Supporting Information

Transition-metals-catalyzed one-pot selenylation of electrophilic arylating agents using triphenyltin chloride/Se as a phenylselenating agent

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I. Characterization of $NiFe_2O_4$ MNPs

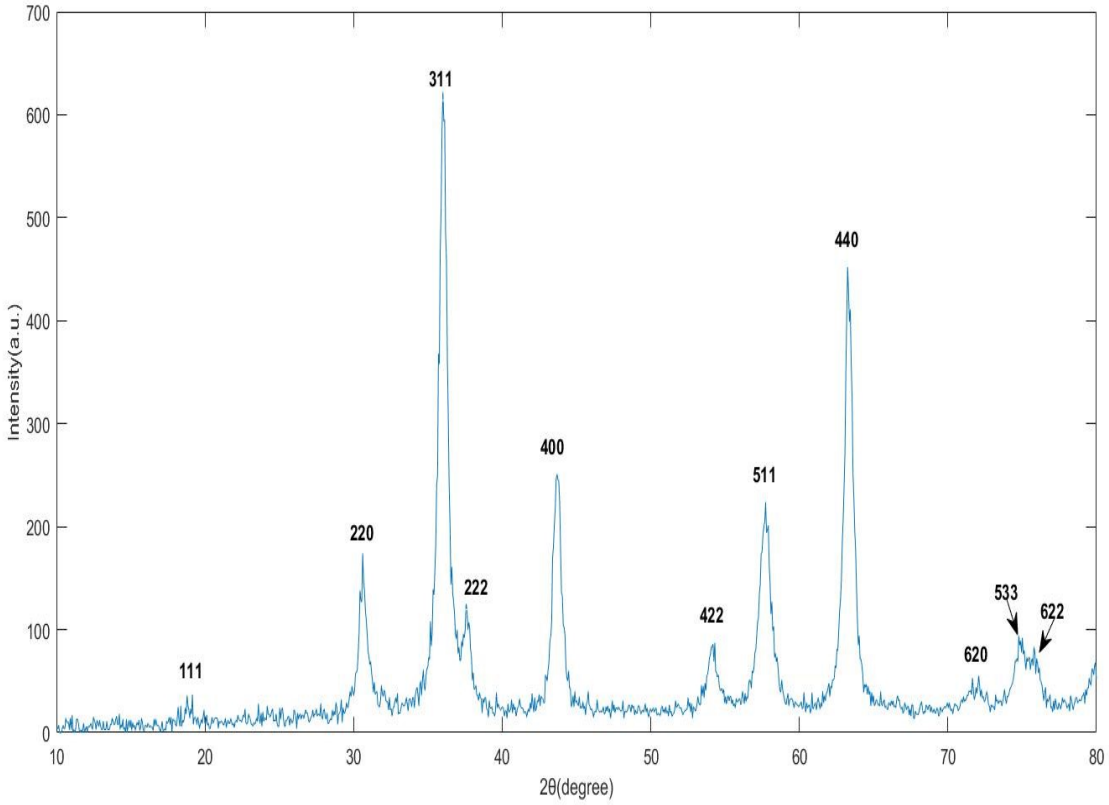


Fig. S1 XRD pattern of $NiFe_2O_4$ MNPs.

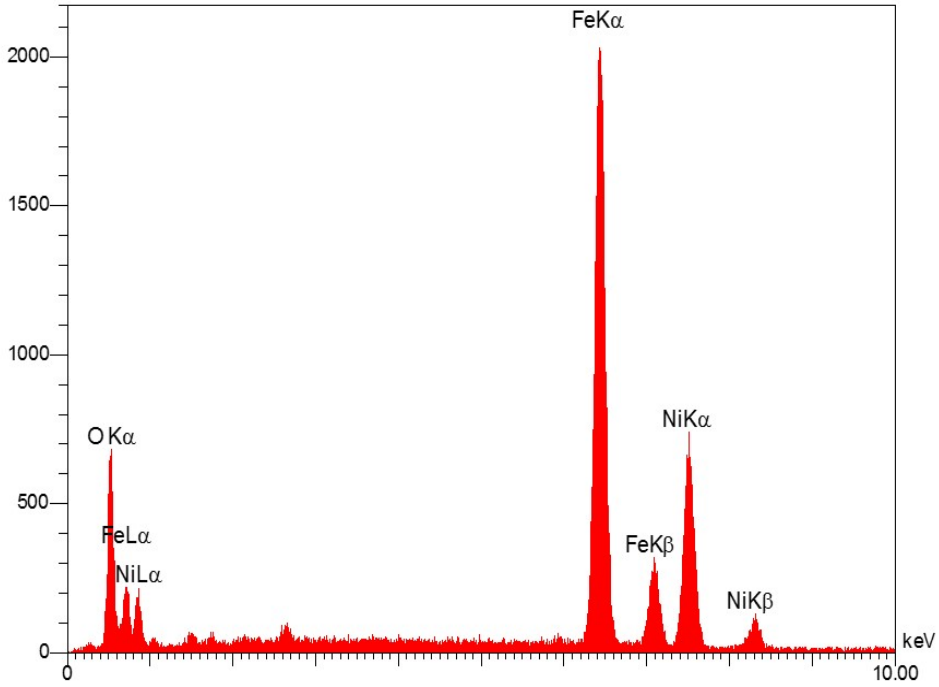


Fig. S2 EDS spectrum of $NiFe_2O_4$ MNPs.

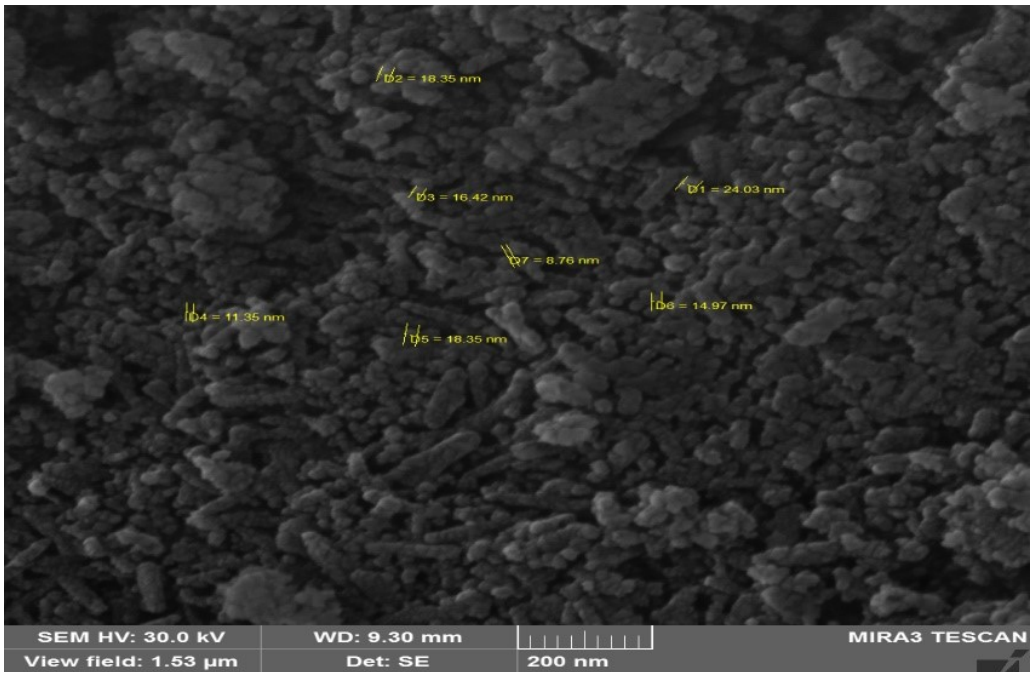


Fig. S3 SEM image of $NiFe_2O_4$ MNPs.

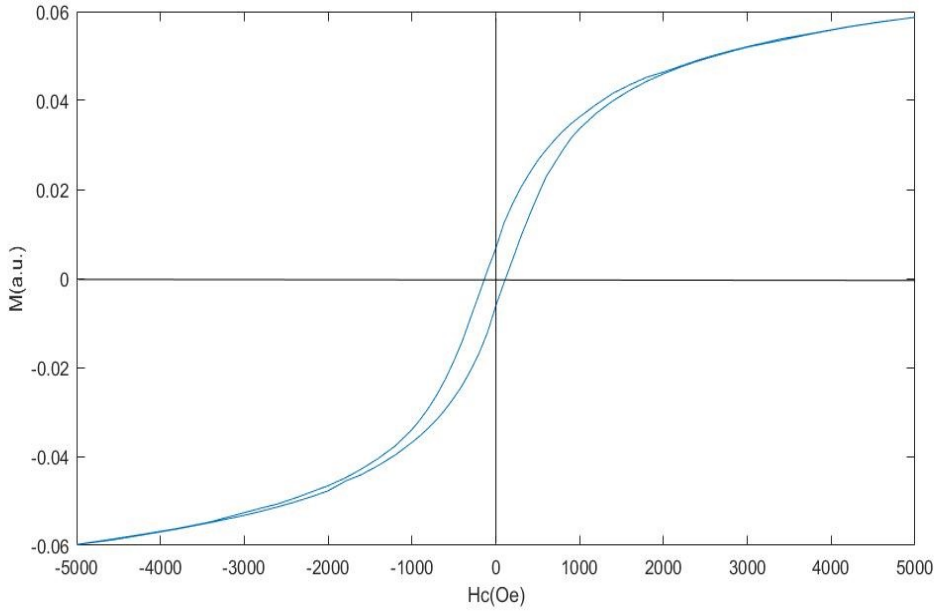


Fig. S4 Magnetization curve for $NiFe_2O_4$ MNPs.

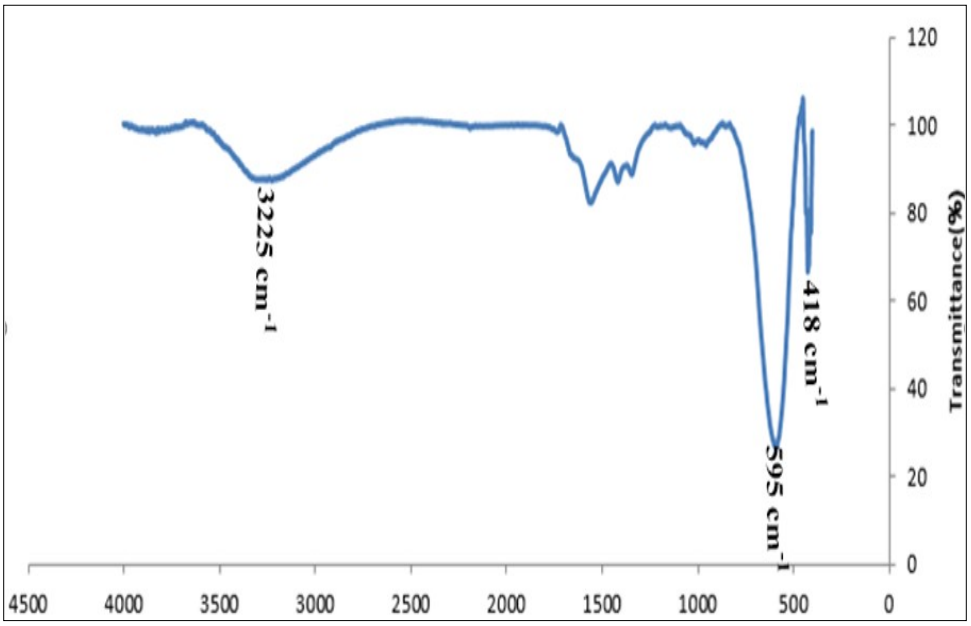
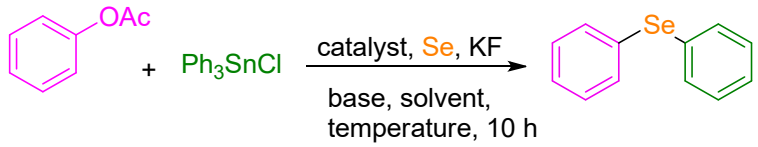


Fig. S5 FT-IR spectra of $NiFe_2O_4$ MNPs.

II. Reaction optimization studies

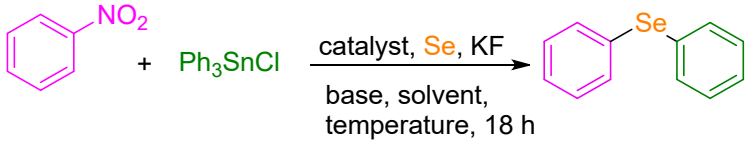
Table S1. Optimization of the reaction conditions for the reaction of phenyl acetate, triphenyltin chloride, and elemental selenium in the presence of homogenous[a] and heterogeneous[b] catalysts



Entry	Catalyst	Base	Solvent	Temperature. (°C)	GC Yield (%)
1	$Cu(OAc)_2$	K_2CO_3	Dioxane	100	35
2	$Cu(OAc)_2$	K_2CO_3	DMF	100	80
3[a]	**$Cu(OAc)_2$**	**K_2CO_3**	**PEG200**	**100**	**100**
4	$Cu(OAc)_2$	KOH	PEG200	100	trace
5	$Cu(OAc)_2$	NaOH	PEG200	100	trace
6	$Cu(OAc)_2$	Cs_2CO_3	PEG200	100	40
7	$CuCl_2$	K_2CO_3	PEG200	100	47
8	CuI	K_2CO_3	PEG200	100	55
9	$Cu(OAc)_2$	K_2CO_3	PEG200	80	61
10	$Cu(OAc)_2$	K_2CO_3	PEG200	90	78
11	$NiFe_2O_4$	K_2CO_3	PEG200	100	79
12	$NiFe_2O_4$	K_2CO_3	PEG200	110	89
13[b]	**$NiFe_2O_4$**	**K_2CO_3**	**PEG200**	**120**	**99**
14	$CuFe_2O_4$	K_2CO_3	PEG200	120	88
15	$CuNiFe_2O_4$	K_2CO_3	PEG200	120	87

[a]Reactions conditions: phenyl acetate (1 mmol), triphenyltin chloride (0.5 mmol), Se (1.5 mmol), $Cu(OAc)_2$ (25 mol %), KF (3 mmol), K_2CO_3 (2 mmol), solvent (2 mL).
[b]Reactions conditions: phenylacetate (1 mmol), triphenyltin chloride (0.5 mmol), Se (1.5 mmol), $NiFe_2O_4$ (25 mol %), KF (3 mmol), K_2CO_3 (2 mmol), solvent (2 mL).
[a],[b] Most effective reaction conditions.

Table S2. Optimization of the reaction conditions for the reaction of nitrobenzene, triphenyltin chloride and elemental selenium in the presence of homogenous[a] and heterogeneous[b] catalyst



Entry	Catalyst	Base	Solvent	Temperature (°C)	GC Yield (%)
1	$Cu(OAc)_2$	K_2CO_3	Dioxane	110	20
2	$Cu(OAc)_2$	K_2CO_3	DMF	110	65
3[a]	**$Cu(OAc)_2$**	**K_2CO_3**	**PEG200**	**110**	**100**
4	$Cu(OAc)_2$	KOH	PEG200	110	trace
5	$Cu(OAc)_2$	NaOH	PEG200	110	trace
6	$Cu(OAc)_2$	Cs_2CO_3	PEG200	110	28
7	$CuCl_2$	K_2CO_3	PEG200	110	36
8	CuI	K_2CO_3	PEG200	110	49
9	$Cu(OAc)_2$	K_2CO_3	PEG200	90	58
10	$Cu(OAc)_2$	K_2CO_3	PEG200	100	70
11	$NiFe_2O_4$	K_2CO_3	PEG200	110	74
12	$NiFe_2O_4$	K_2CO_3	PEG200	120	85
13[b]	**$NiFe_2O_4$**	**K_2CO_3**	**PEG200**	**130**	**98**
14	$CuFe_2O_4$	K_2CO_3	PEG200	130	85
15	$CuNiFe_2O_4$	K_2CO_3	PEG200	130	83

[a]Reactions conditions: nitrobenzene (1 mmol), triphenyltin chloride (0.5 mmol), Se (1.5 mmol), $Cu(OAc)_2$ (20 mol %), KF (3 mmol), K_2CO_3 (4 mmol), solvent (2 mL).

[b]Reactions conditions: nitrobenzene (1 mmol), Se (1.5 mmol), triphenyltin chloride (0.5 mmol), $NiFe_2O_4$ (25 mol %), KF (3 mmol), K_2CO_3 (4 mmol), solvent (2 mL).

III. Mass, ^{1}H NMR

Diphenyl-selenid

6H); ^{13}C NMR ($CDCl_3$,

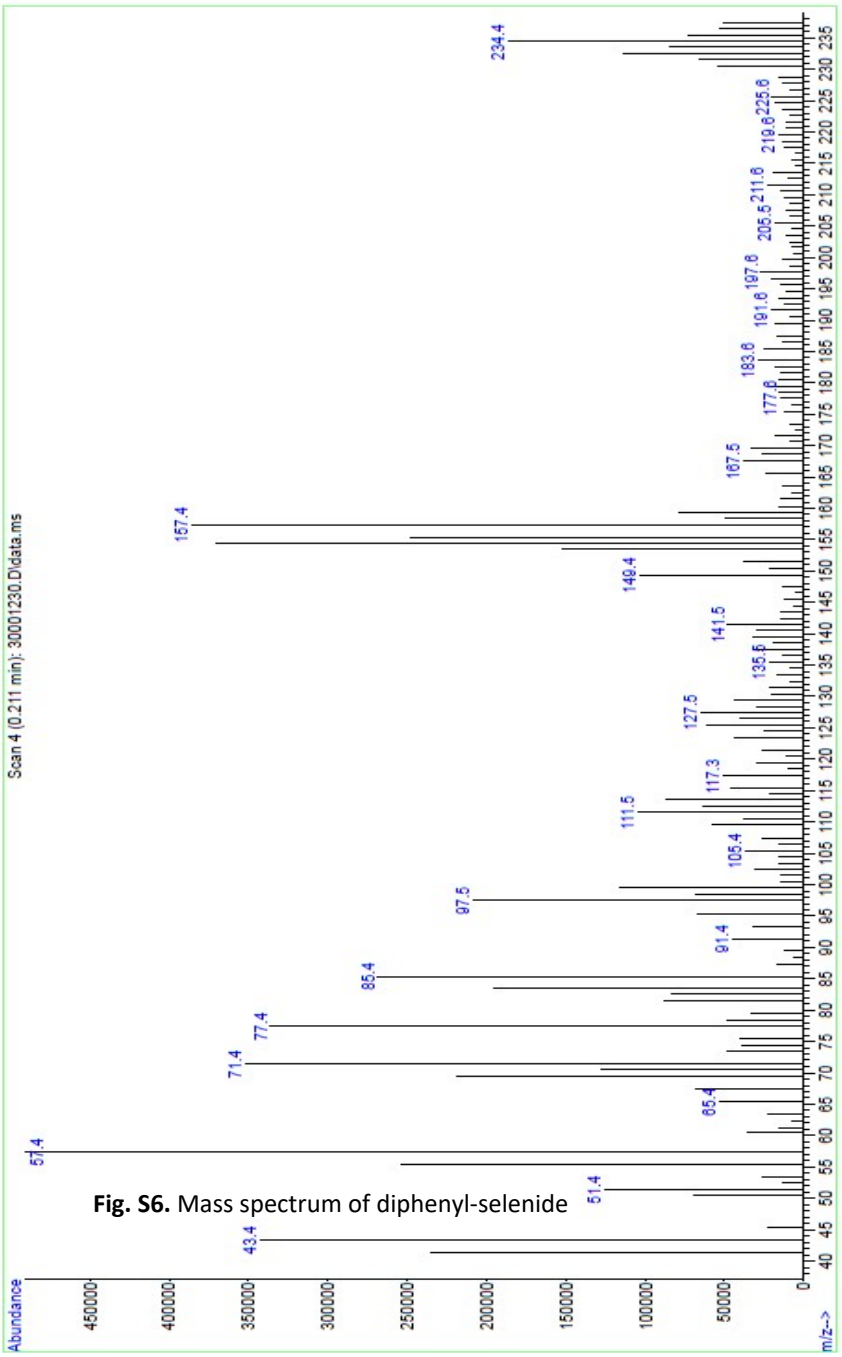


Fig. S6. Mass spectrum of diphenyl-selenide

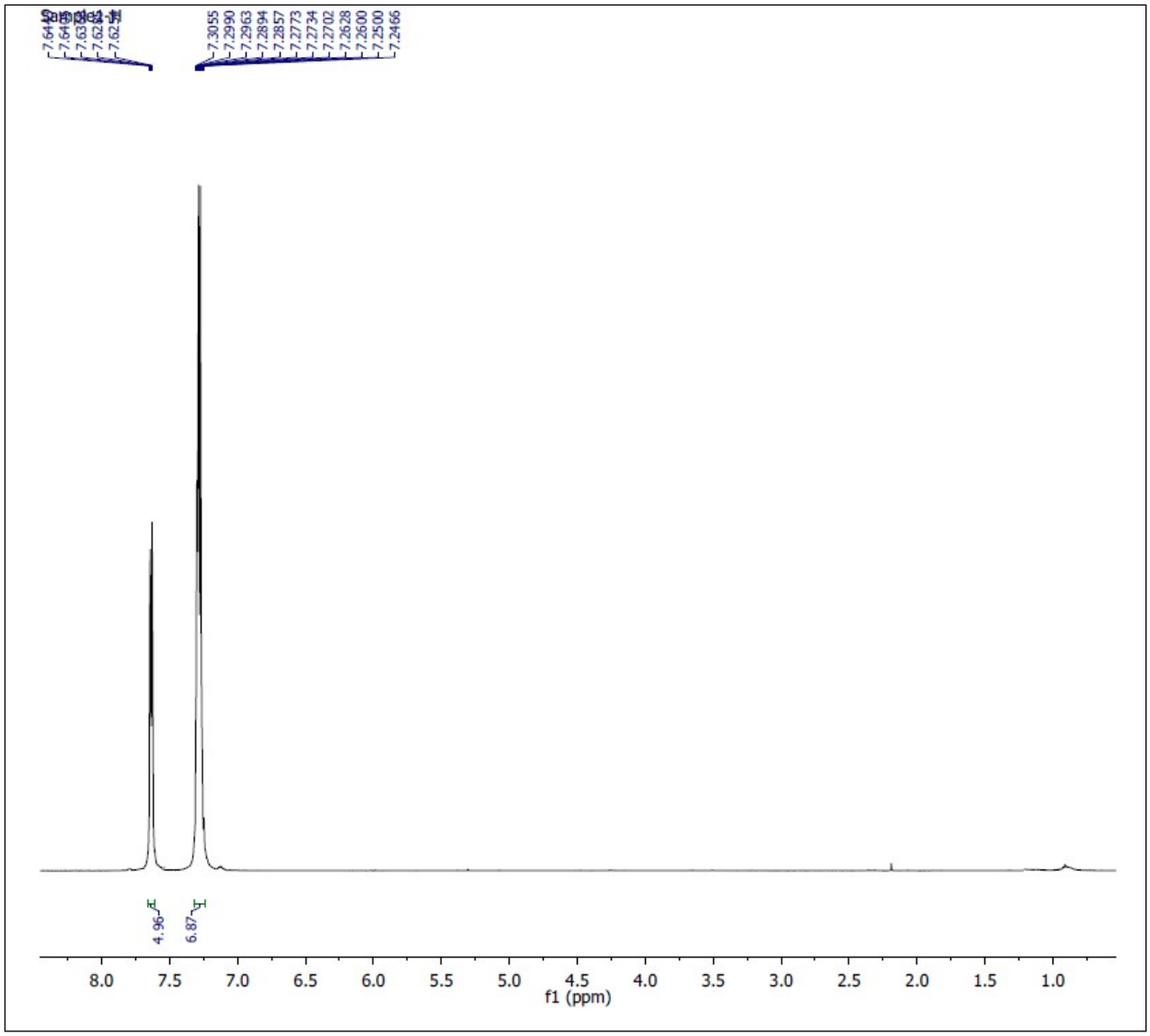


Fig. S7. ^{1}H NMR spectrum of diphenyl-selenide in $CDCl_3$

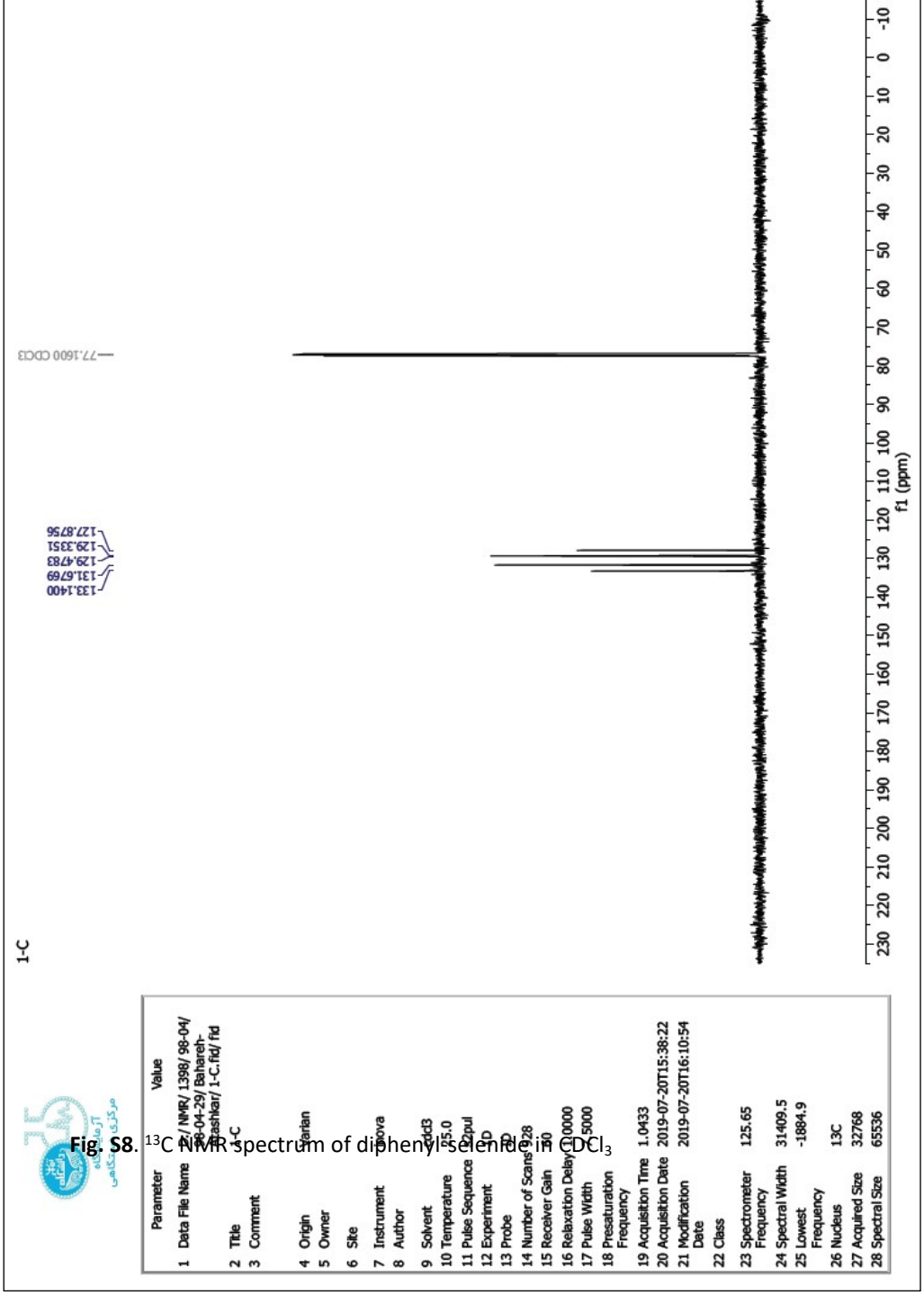


Fig. S8. ^{13}C NMR spectrum of diphenyl selenide in $CDCl_3$

4-Tolyl-phenyl-selenide [1]: oil: MS: 248.7 m/z; ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.67-7.65 (m, 2H); 7.47-7.46 (m, 2H); 7.32-7.26 (m, 3H); 7.16-7.11 (m, 2H); 2.38 (s, 3H); ^{13}C NMR ($CDCl_3$, 500 MHz): 134.0, 132.2, 131.7, 130.3, 129.3, 127.9, 127.0, 29.8.

Fig. S10. Expanded mass spectrum of 4-Tolyl-phenyl-selenide

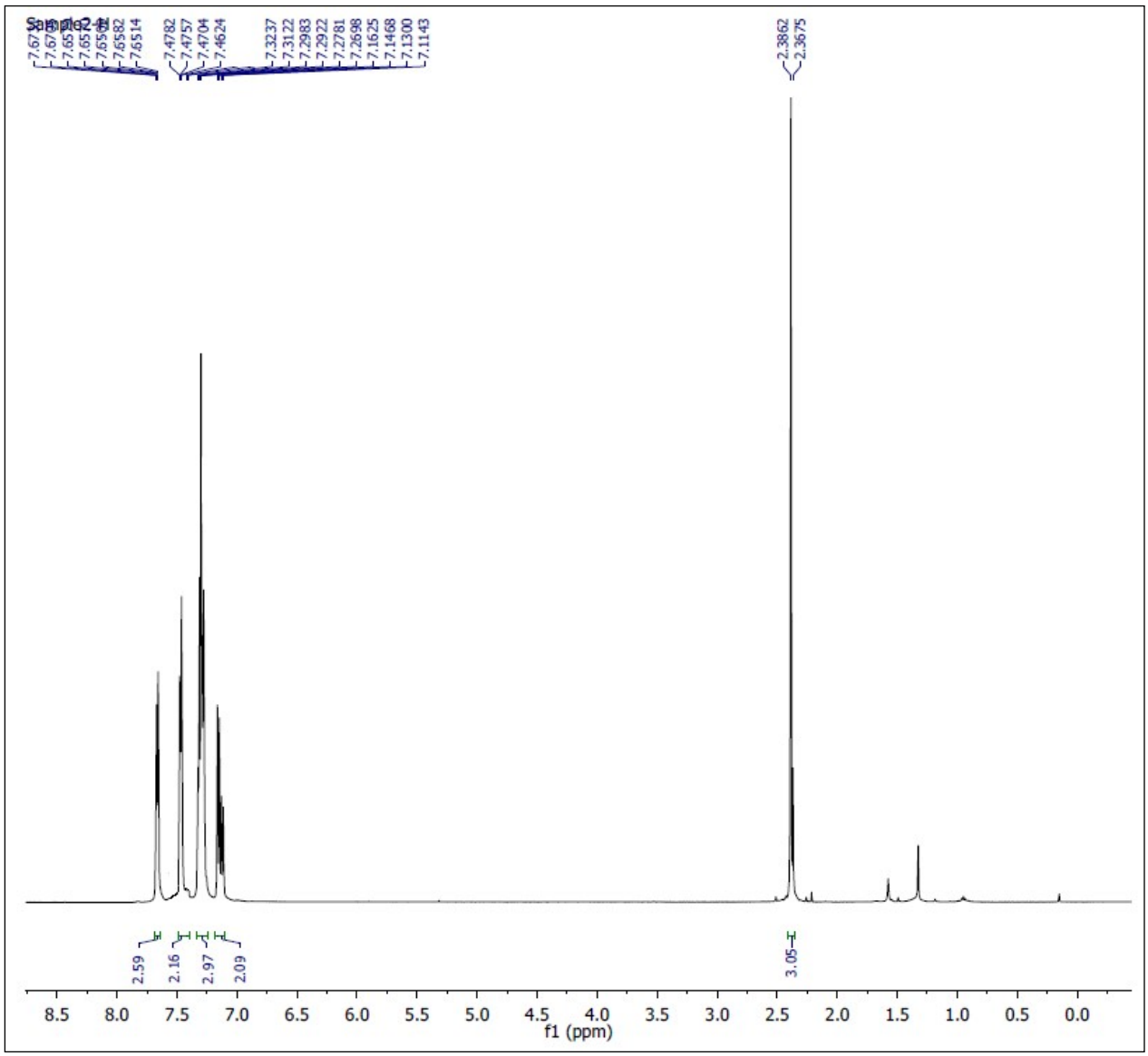


Fig. S11. ^{1}H NMR spectrum of 4-Tolyl-phenyl-selenide

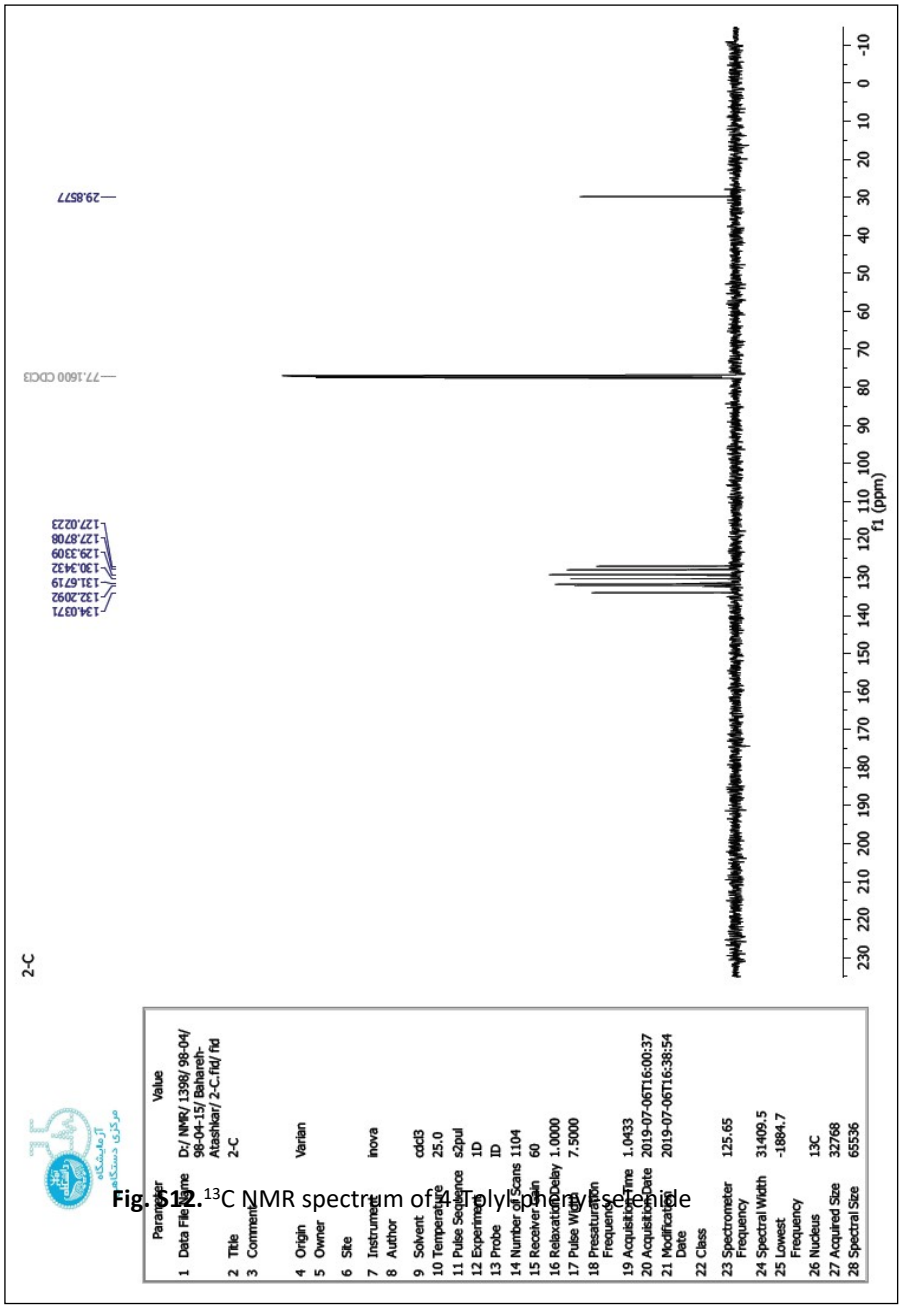


Fig. S12. ^{13}C NMR spectrum of 4-Tolyl phenylselenide

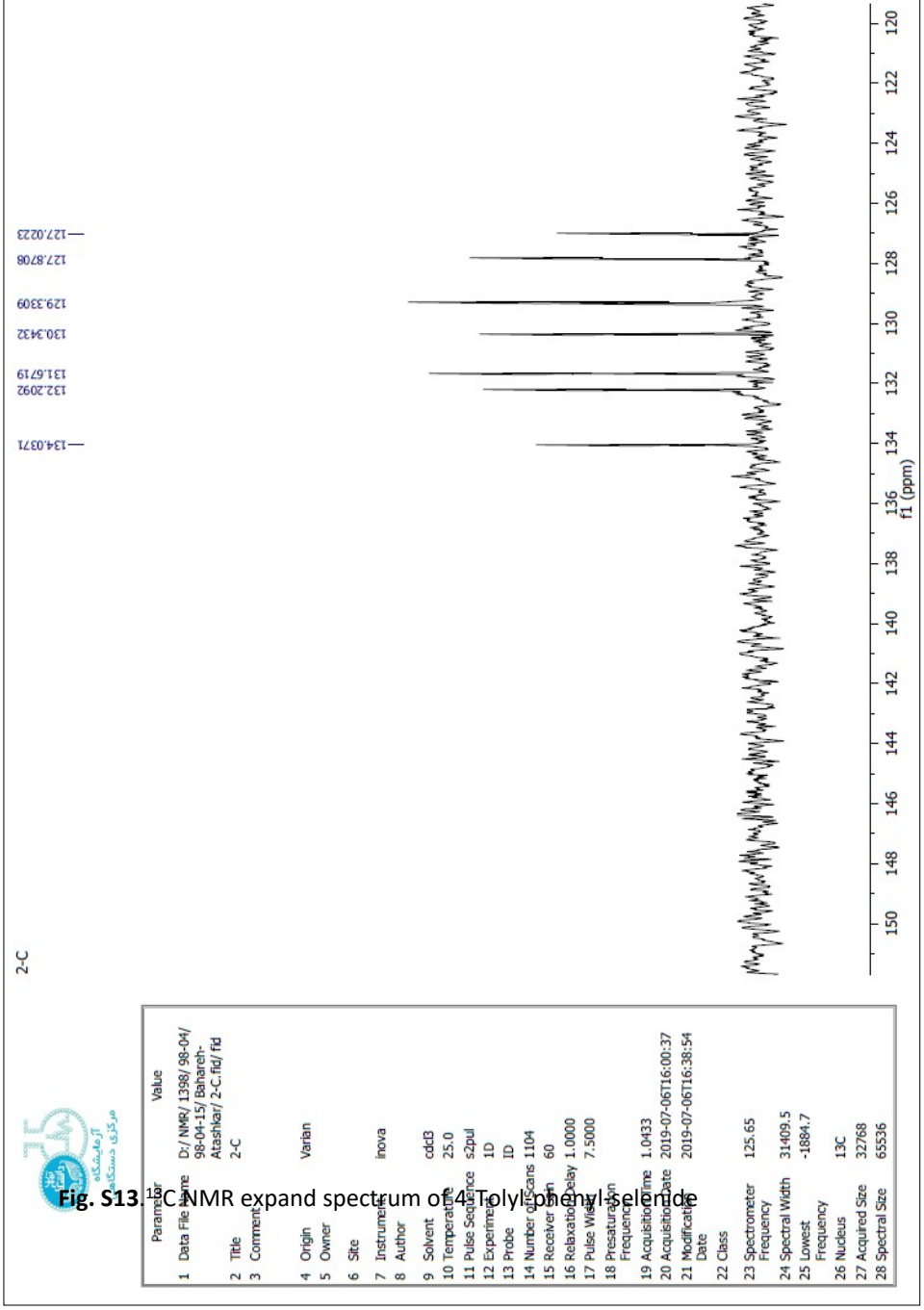


Fig. S13. ^{13}C NMR expand spectrum of 4-Tolyl-phenyl-selenide

4-Chlorophenyl-phenyl-selenide [1]: oil: MS: 268 m/e; ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.73 (d, J = 10 Hz, 2H); 7.61 (d, J = 10 Hz, 2H); 7.28-7.26 (m, 3H); 7.24-7.12 (m, 2H); ^{13}C NMR ($CDCl_3$, 500 MHz): 134.9, 133.7, 133.1, 131.9, 130.7, 129.9, 128.1.

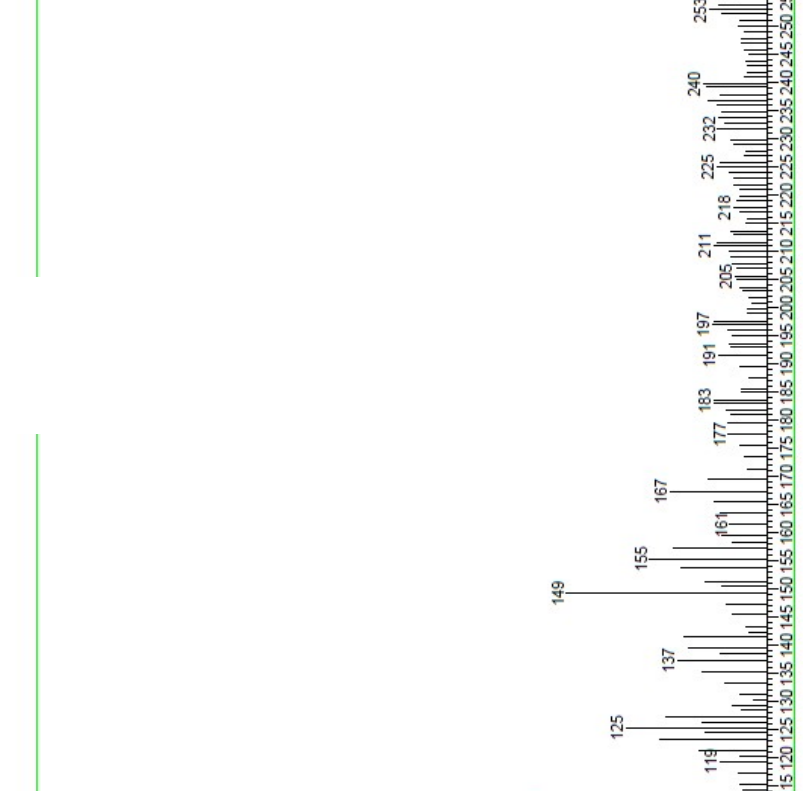


Fig. S14. Mass spectrum of

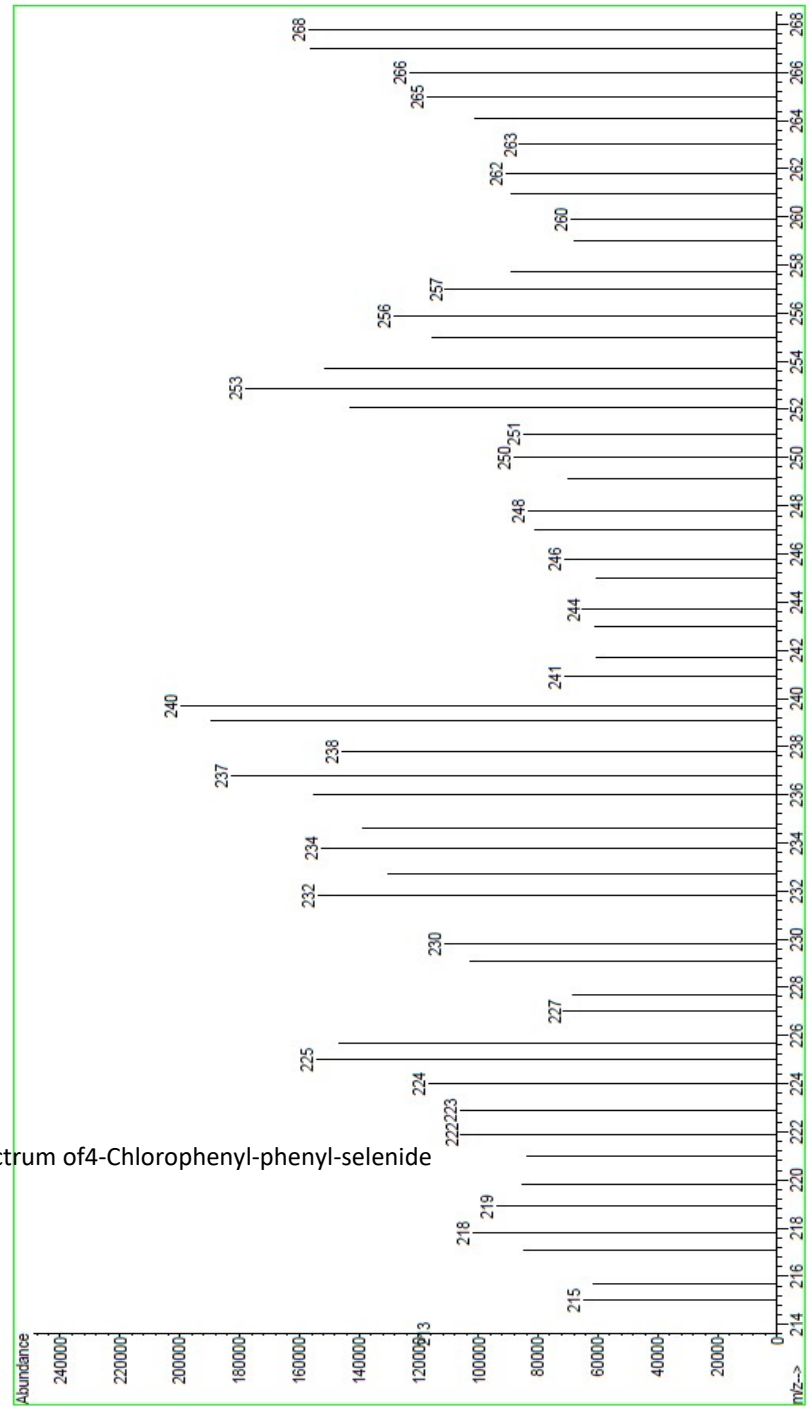


Fig. S15. Expanded mass spectrum of4-Chlorophenyl-phenyl-selenide

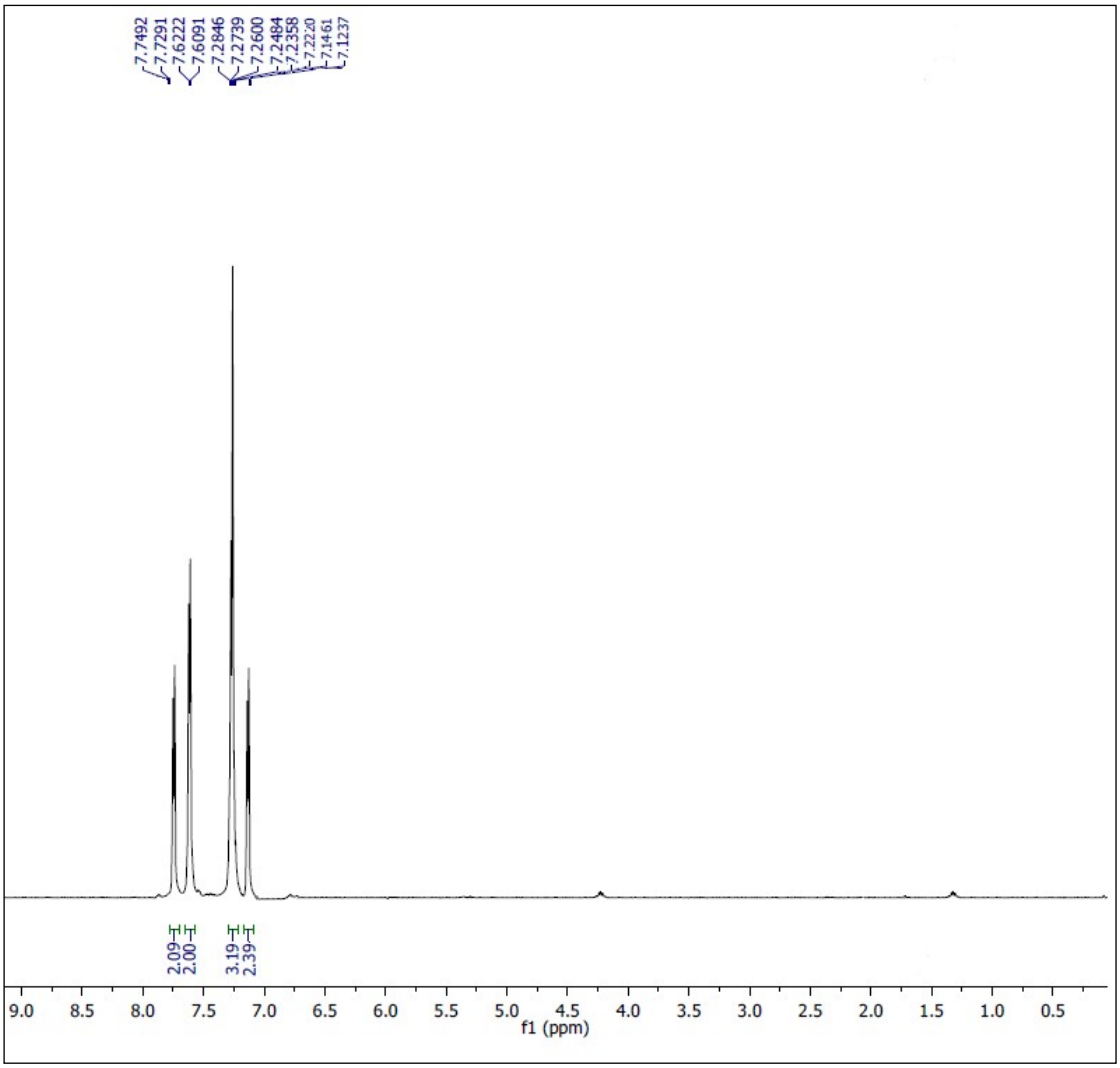


Fig. S16. ^{1}H NMR spectrum of 4-Chlorophenyl-phenyl-selenide

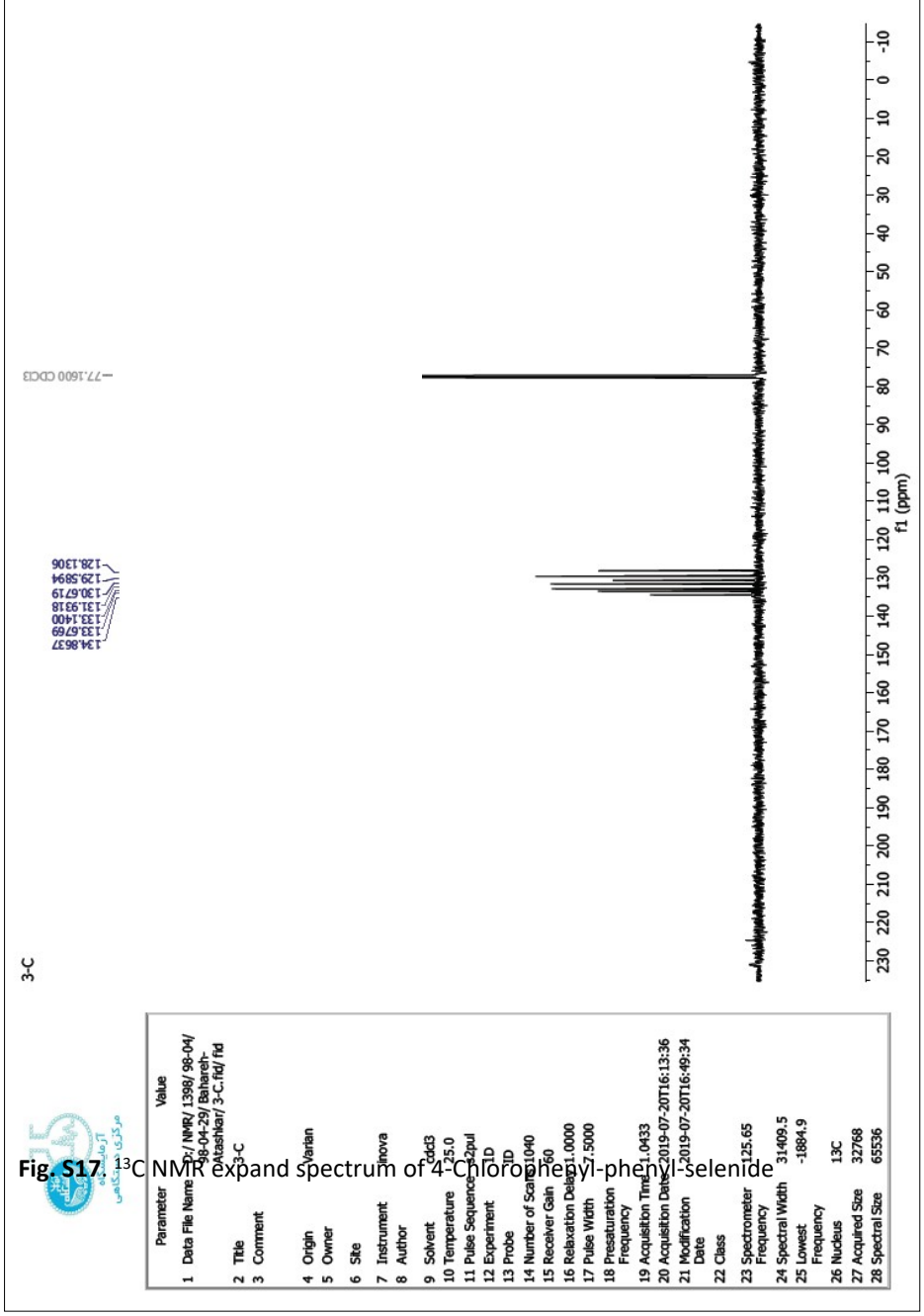


Fig. S17. ^{13}C NMR expand spectrum of 4-Chlorophenyl-phenyl-selenide

2-Tolyl-phenyl-selenide [1]**:** oil: MS: 248.1 m/e; ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.62-7.49 (m, 2H); 7.48-7.47 (m, 1H); 7.27-7.25 (m, 5H); 7.23-7.22 (m, 1H); 2.43 (s, 3H).

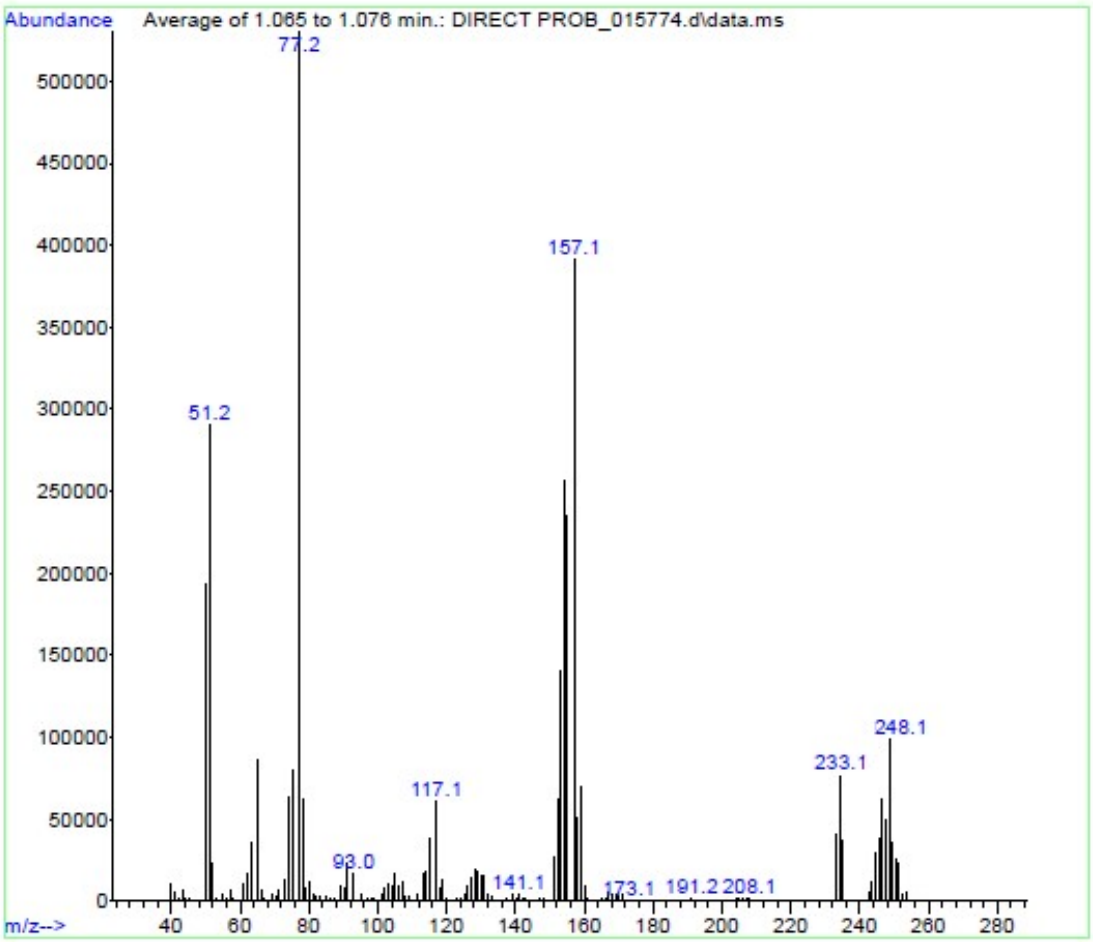


Fig. S18. Mass spectrum of 2-Tolyl-phenyl-selenide

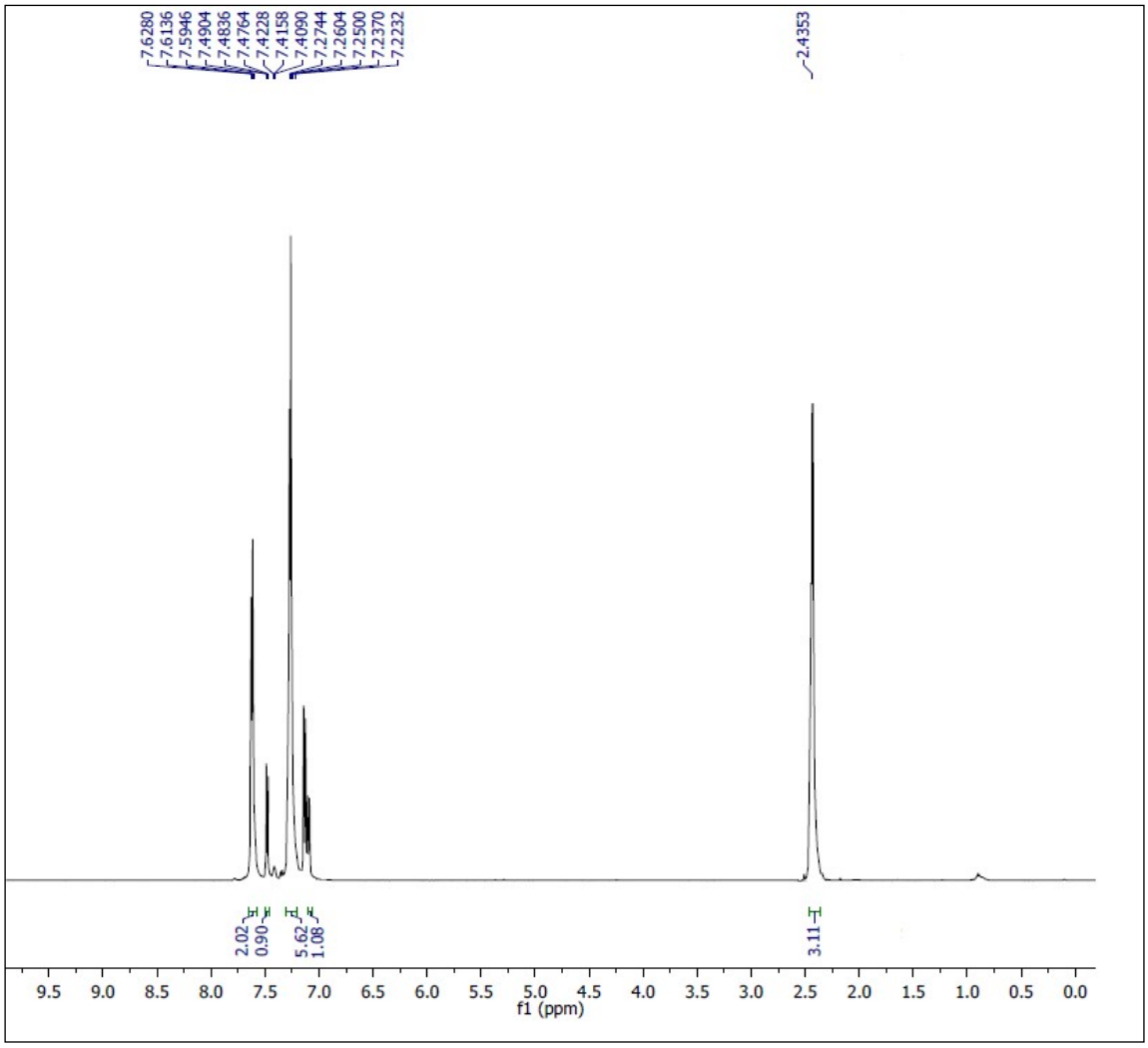


Fig. S19. ^{1}H NMR spectrum of 2-Tolyl-phenyl-selenide

2-Nitrophenyl-phenyl $_3$, 500 MHz):

δ 8.31 (dd, *J* = 9.15, 0.6 Hz 7.75, 1H).

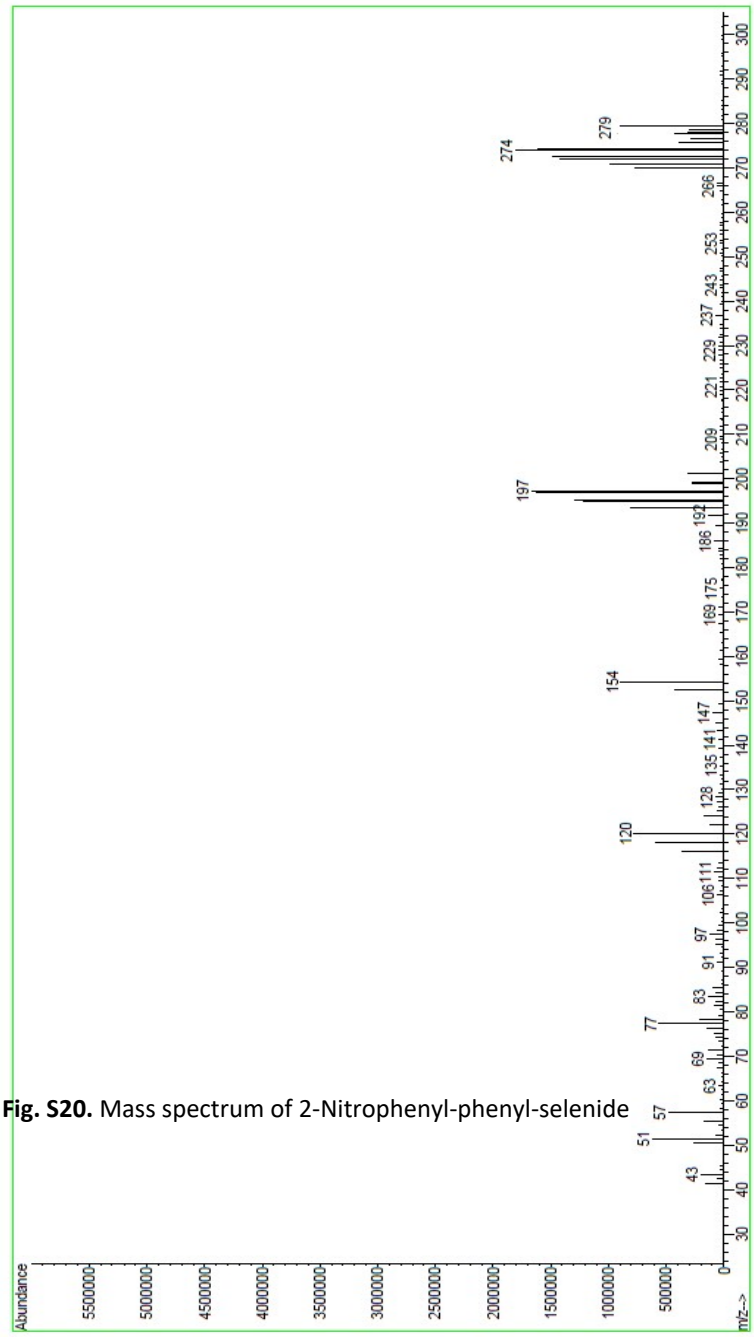


Fig. S20. Mass spectrum of 2-Nitrophenyl-phenyl-selenide

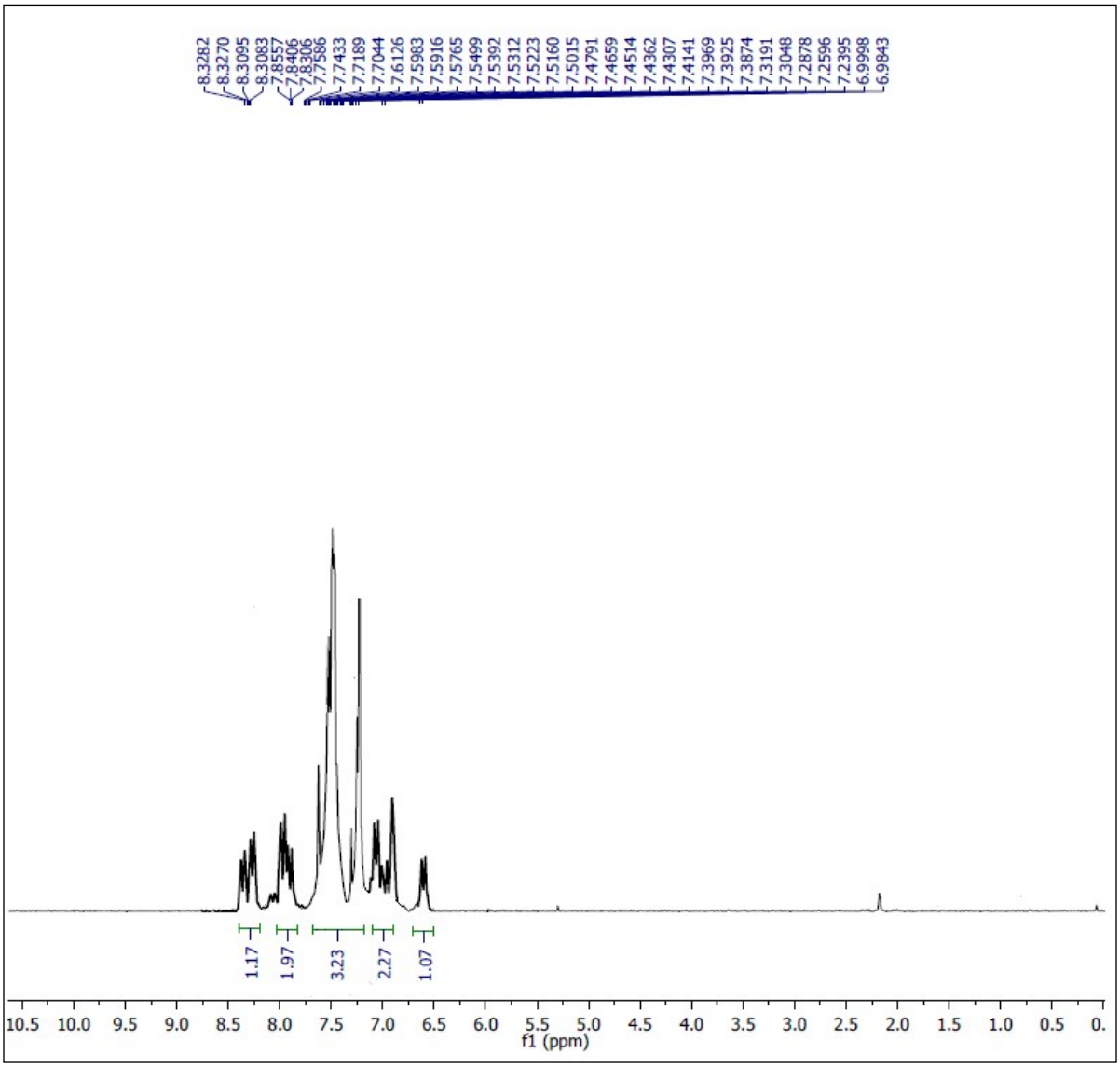


Fig. 21S. ^{1}H NMR spectrum of 2-Nitrophenyl-phenyl-selenide

3-Nitrophenyl-phen

. (s, 1H);

8.07 (dd, J = 10, 2 Hz, 1H

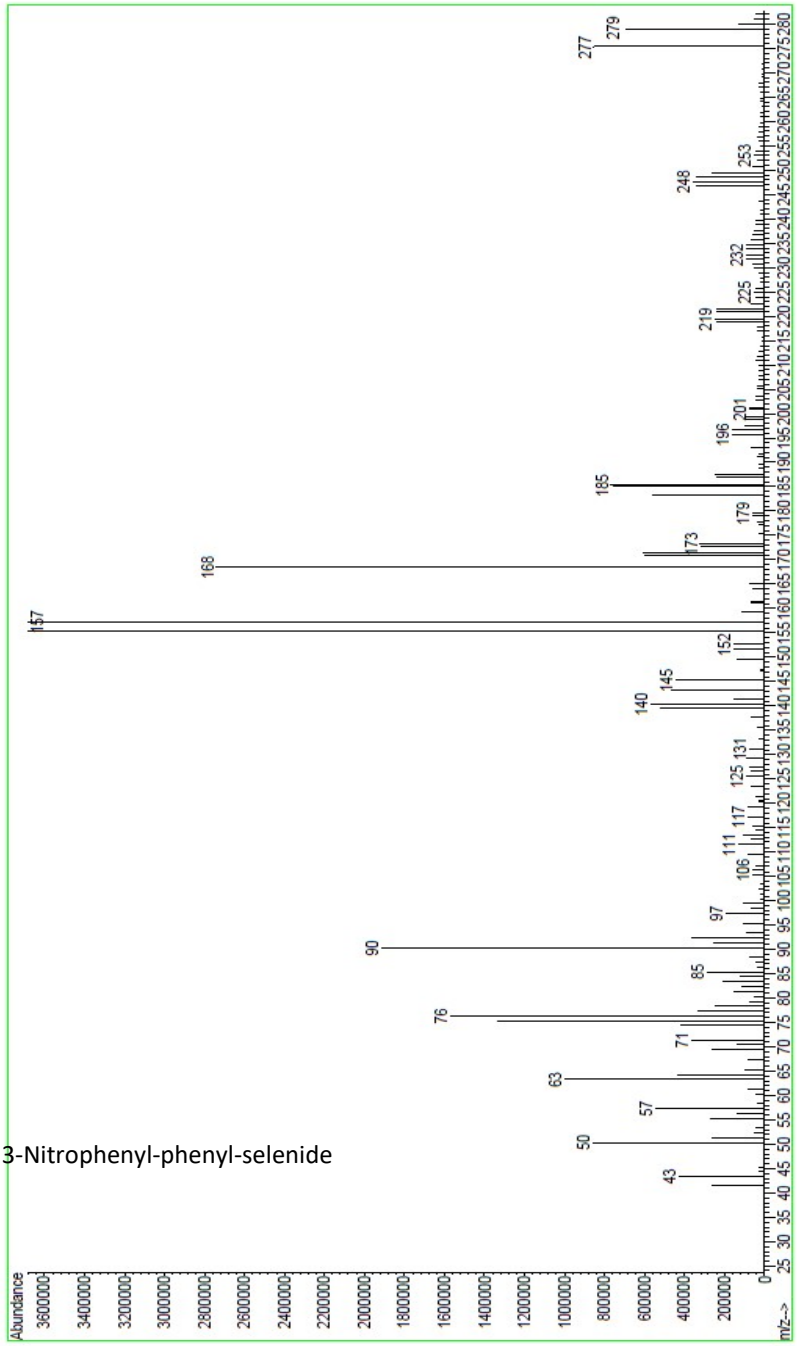


Fig. S22. Mass spectrum of 3-Nitrophenyl-phenyl-selenide

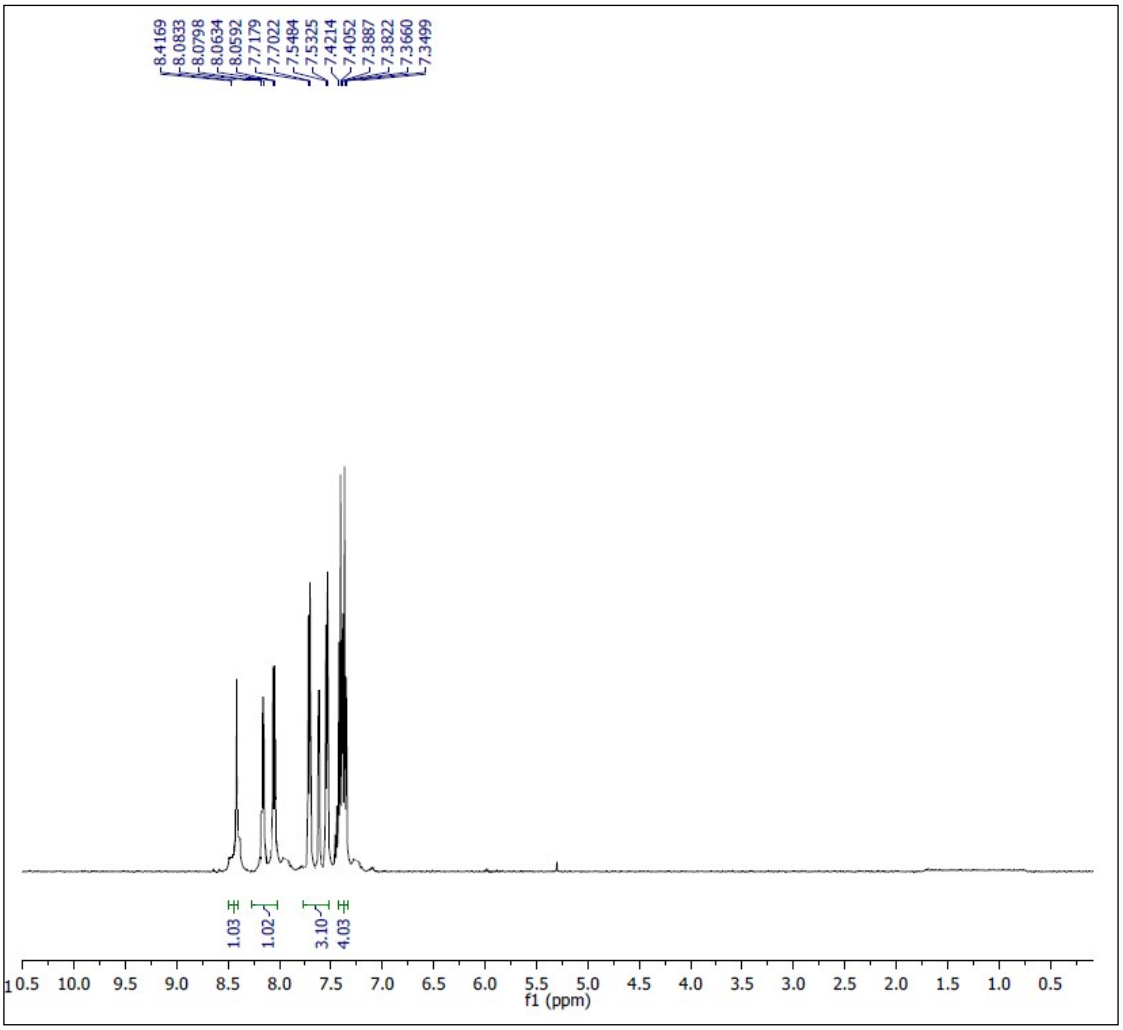


Fig. S23.^{1}H NMR spectrum of 3-Nitrophenyl-phenyl-selenide

Naphthalen-2-yl(phenyl

8.01 (m, 1H); 7.62-7.59 (m, 1H

5 8.12-

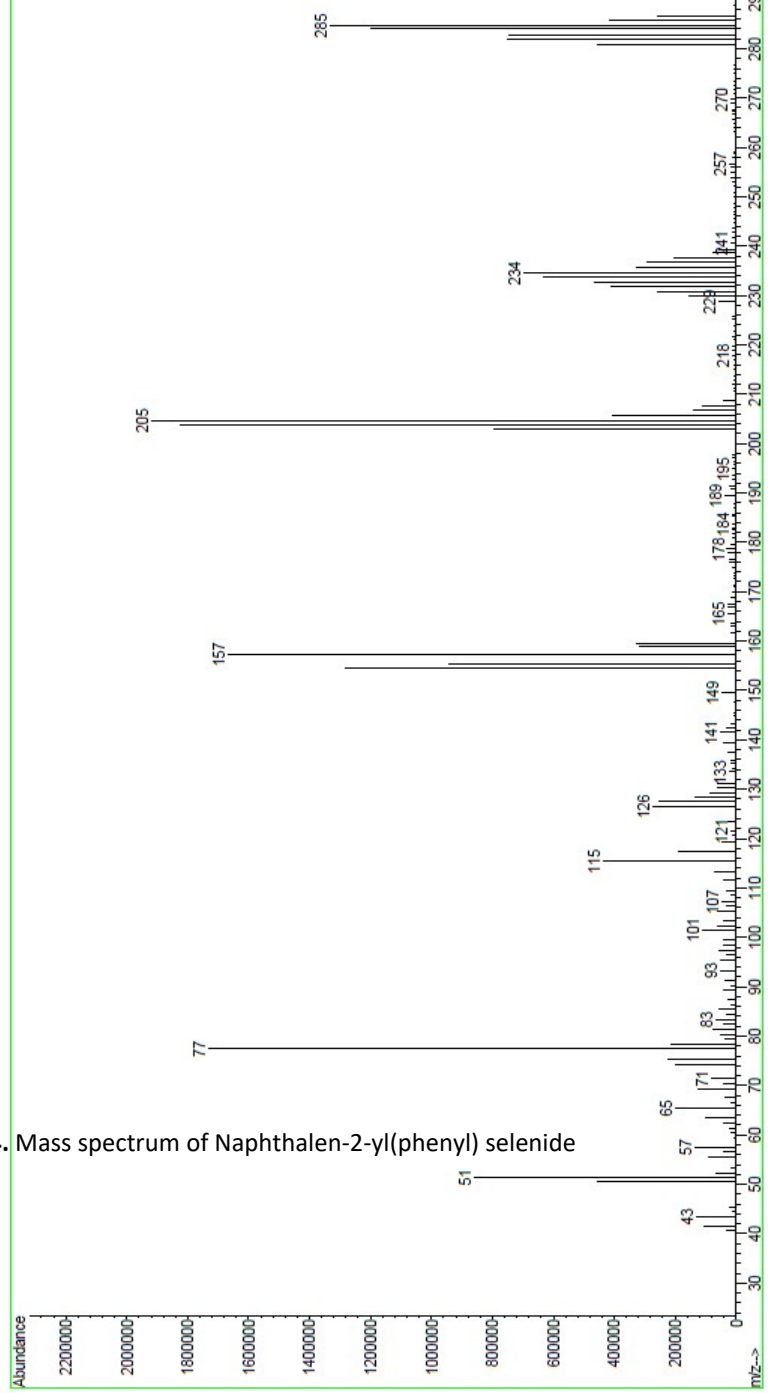


Fig. S24. Mass spectrum of Naphthalen-2-yl(phenyl) selenide

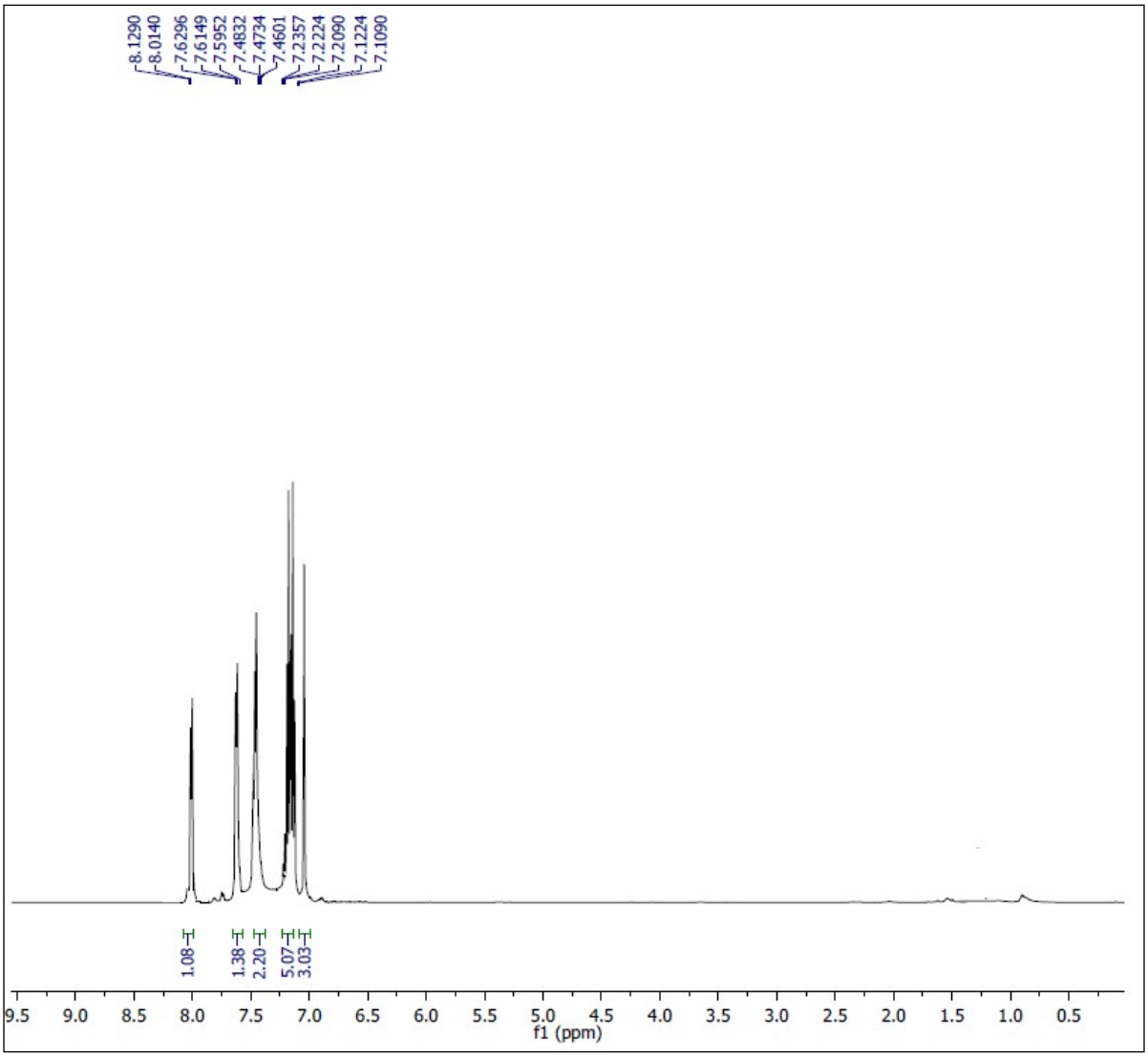


Fig. S25. ^{1}H NMR spectrum of Naphthalen-2-yl(phenyl) selenide

3,5-Bis(trifluoromethyl)phenyl phenyl selenide [5]**:** Colorless oil: MS: 370 m/z; ^{1}H NMR ($CDCl_3$, 500 MHz): *δ* 8.03 (s, 2H); 7.73 (s, 1H); 7.30-7.29 (m, 2H); 7.28-7.25 (m, 3H).

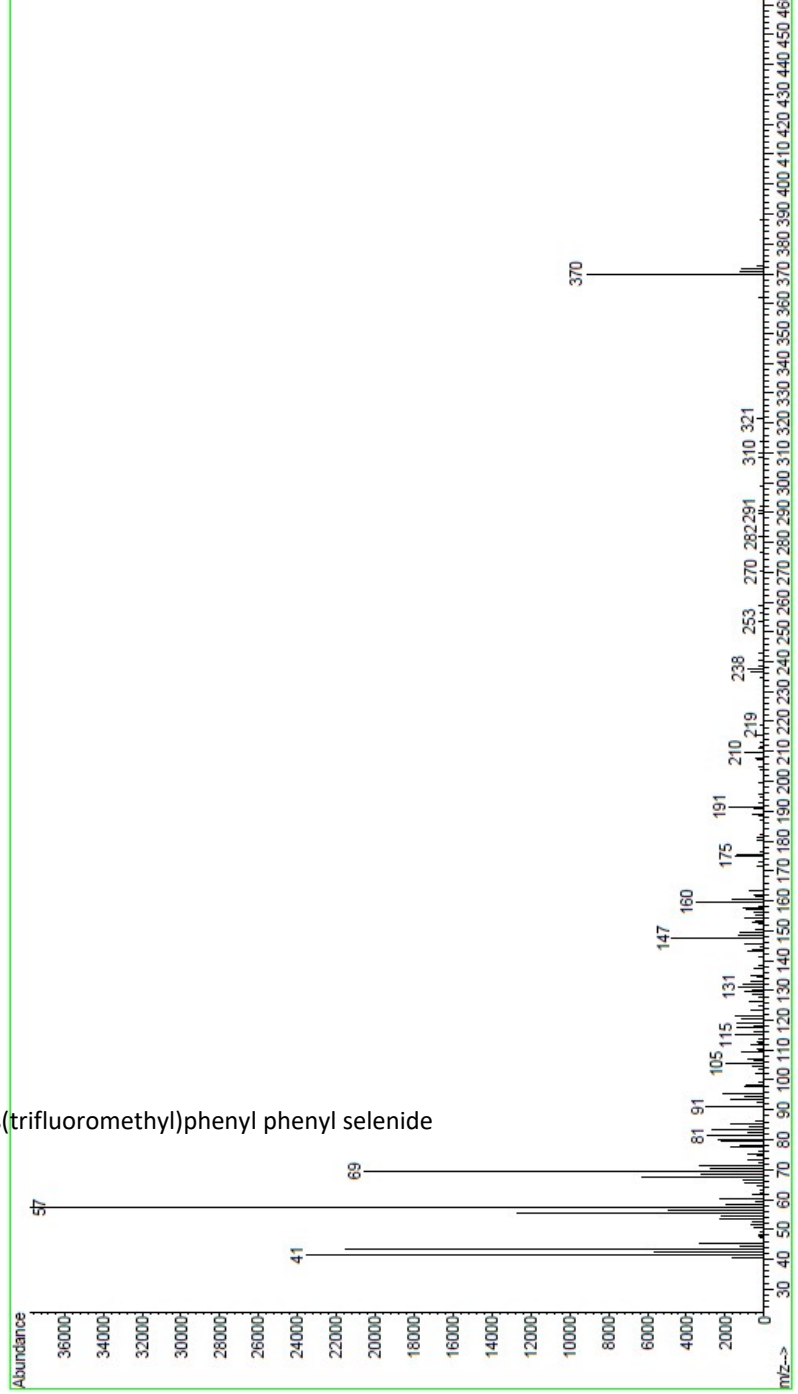


Fig. S26. Mass spectrum of 3,5-Bis(trifluoromethyl)phenyl phenyl selenide

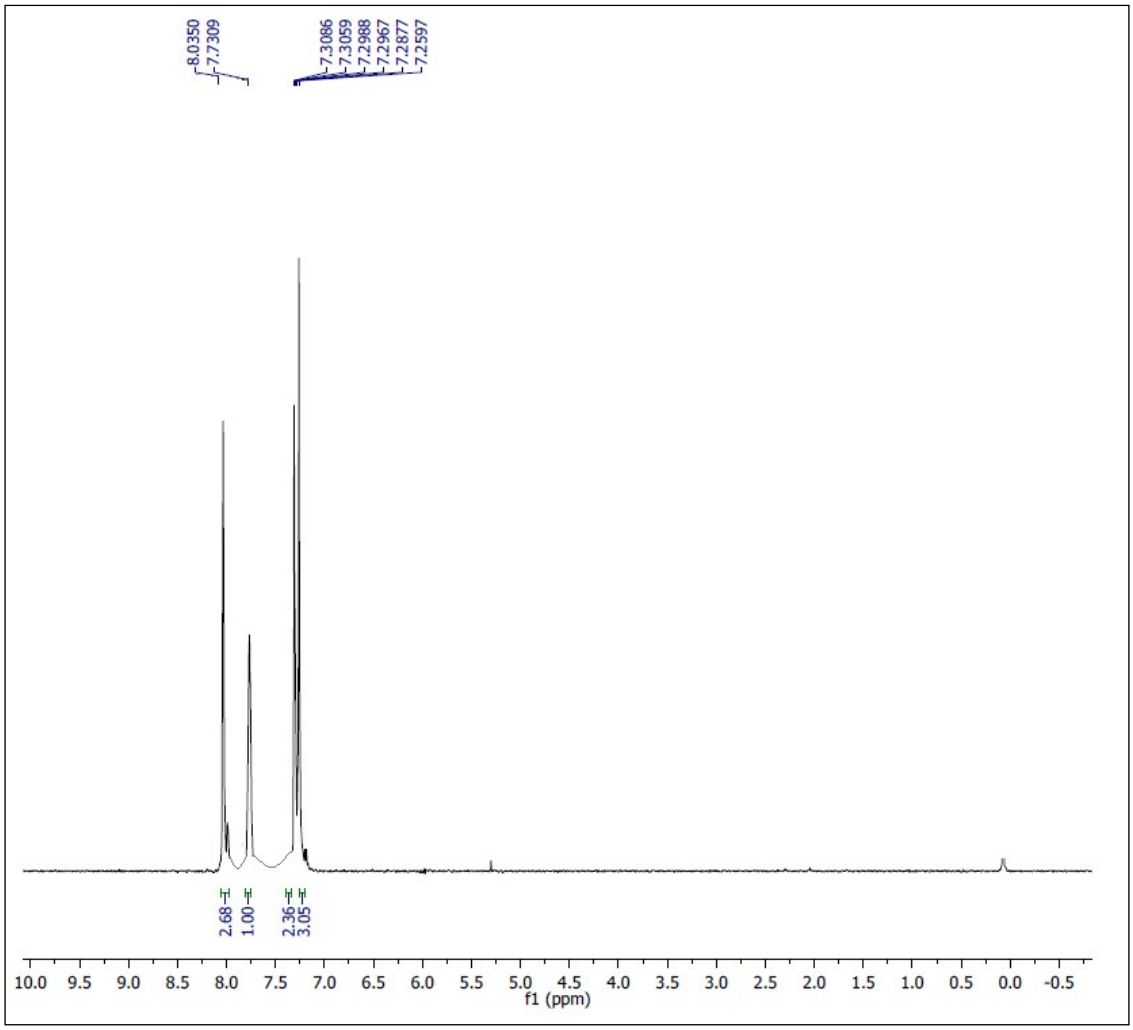


Fig. S27. ^{1}H NMR spectrum of 3,5-Bis(trifluoromethyl)phenyl phenyl selenide

Naphthalen-1-yl(phenyl) s ·7.74
(m, 1H); 7.62-7.61 (m, 2H); 7.45

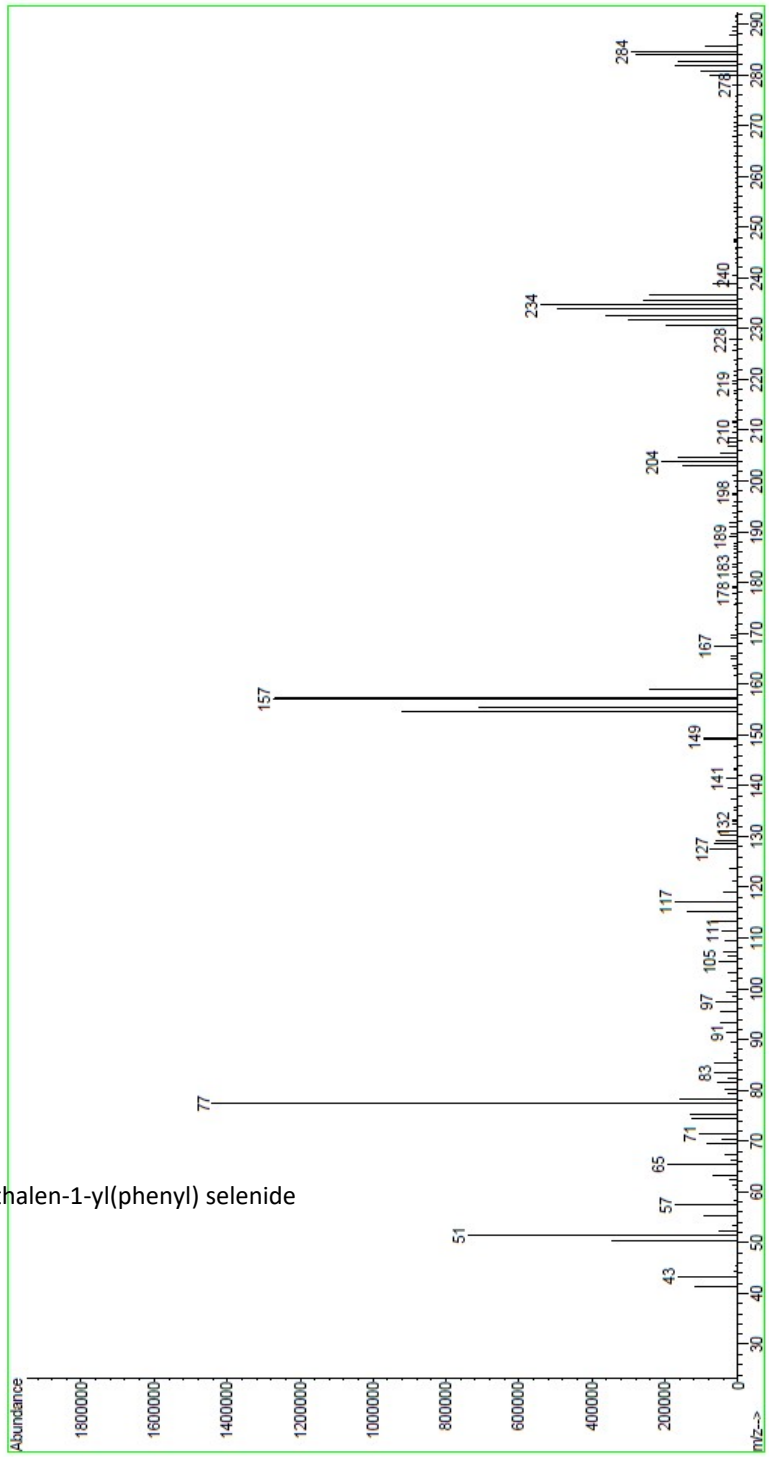


Fig. S28. Mass spectrum of Naphthalen-1-yl(phenyl) selenide

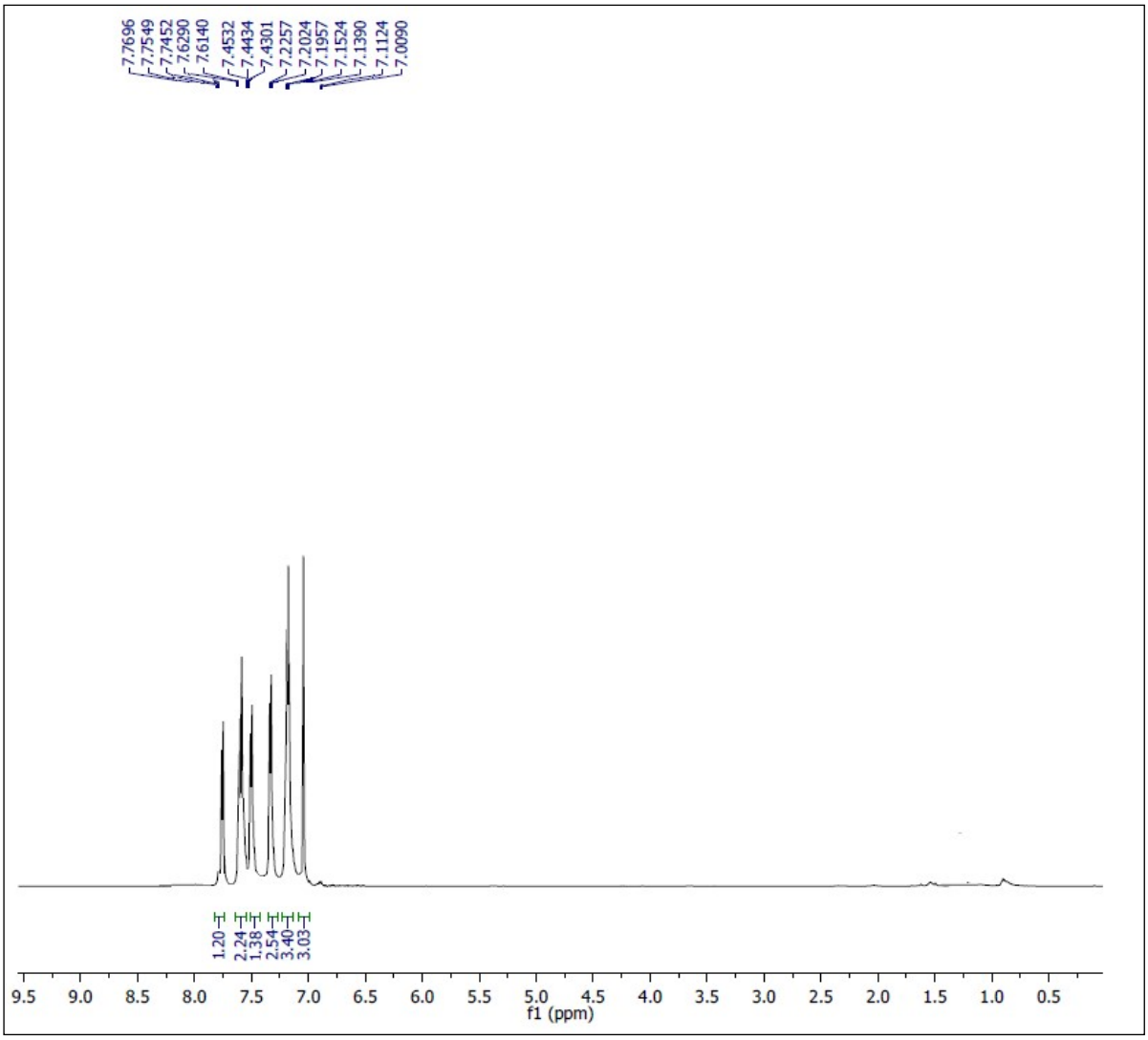


Fig. S29.[1]H NMR spectrum of Naphthalen-1-yl(phenyl) selenide

4-Flourophenyl-phen 59(m,

2H), 7.28-7.22 (m, 6H), 6.9

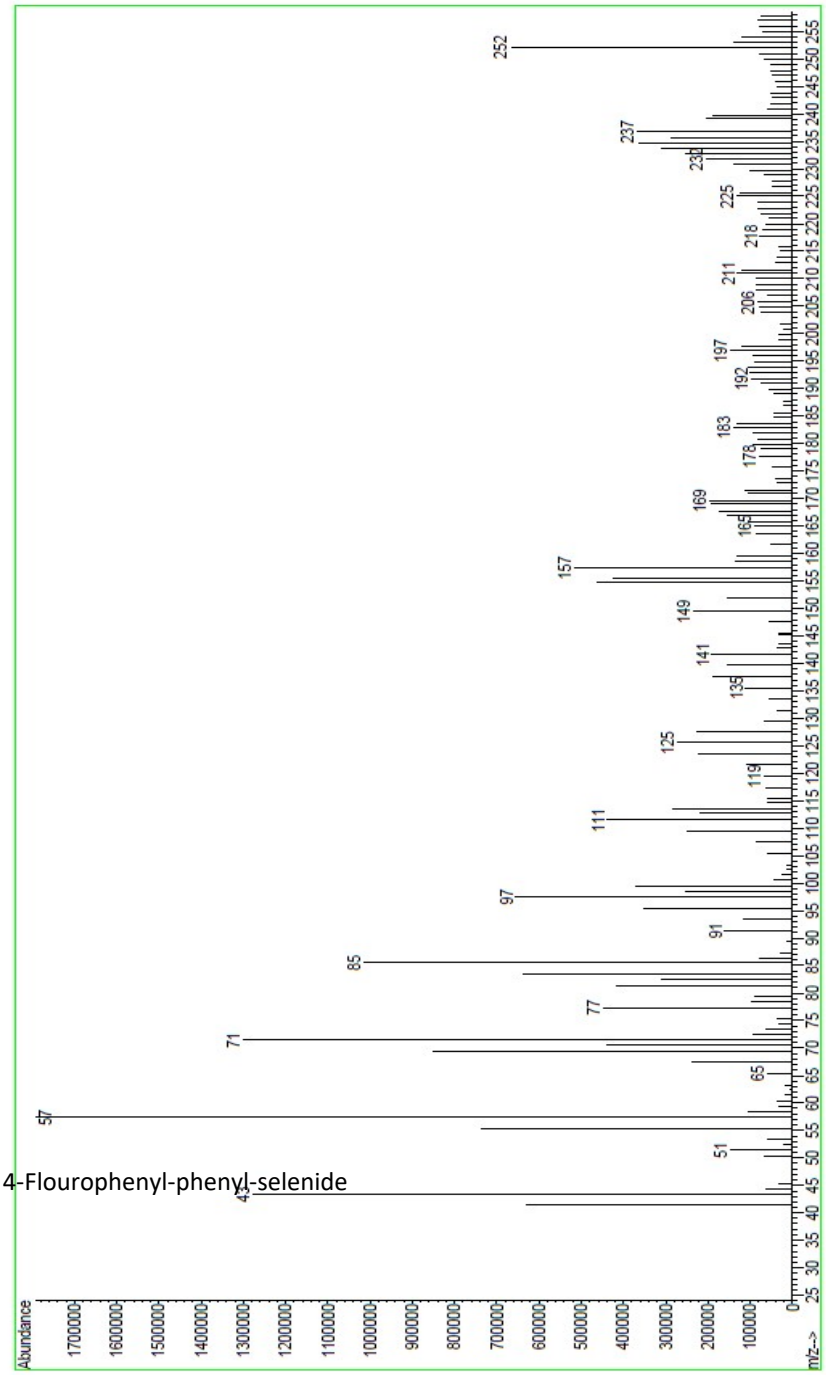


Fig. S30. Mass spectrum of 4-Flourophenyl-phenyl-selenide

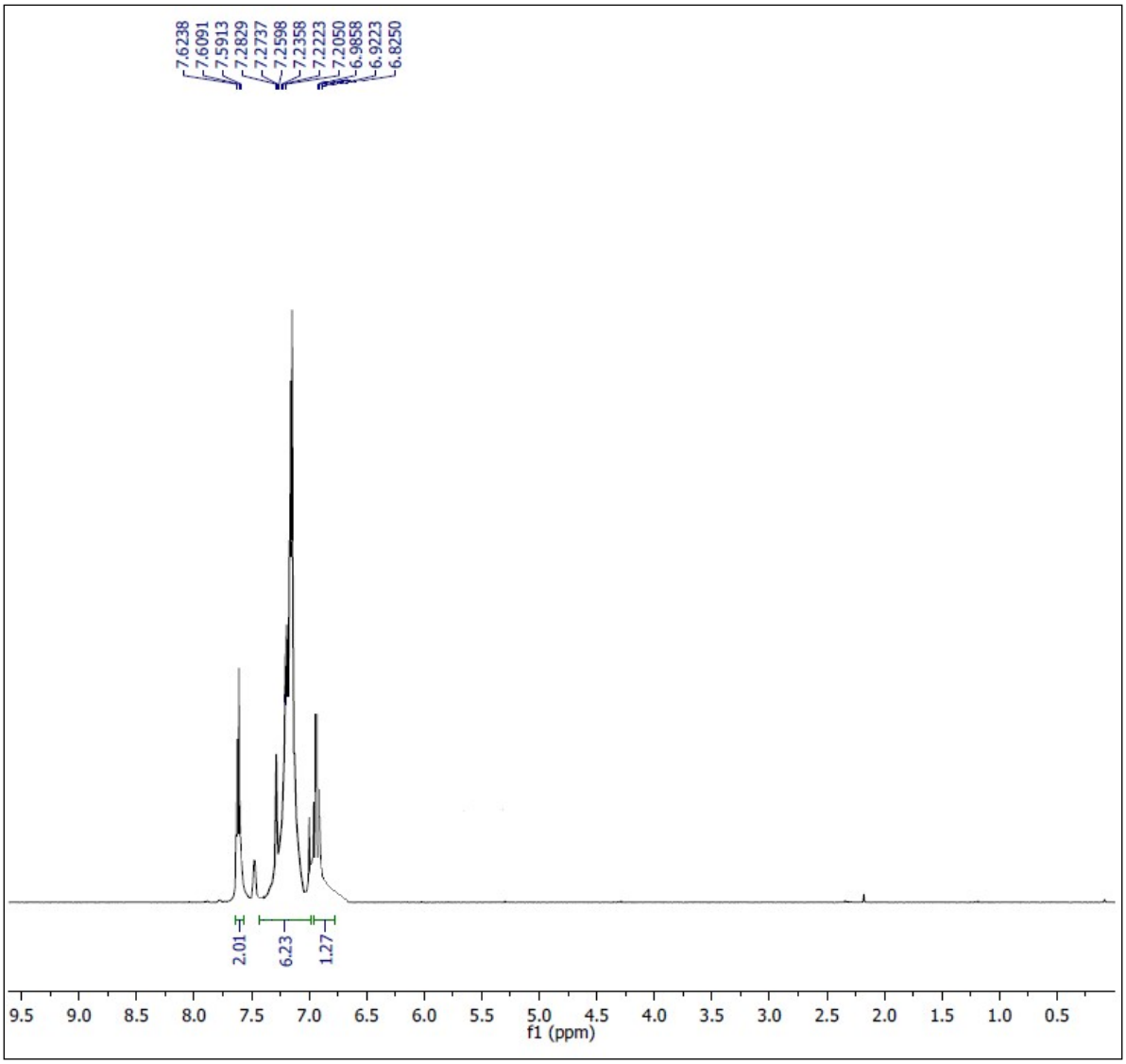
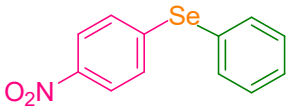


Fig. S31.[1]H NMR spectrum of 4-Flourophenyl-phenyl-selenide

4-Nitrophenyl-phenyl-se $CDCl_3$, 500 MHz): δ 8.05 (dd, J = 10, 2 Hz,



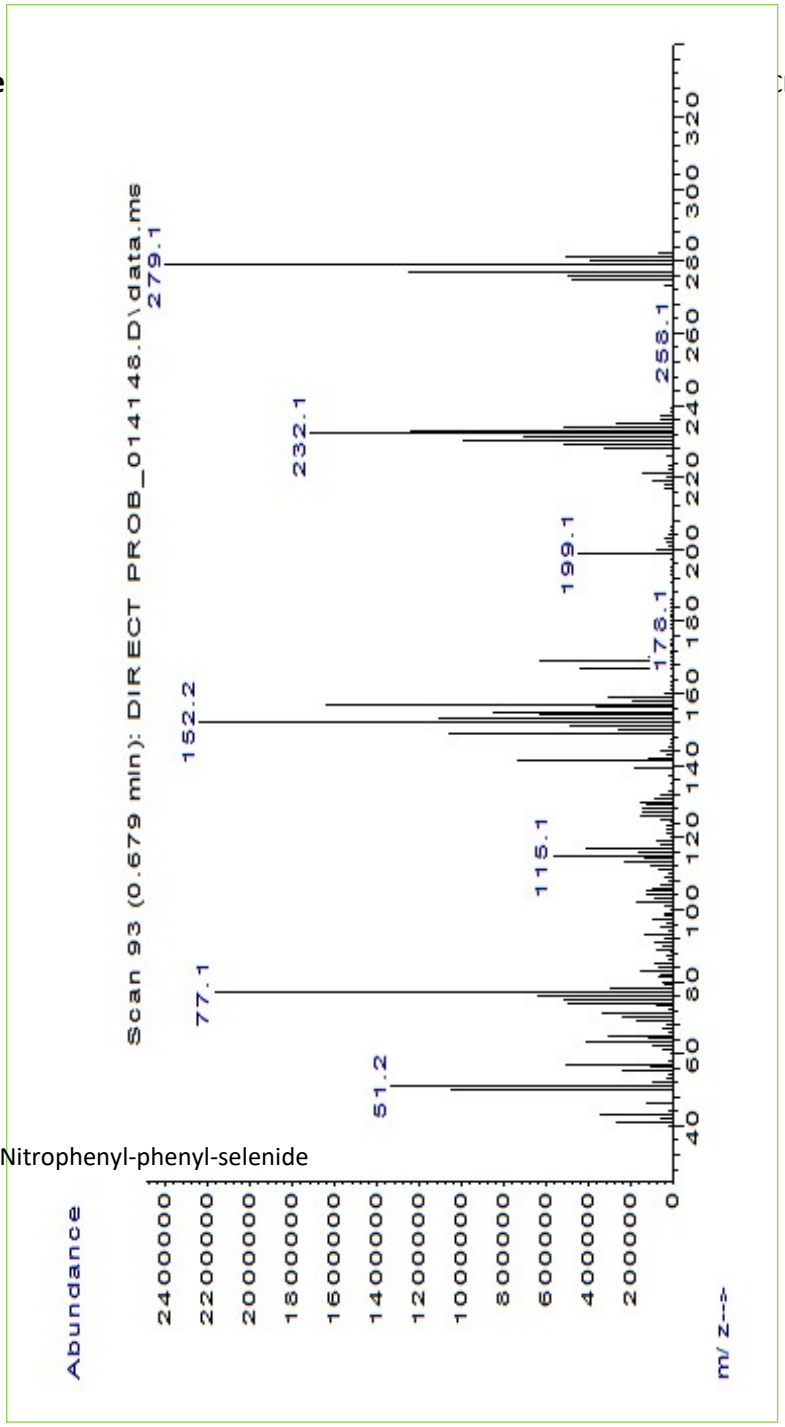


Fig. S32. Mass spectrum of 4-Nitrophenyl-phenyl-selenide

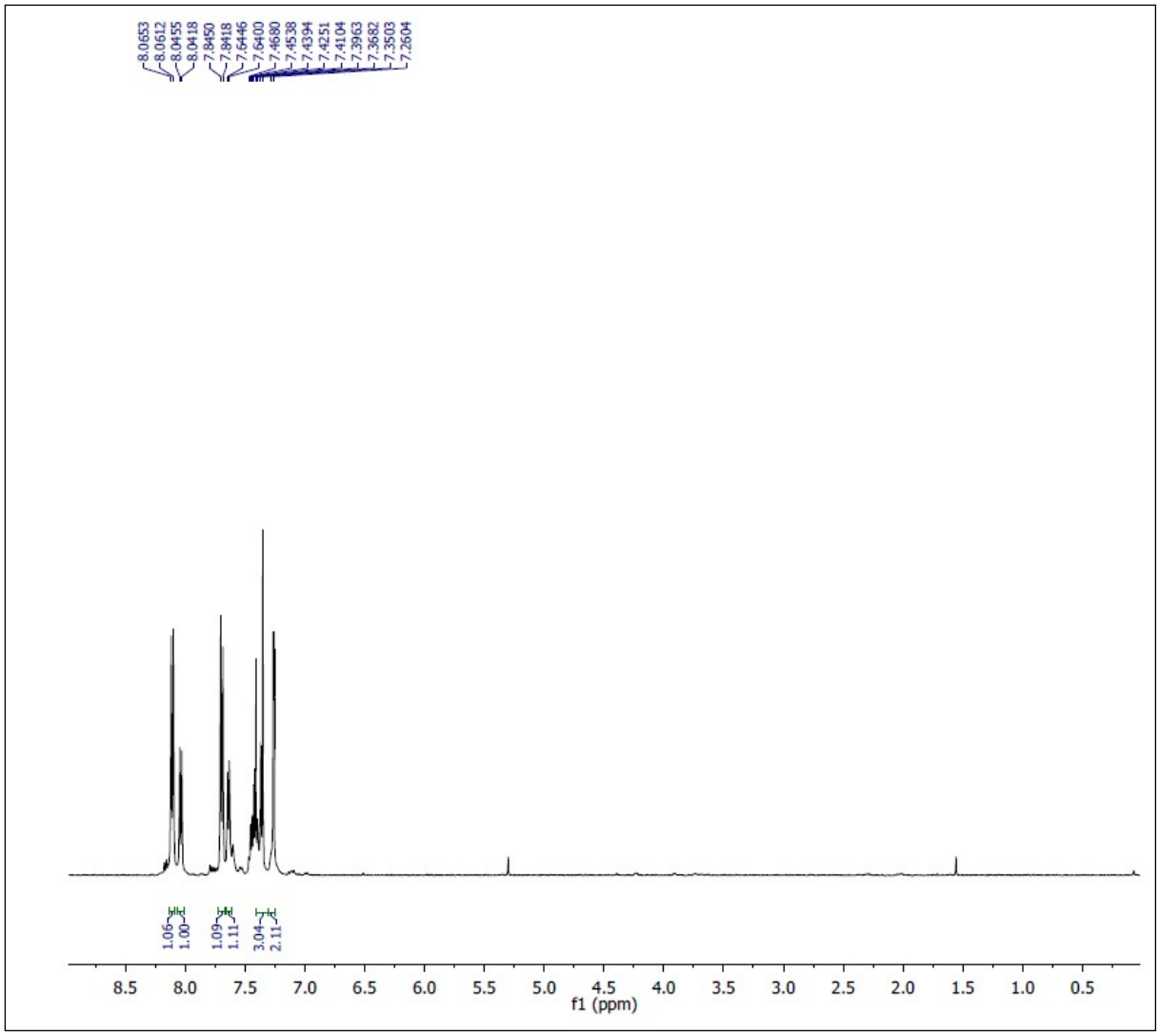


Fig. S33. ^{1}H NMR spectrum of 4-Nitrophenyl-phenyl-selenide

2-Pyridine-phenyl-seler 12 (d, *J* = 5 Hz, 1H); 7.74-7.70 (m, 2H); 7.40

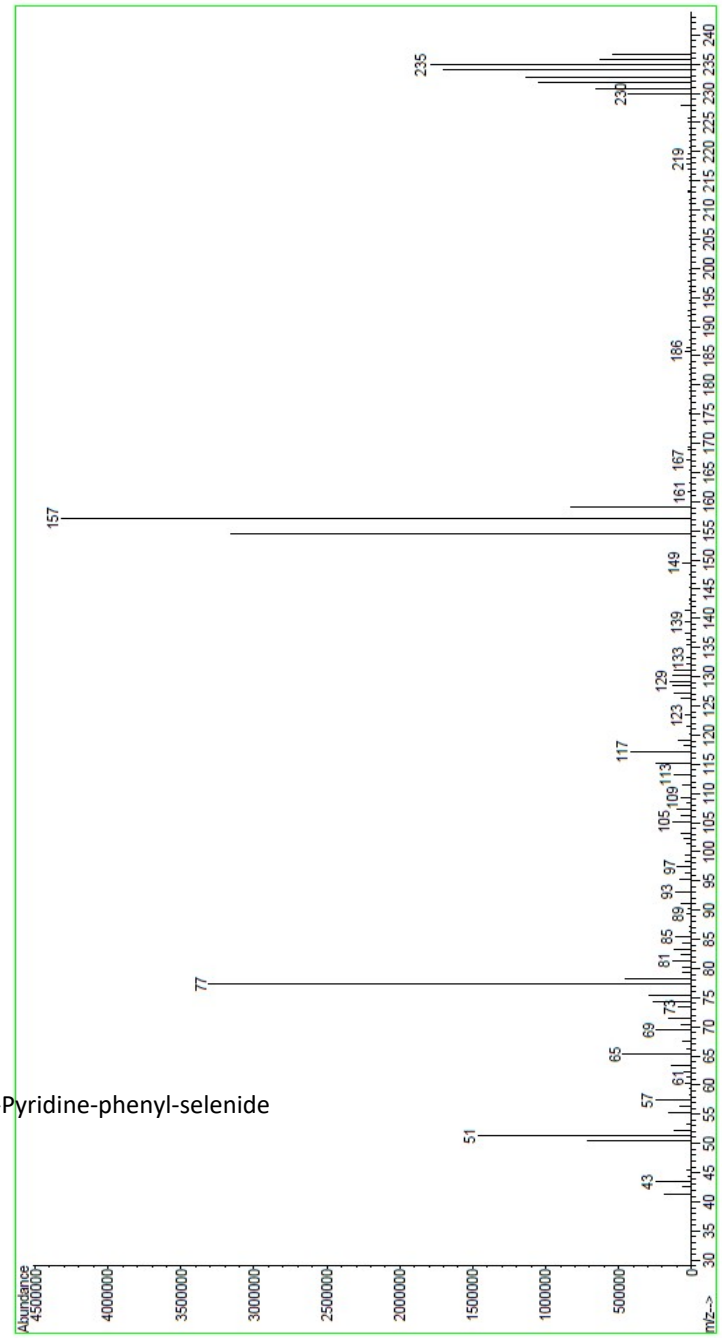


Fig. S34. Mass spectrum of 2-Pyridine-phenyl-selenide

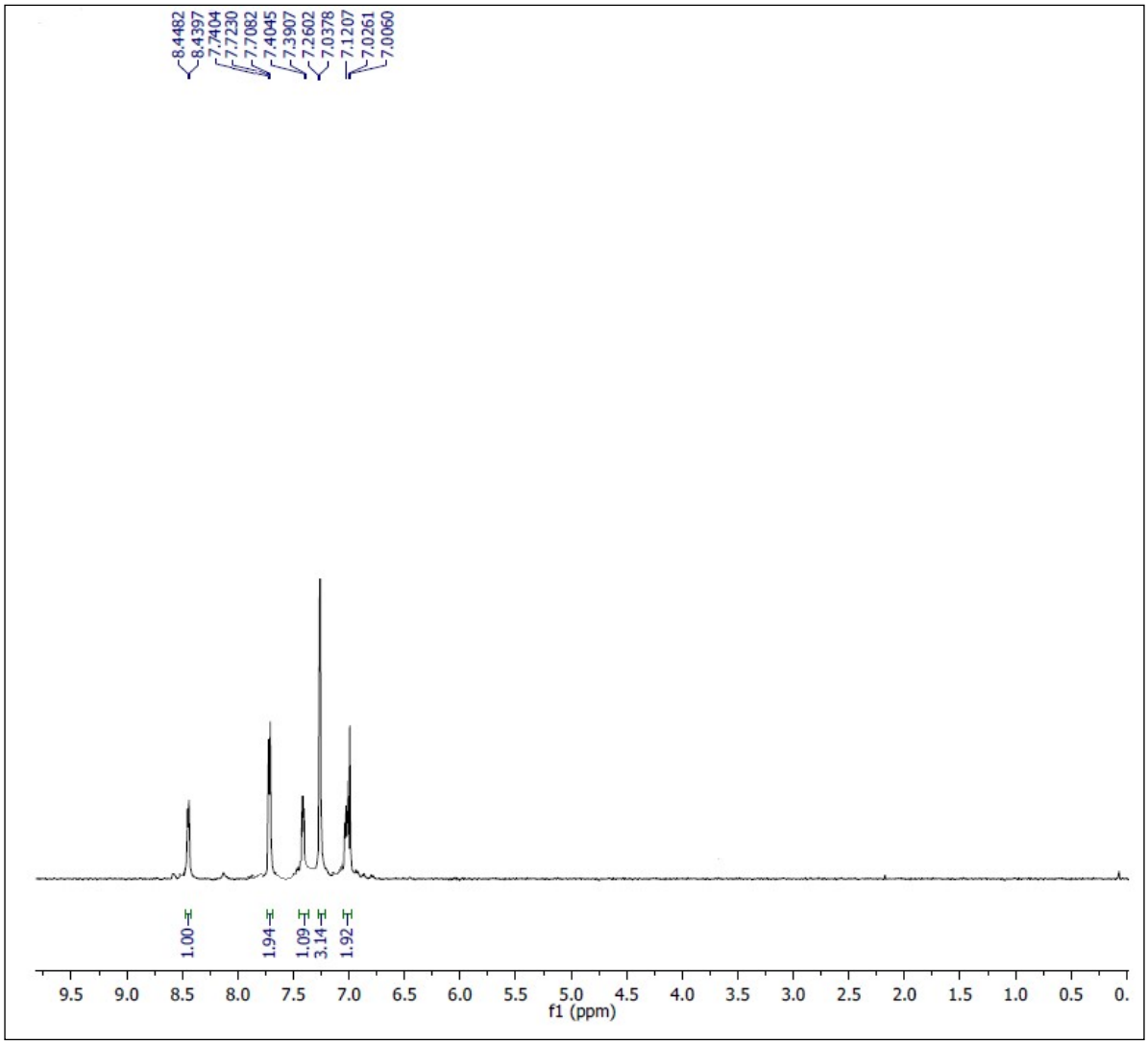


Fig. S35. ^{1}H NMR spectrum of 2-Pyridine-phenyl-selenide

IV. References

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