



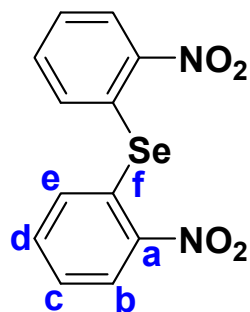
STRUCTURAL
CHEMISTRY

Volume 77 (2021)

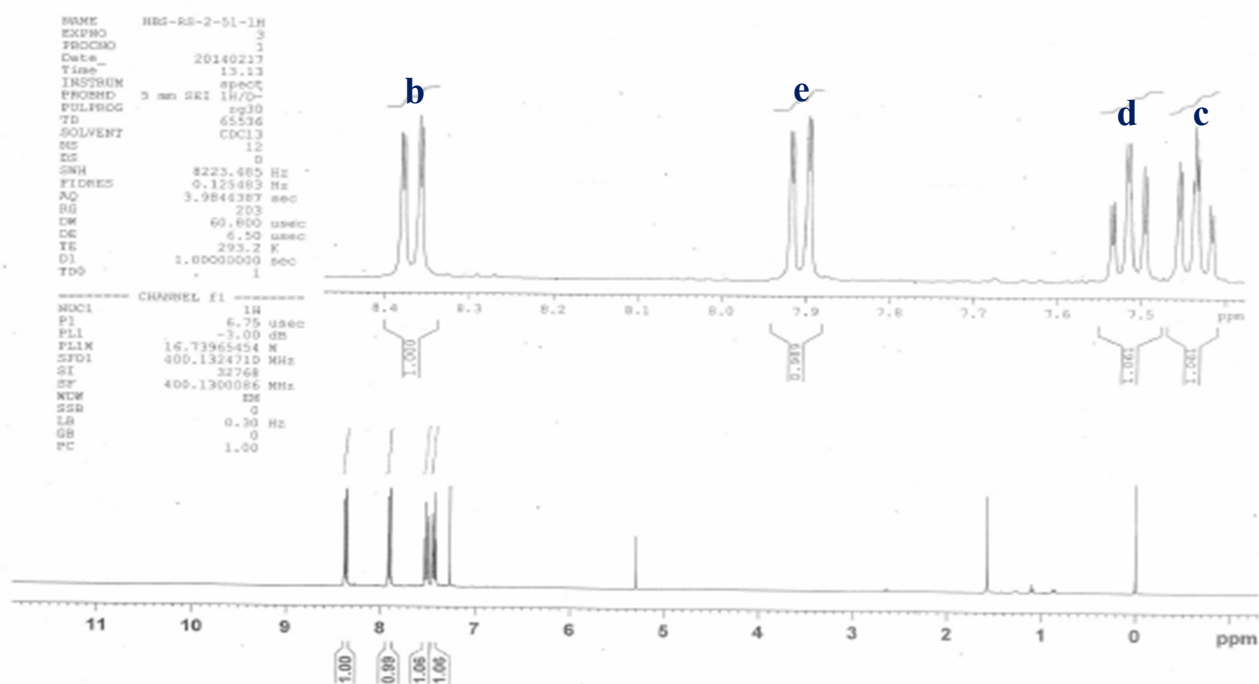
Supporting information for article:

Bis(2-nitrophenyl) selenide, bis(2-aminophenyl) selenide and bis(2-aminophenyl) telluride: structural and theoretical analysis

Raju Saravanan, Harkesh B. Singh and Ray J. Butcher



4 HDS-Kb-2-51-1H



Feb 17, 2014 (1:17:18 PM) HBS-RS-2-51-13C 3 1 D:\Feb17-2014... Page 1/1

Peak v(F1)	[ppm]	v(F1) [Hz]	Intensity [rel]
1	0.3806	1353.3295	11.99
2	0.3770	3351.8891	11.55
3	0.3602	3345.1669	13.09
4	0.3566	3343.7264	12.24
5	7.9185	3168.4295	12.16
6	7.9154	3167.1891	12.11
7	7.8993	3160.3468	13.45
8	7.8952	3159.1064	13.23
9	7.5359	3015.3397	6.44
10	7.5322	3013.8593	6.62
11	7.5178	3008.0978	11.29
12	7.5142	3006.6569	11.48
13	7.5123	3005.8967	7.04
14	7.4978	3000.0948	9.50
15	7.4940	2998.5743	8.71
16	7.4564	2983.5294	9.89
17	7.4530	2982.1690	9.30
18	7.4382	2976.2470	0.43
19	7.4356	2975.2067	12.78
20	7.4327	2974.0463	10.19
21	7.4180	2968.1644	6.48
22	7.4166	2966.8040	5.82
23	7.2642	2906.6248	14.20
24	5.3039	2122.2496	7.17
25	1.5764	630.7649	12.99
26	0.0000	0.0000	15.00

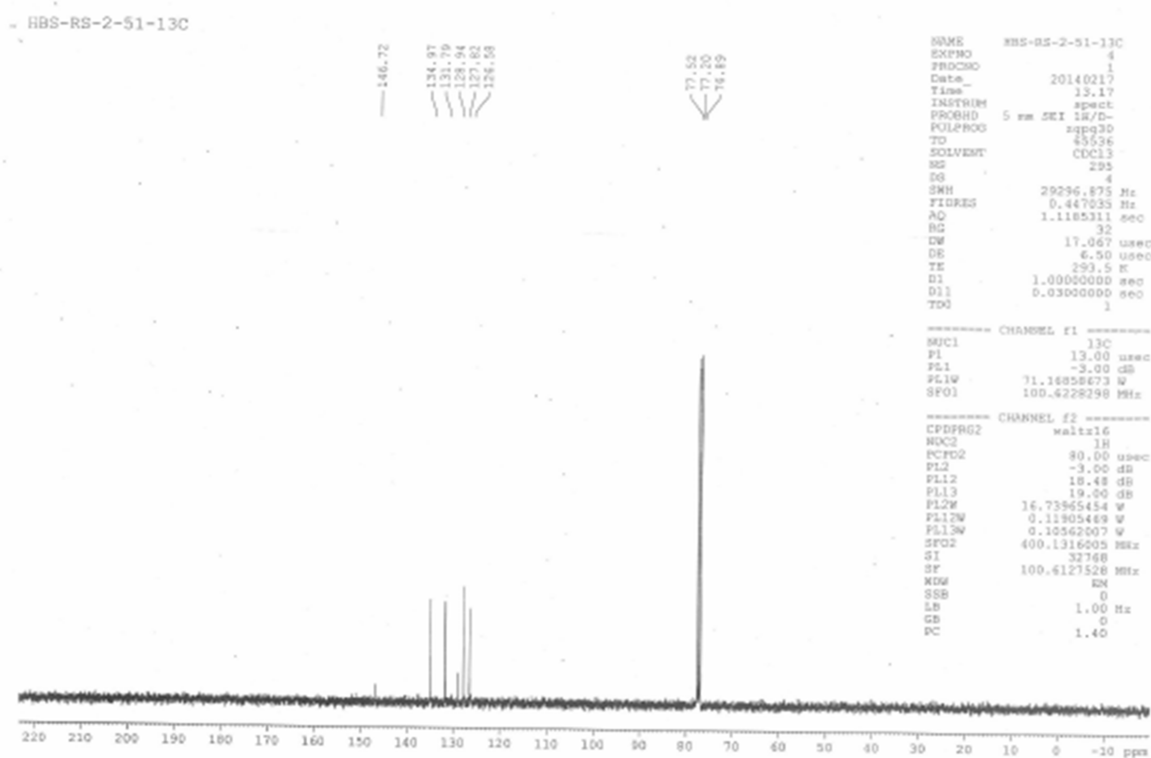
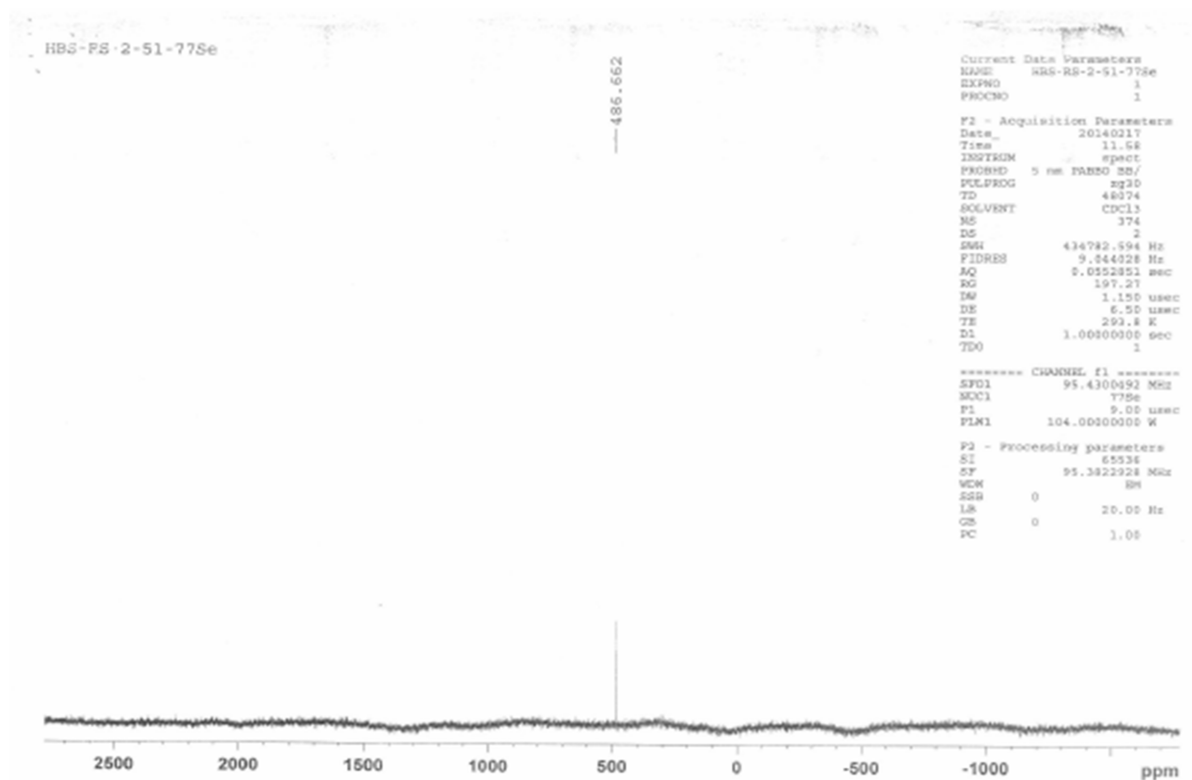
Fig.S1 ¹H NMR spectrum of Compound 2

Fig.S2 ^{13}C NMR spectrum of Compound 2**Fig.S3** ^{77}Se NMR spectrum of Compound 2

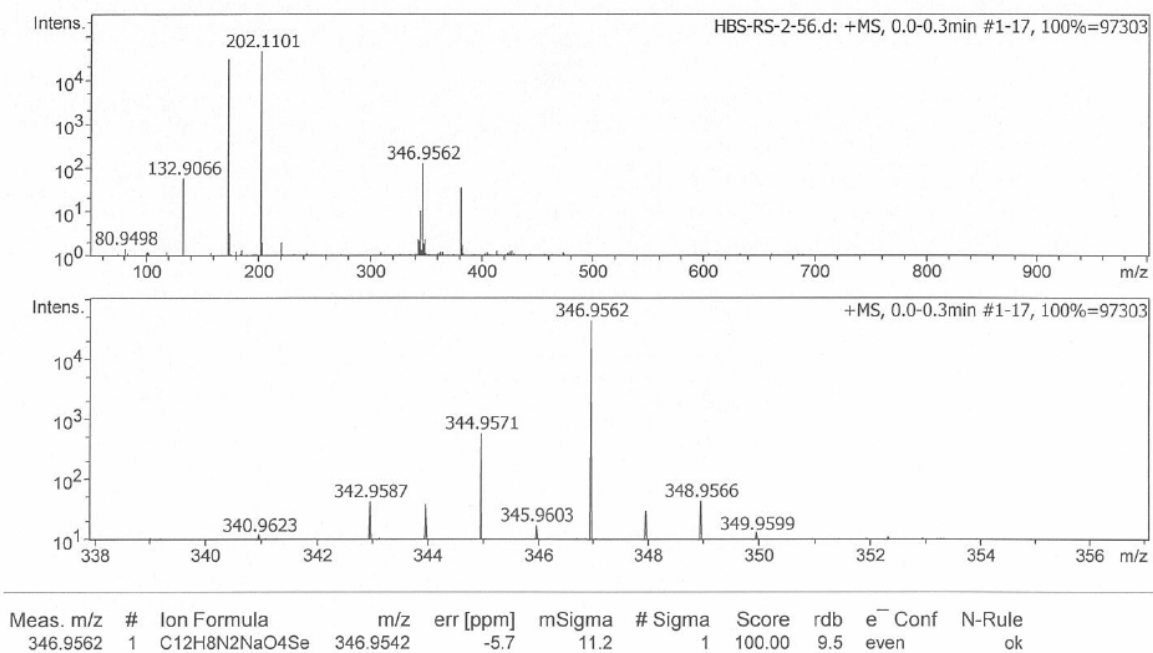
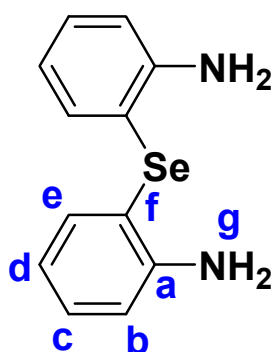


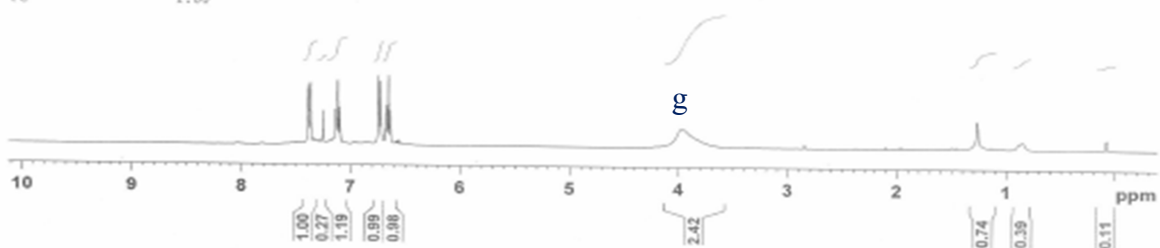
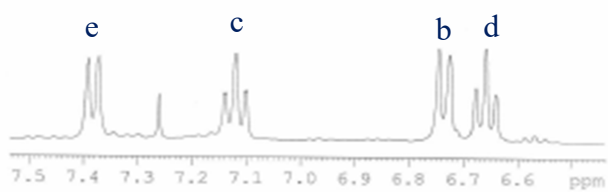
Fig.S4 LR-MS Mass spectrum of Compound 2



HBS-RS-2-66B-1H

NAME HBS-RS-2-66B-1H
EXPNO 12
PROCNO 1
Date_ 20180409
Time 11.09
INSTRUM spect
PROBHD 5 mm DEL 1H/2D-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 0
DS 0
SMH 8223.685 Hz
FIDRES 0.129483 Hz
AQ 3.9846387 sec
RG 80.6
DM 60.800 usec
DE 6.50 usec
TE 296.8 K
D1 1.00000000 sec
TD 1

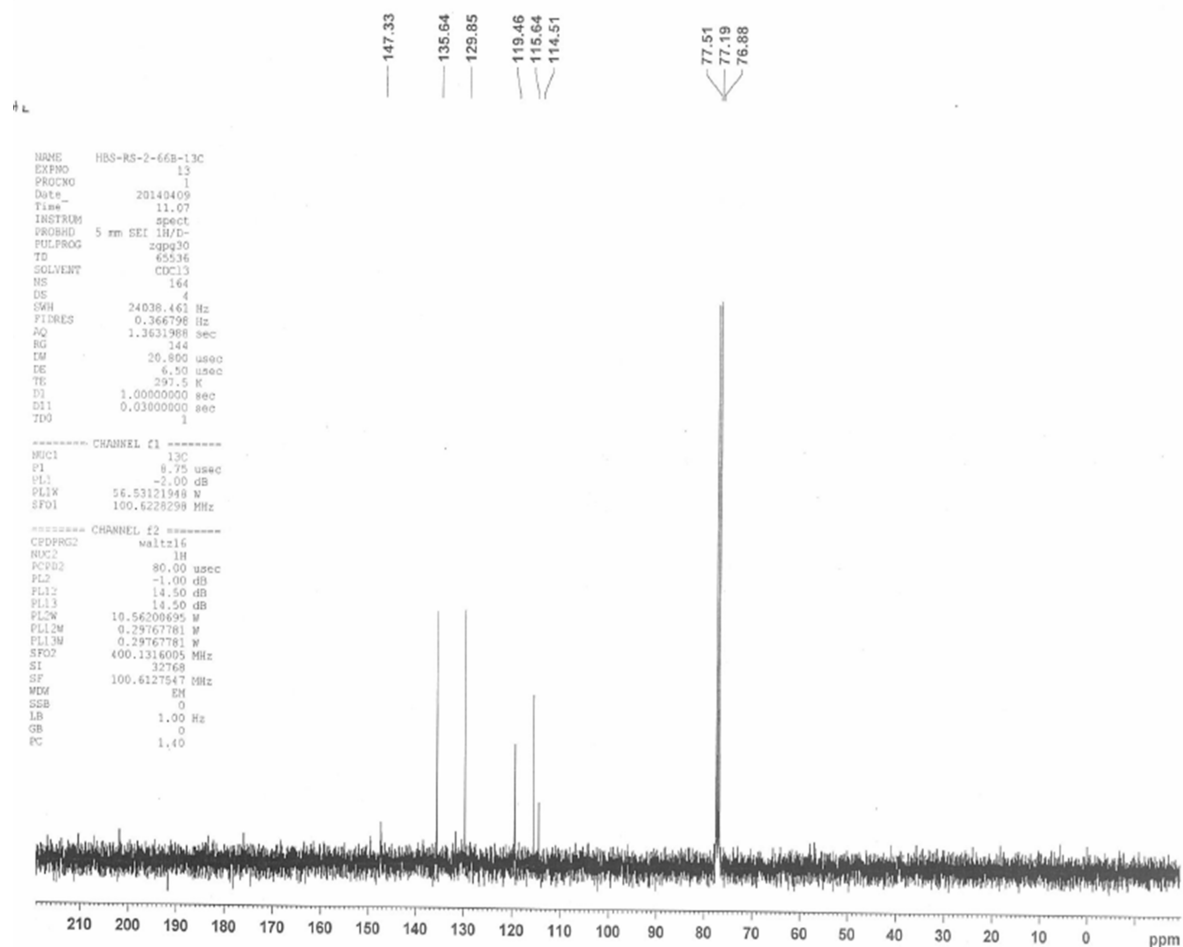
----- CHANNEL f1 -----
NUC1 1H
P1 6.75 usec
PL1 -9.00 dB
PLW 16.73965454 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300102 MHz
WDW EN
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Apr 9, 2014 (11:07:48 AM) HBS-BS-2-66B-1H 12 1 *D:\APR 09-... Page 1/1

Peak	ν (F1) [ppm]	ν (F1) [Hz]	Intensity [rel]
1	7.3946	2958.8014	12.00
2	7.3921	2957.8010	13.09
3	7.3756	2951.1989	12.63
4	7.3728	2950.0785	13.47
5	7.2612	2905.4240	7.45
6	7.1415	2857.5285	7.74
7	7.1382	2856.2080	7.78
8	7.1204	2849.0857	14.00
9	7.1032	2842.2035	8.08
10	7.1001	2840.9631	8.25
11	6.7458	2699.1970	14.98
12	6.7261	2694.3145	13.91
13	6.6793	2670.5884	8.69
14	6.6771	2674.7081	8.67
15	6.6600	2664.8659	15.00
16	6.6419	2657.6235	7.70
17	6.6398	2656.7830	7.47
18	3.9720	1589.3164	4.09
19	1.2685	507.5649	6.28
20	0.8886	355.5555	1.39
21	0.8598	344.0318	1.79
22	0.0876	35.0514	2.24
23	0.0855	34.2111	2.07
24	0.0791	31.6503	2.36

Fig.S5 ^1H NMR spectrum of Compound 3

**Fig.S6** ^{13}C NMR spectrum of Compound 3

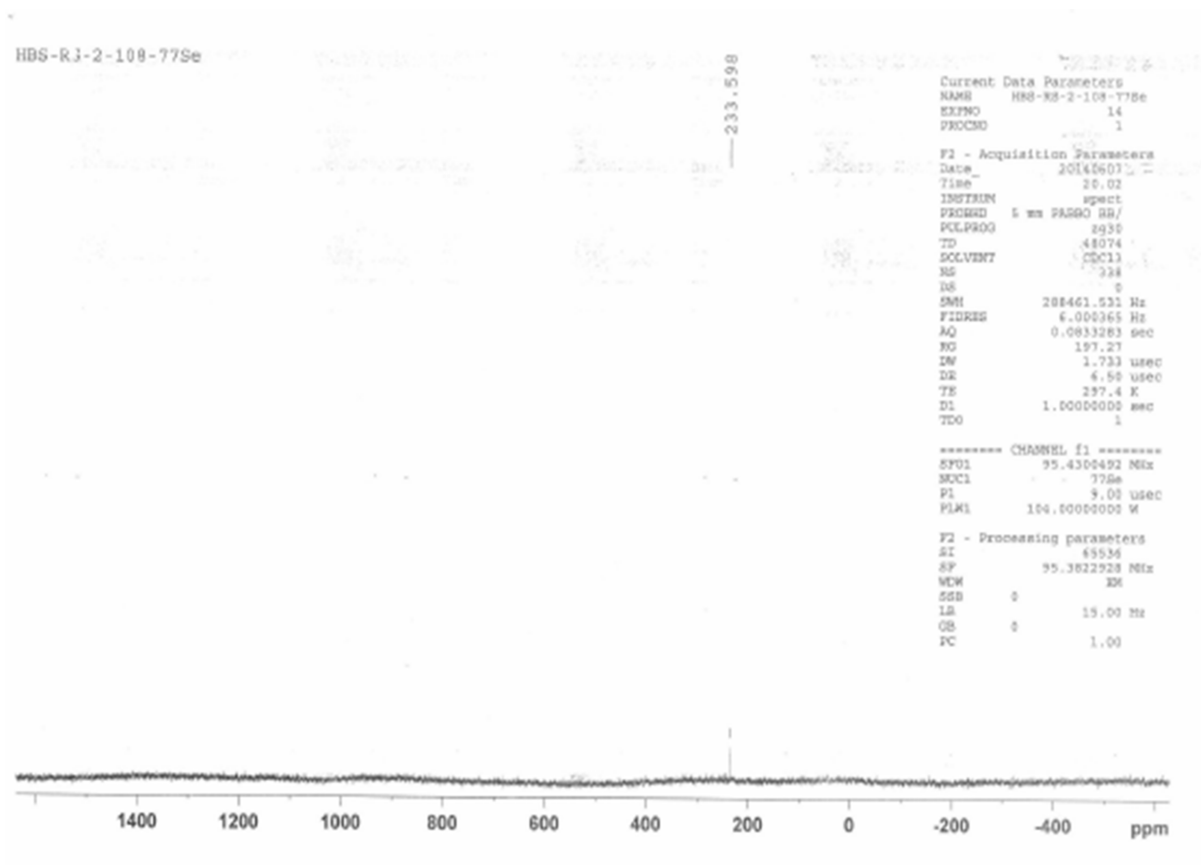
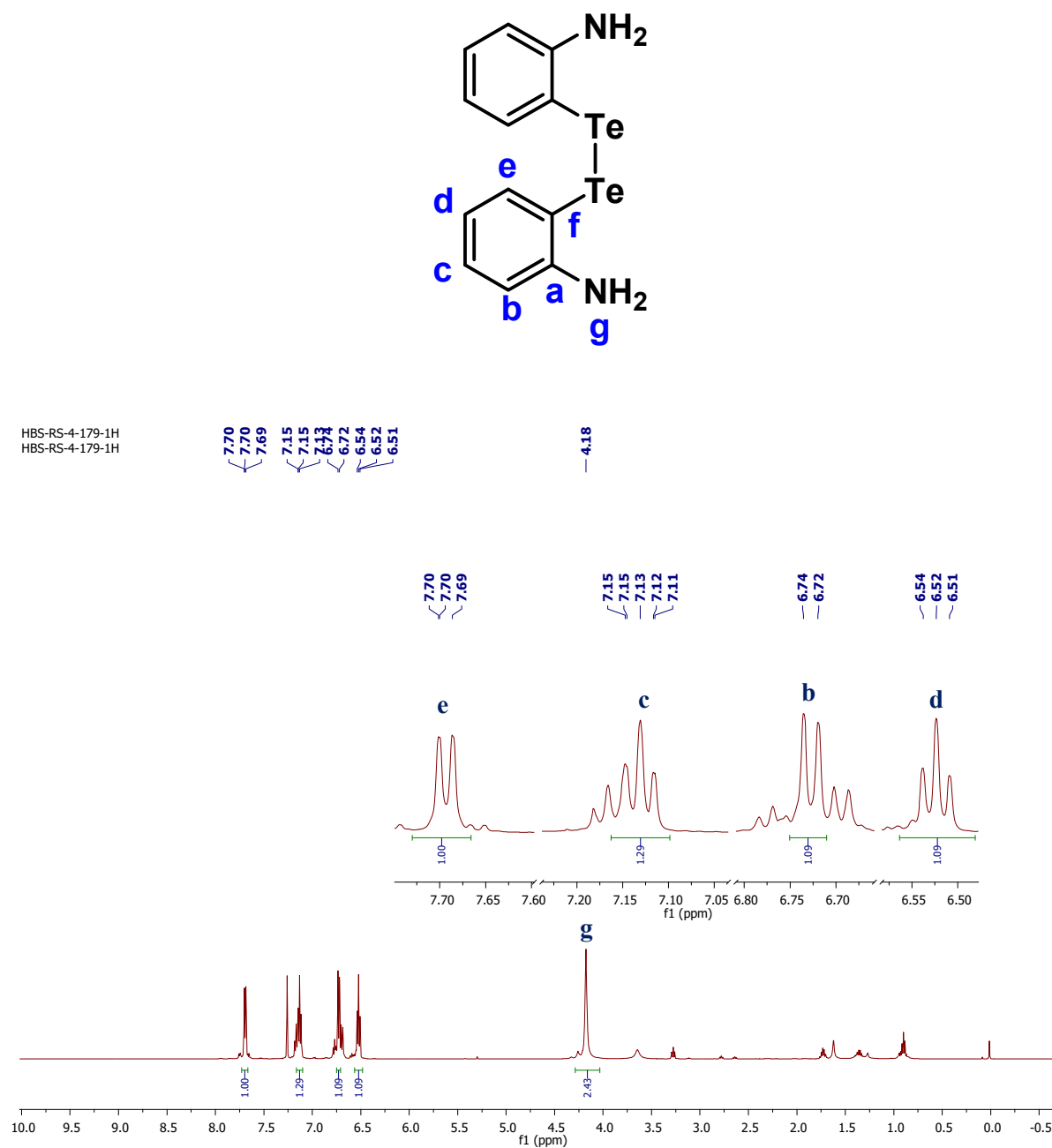


Fig. S7 ^{77}Se NMR spectrum of Compound 3

Fig.S8 ¹H NMR spectrum of Compound 6

HBS-RS-4-179-13C
HBS-RS-4-179-13C

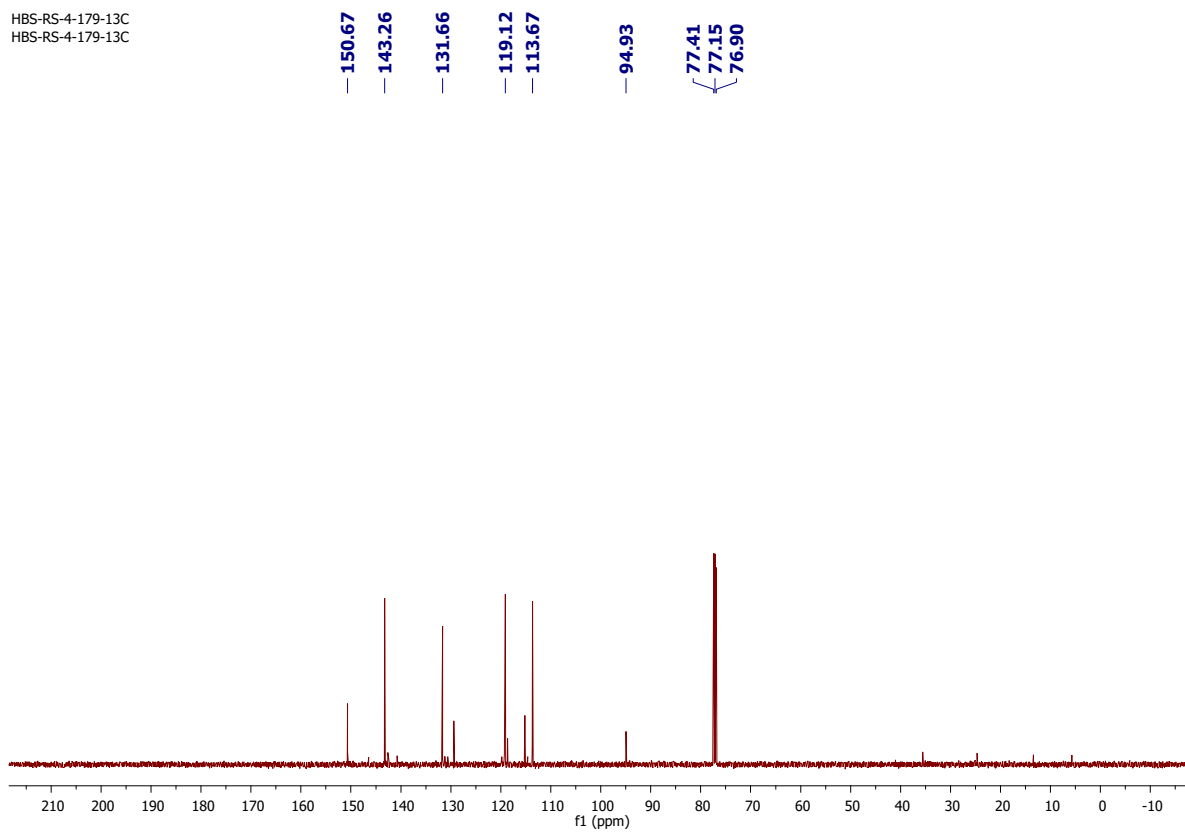


Fig.S9 ^{13}C NMR spectrum of Compound **6**

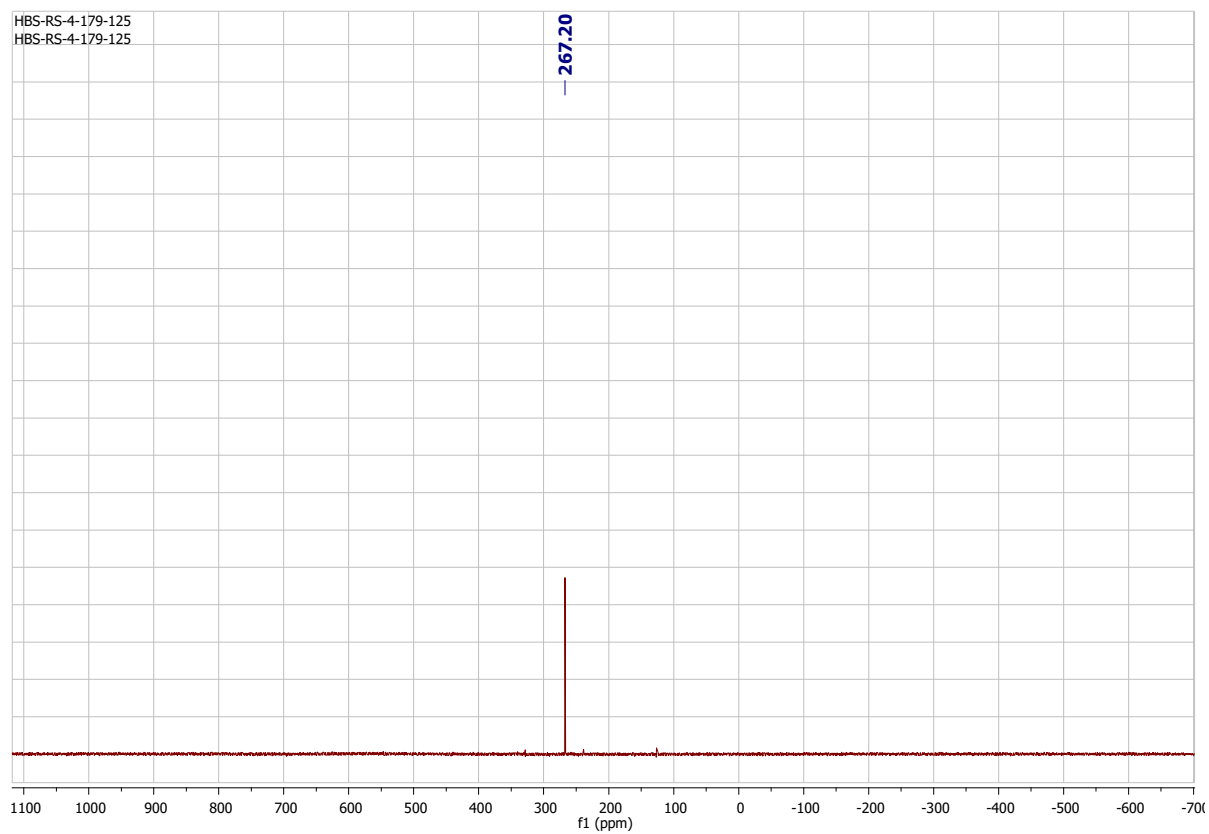
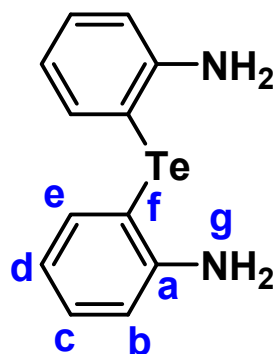


Fig.S10 ^{125}Te NMR spectrum of Compound 6



HBS-RS-4-194-1H
HBS-RS-4-194-1H

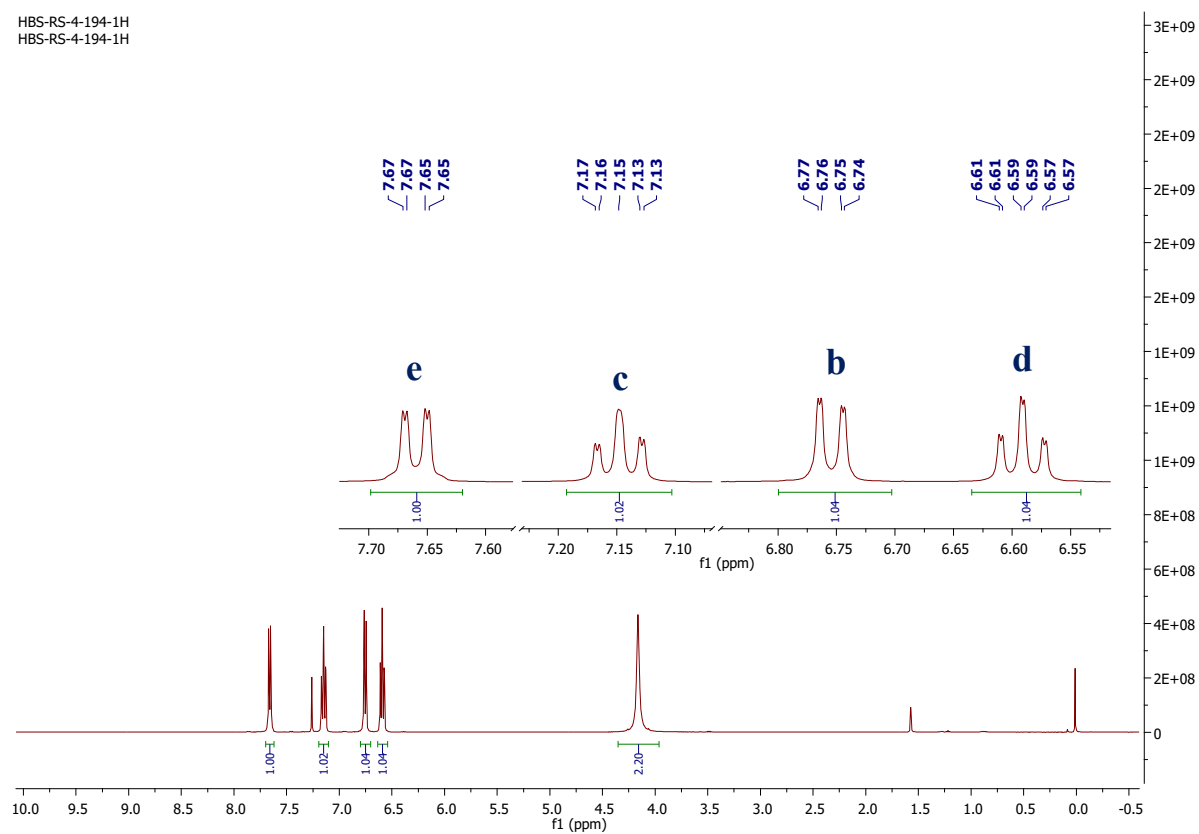


Fig.S11 ^1H NMR spectrum of Compound 7

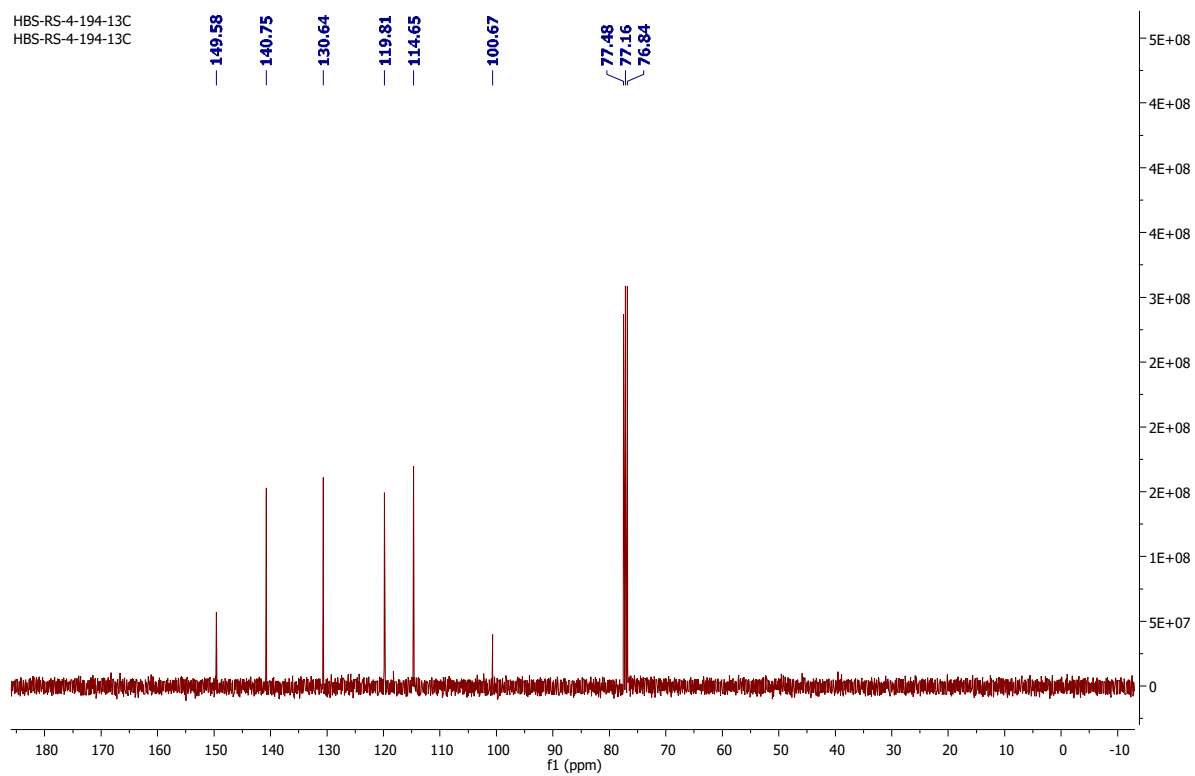


Fig.S12 ^{13}C NMR spectrum of Compound 7

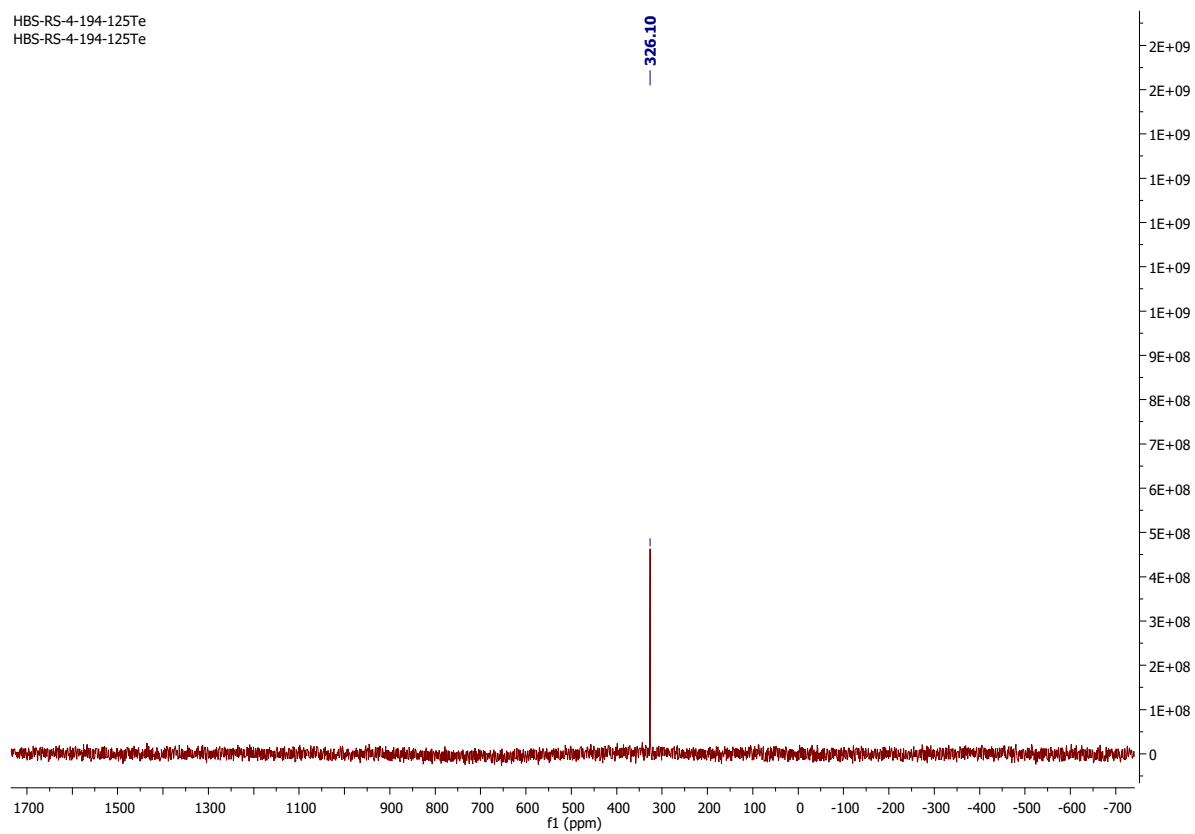
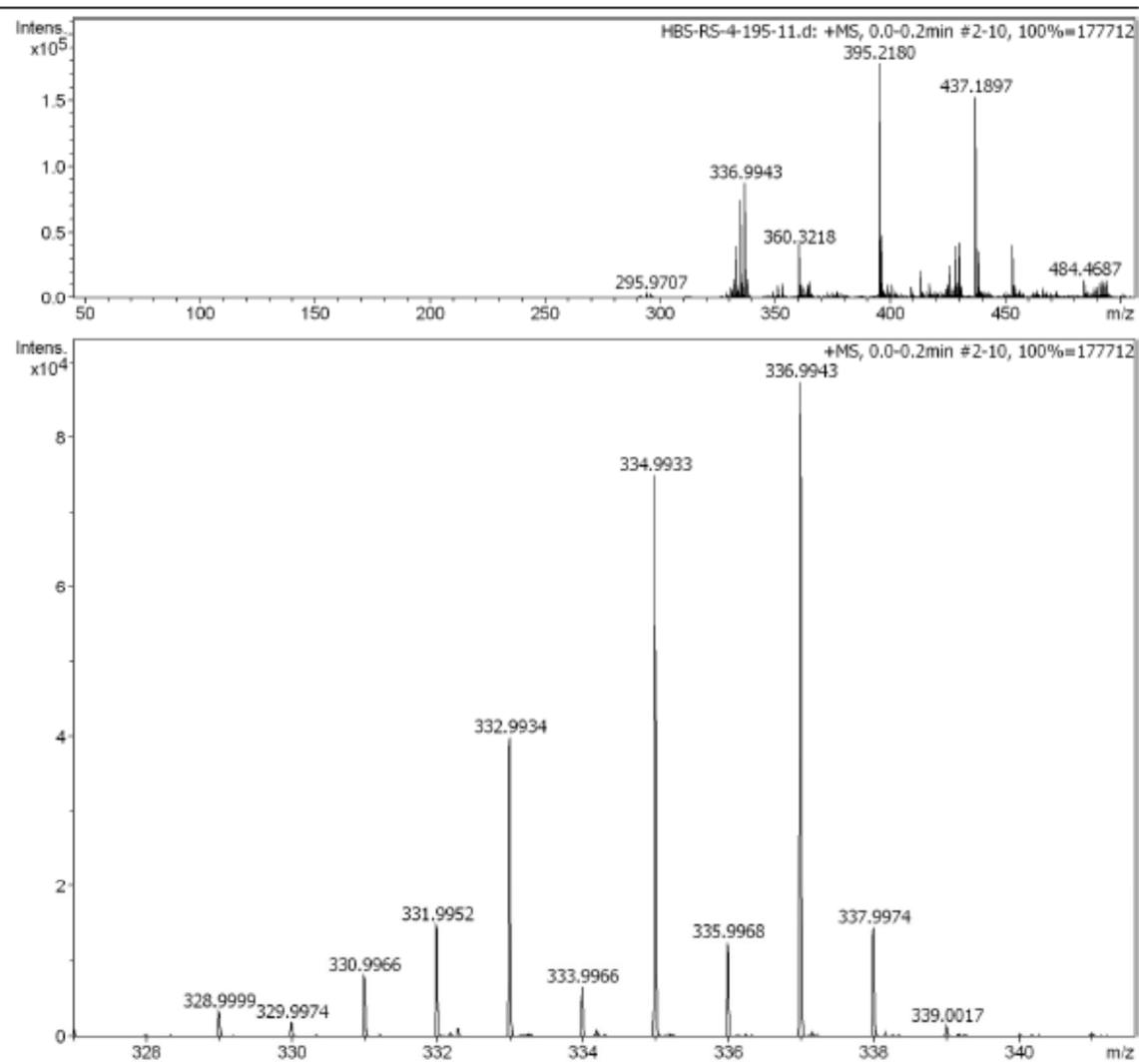


Fig.S13 ^{125}Te NMR spectrum of Compound 7



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Fig.S14 HR-MS spectrum of Compound 7