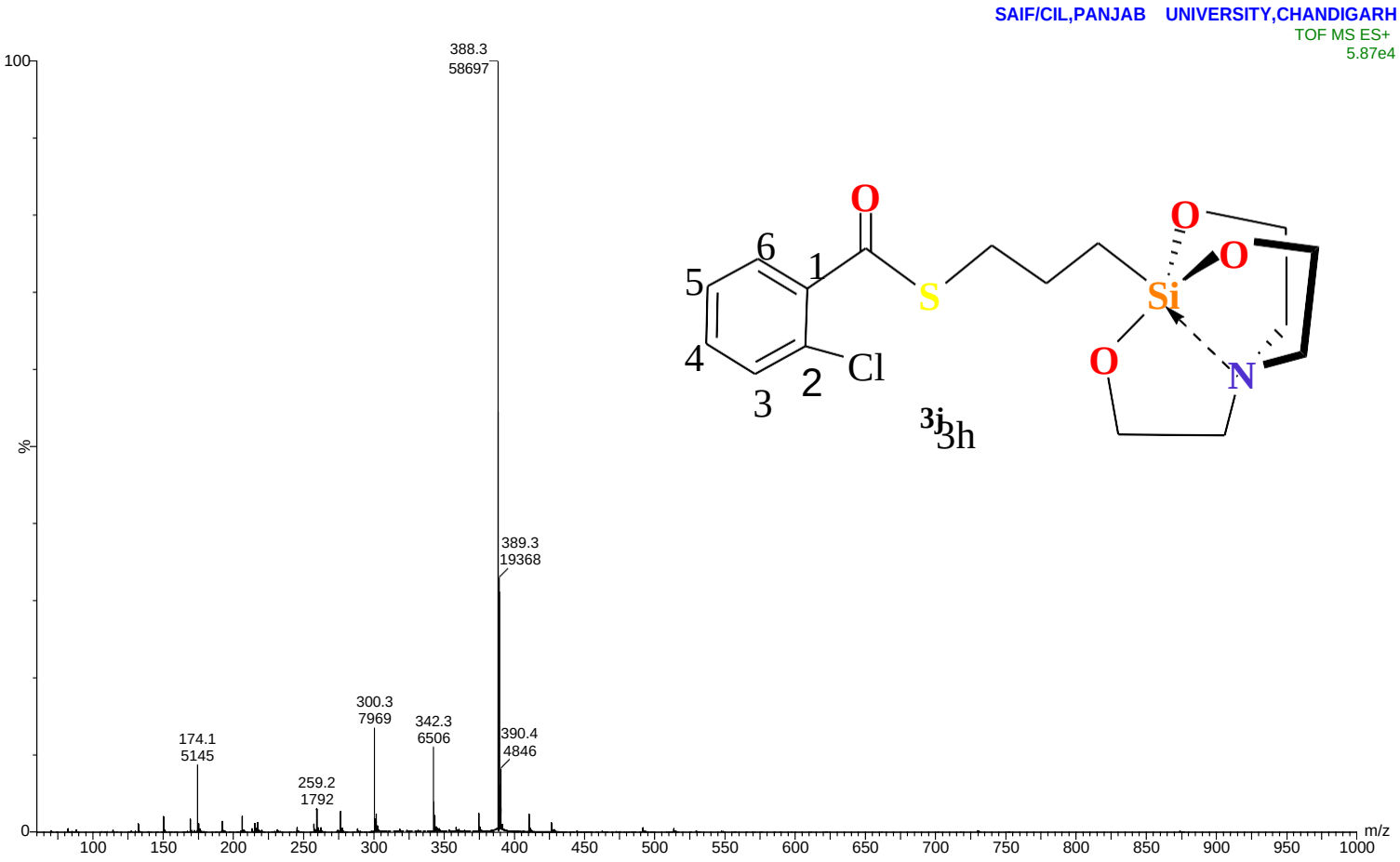


Fig. S39 Mass spectrum of **3j**

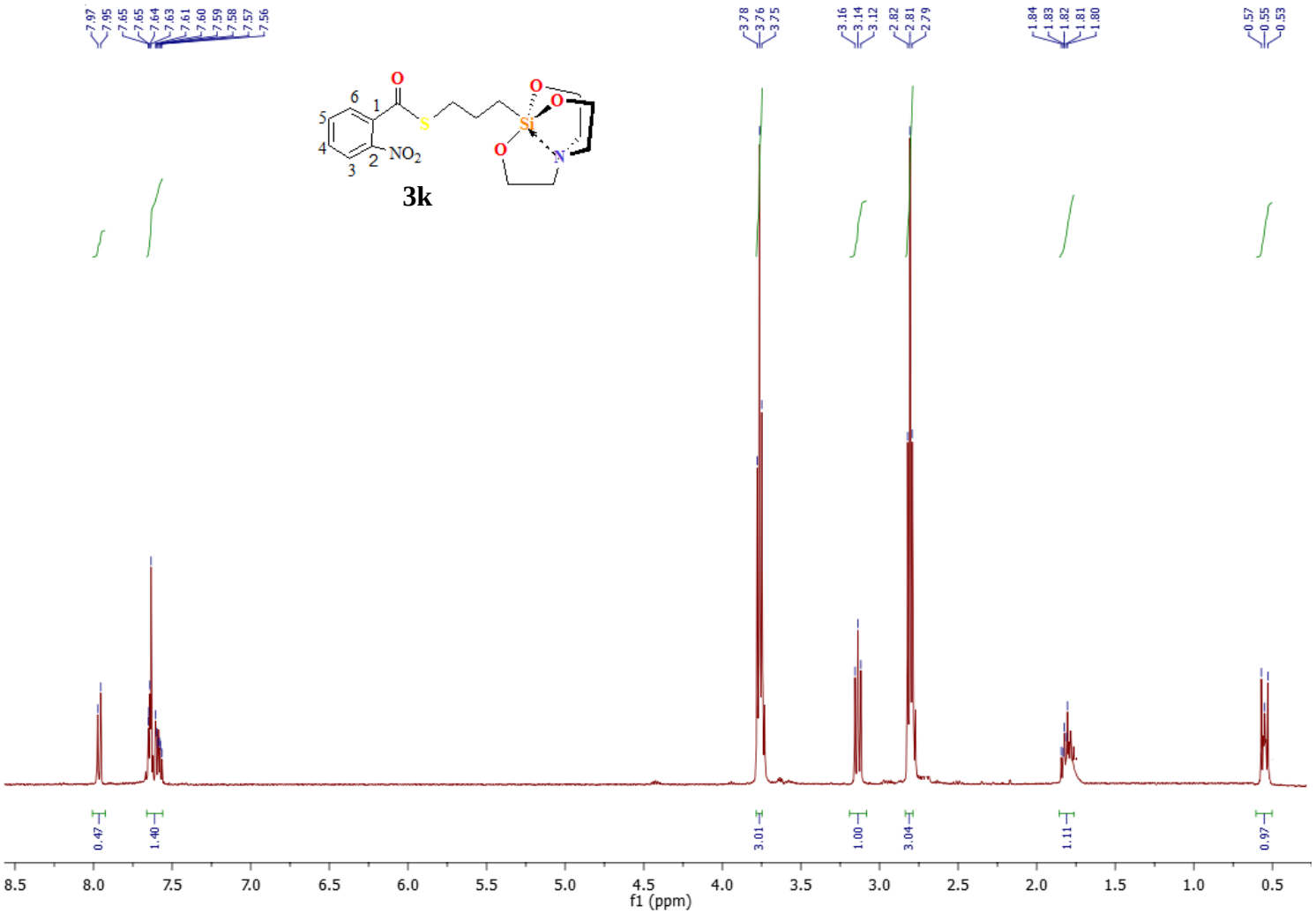


Fig. S40 ^{1}H spectrum of **3k**

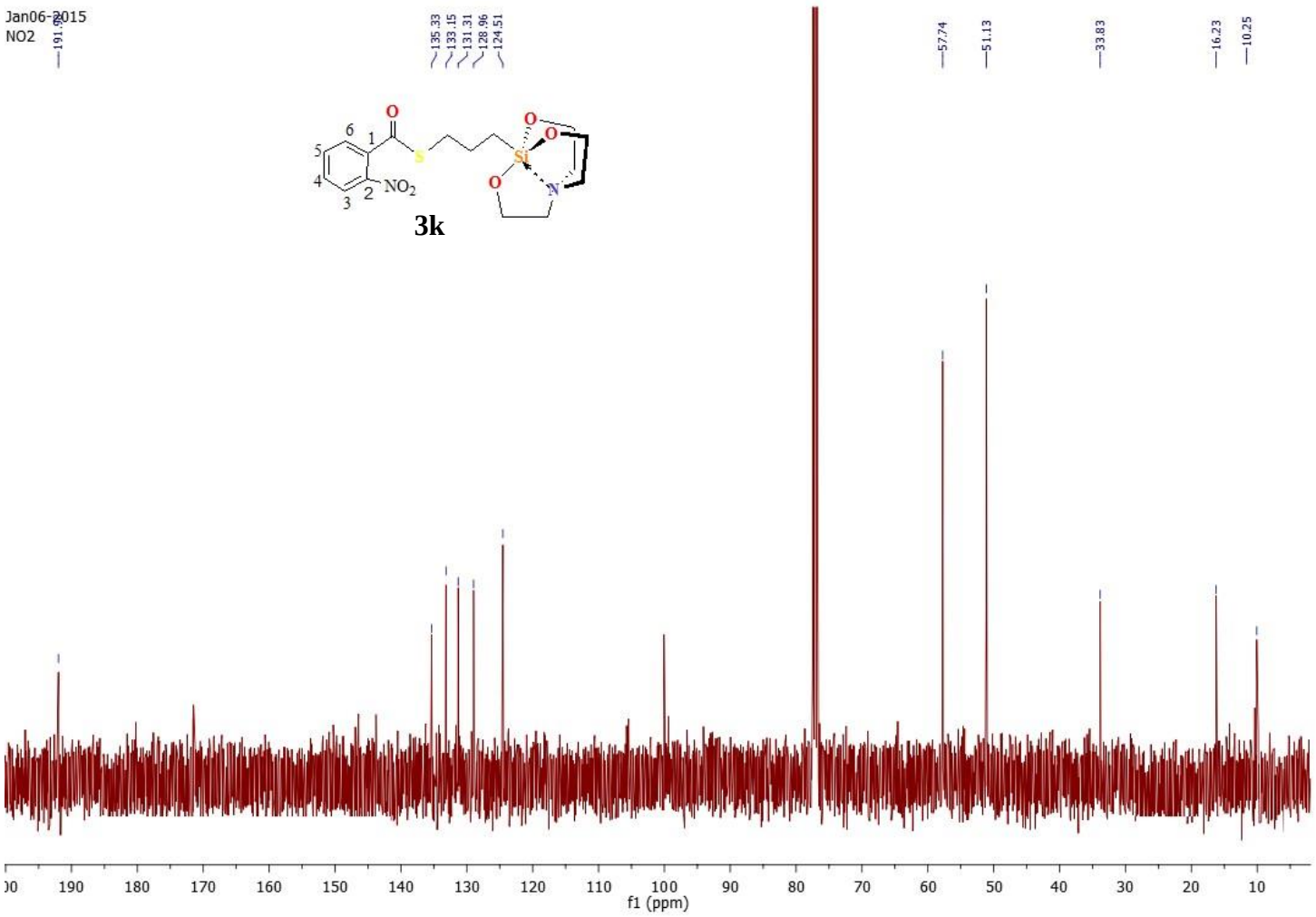


Fig. S41 ^{13}C spectrum of **3k**

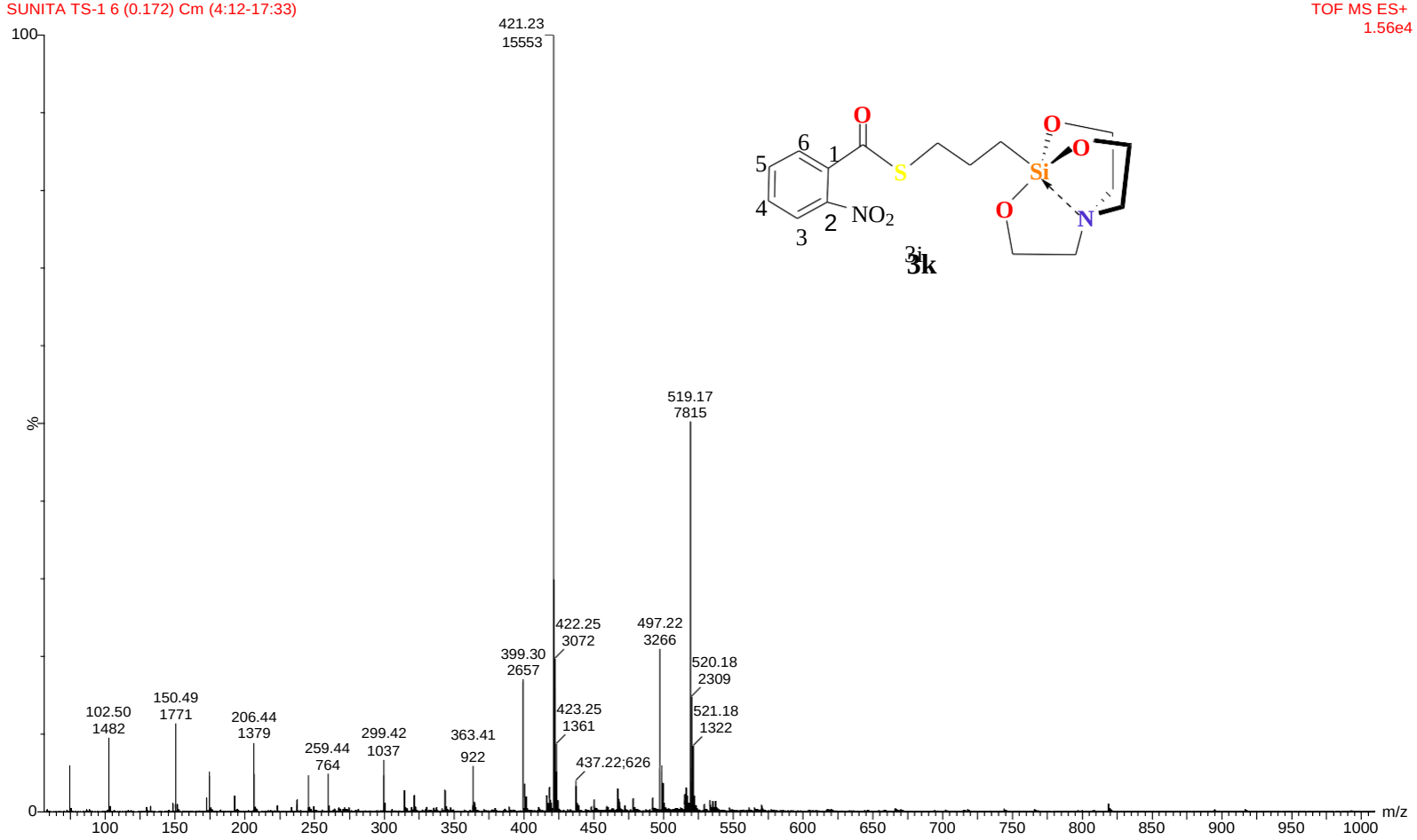


Fig. S42 Mass spectrum of **3k**

Table T1 Selected crystal data and details on the structure determinations from single crystal data for compound **3c** and **3f.**

Compound	***3c***	***3f***
Formula	$C_{22}H_{27}NO_4SSi$	$C_{17}H_{25}NO_5SSi$
MW [g·mol^{-1}]	429.59	383.53
Crystal system	Monoclinic	Orthorhombic
Space group	$P2_1$	$P2_12_12_1$
a [Å]	7.2068(2)	8.3421(6)
b [Å]	8.9671(3)	13.3327(0)
c [Å]	16.5006(6)	16.7969(1)
α [deg]	90	90
β [deg]	93.343(1)	90
γ [deg]	90	90
V [Å^3]	1064.52(6)	1868.2(2)
T [K]	170(2)	170(2)
Z	2	4
ρ_{calc} [g·cm^{-3}]	1.340	1.364

μ [mm^{-1}]	0.237	0.264
Min/max transmission	0.958/0.974	0.953/0.968
θ_{max} [deg]	28.386	28.330
Measured reflections	18186	33751
Unique reflections	5321	4651
Reflections [$F_0 > 4\sigma(F_0)$]	5035	4370
Parameter	262	244
R_{int}	0.0269	0.0251
R_1 [$F_0 > 4\sigma(F_0)$]	0.0287	0.0373
wR_2 [all data]	0.0726	0.0994
GOF	1.037	1.017
$\Delta\rho_{max}/\Delta\rho_{min}$ [e·Å^{-3}]	0.288/-0.157	0.476/-0.411

Table T2: Quantity of thionyl chloride used

Acid chloride	Thionyl chloride (in ml)[a]
1a	6.00
1b	4.33
1c	3.74
1d	4.37
1e	5.33
1f	4.77
1g	5.26
1h	4.71
1j	4.65
1k	4.35

a: amount of thionyl chloride for each 1.00 g of corresponding carboxylic acid used