Electronic Supplementary Material (ESI) for Dalton Transactions.

ESI for

Complexes of (η^6-benzene)ruthenium(II) with 1,4-bis(phenylthio/seleno-methyl)-1,2,3-triazoles: synthesis, structure and applications in catalytic activation of oxidation and transfer hydrogenation

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Table S1 *Crystal data and structural refinements for Complexes* **1− 4**

Compounds	**1**	**2**	**3**	**4**
Empirical formula	C22 H21 Cl N3 Ru S2, F6 P	C22 H21 Cl N3 Ru S Se, F6 P	C22 H21 Cl N3 Ru S Se, F6 P	C22 H21 Cl N3 Ru Se2, F6 P
Formula wt.	673.03	719.94	719.94	766.83
Crystal size [mm]	0.29×0.22×0.20	0.41×0.27×0.17	0.33×0.29×0.21	0.33×0.31×0.29
Crystal system	Monoclinic	Monoclinic	Orthorhombic	Orthorhombic
Space group	$P2_1/c$	$P2_1/c$	$P2_12_12_1$	$P2_12_12_1$
Unit Cell dimension	*a* = 10.729(3)Å *b*= 10.019(3) Å *c* = 24.414(7) Å α = 90.00° β = 96.518(5) γ = 90.00°	*a* = 10.753(19) Å *b* = 10.110(18) Å *c* = 24.622(4) Å α = 90.00° β = 97.496(3)° γ = 90.00°	*a* = 9.3249(8) Å *b* = 10.7293(9) Å *c* = 24.776(2) Å α = 90.00° β = 90.00° γ = 90.00°	*a* = 9.591(5) Å *b*= 10.922(6) Å *c* = 25.180(14) Å α = 90.00° β = 90.00° γ = 90.00°
Volume [$Å^3$]	2607.5(13)	2651.3(8)	2478.8(4)	2638(2)
Z	4	4	4	4
ρ_{calcd} [g/cm^3]	1.714	1.804	1.929	1.931
μ(Mo$K\alpha$) [mm^{-1}]	0.986	2.264	2.421	3.576
F(000)	1344.0	1416	1416.0	1488.0
θ range [°]	1.68–25.00	1.91–25.00	1.64–25.00	1.62 –25.00
Index ranges	$-12\leq h \leq 12$ $-11\leq k \leq 11$ $-29\leq l \leq 29$	$-12\leq h \leq 12$ $-11\leq k \leq 11$ $-29\leq l \leq 21$	$-11\leq h \leq 11$ $-12\leq k \leq 12$ $-29\leq l \leq 29$	$-11\leq h \leq 11$ $-12\leq k \leq 12$ $-29\leq l \leq 29$
Reflections collected	22902	24116	22815	19589
Independent reflections(R_{int}.)	4309 (0.1095)	4656 (0.0701)	4341 (0.0379)	4609 (0.1329)
Completeness to max. θ [%]	94.0	99.7	99.9	98.9
Max./min. Transmission	0.824 / 0.769	0.684/ 0.481	0.604 / 0.451	0.358/ 0.317
Data/restraints/ parameters	4309 / 0 / 325	4656 / 0 / 325	4341 / 0 / 325	4609 / 0 / 325
Goodness-of-fit on F^2	1.241	1.180	1.046	1.099
Final R indices [$I > 2\sigma(I)$]	R_1 = 0.0995, wR_2 = 0.1646	R_1 = 0.0687, wR_2 = 0.1498	R_1 = 0.0202, wR_2 = 0.0524	R_1 = 0.0569, wR_2 = 0.1293
R indices (all data)	R_1 = 0.1219, wR_2 = 0.1736	R_1 = 0.0872, wR_2 = 0.1572	R_1 = 0.0208, wR_2 = 0.0527	R_1 = 0.0844, wR_2 = 0.1432
Largest diff. peak/hole[e.$Å^{-3}$]	0.617 / -1.565	1.581 / -0.707	0.745 / -0.311	1.057 / -1.103
CCDC No.	1401444	1401445	1401446	1401447

Table S2 *Bond Lengths and Bond Angles of* **1− 4**

Compounds	Bond length [Å]	Bond angle [°]
1	C(6)—S(1)1.777(11) C(7)— S(1) 1.832(11) C(8) —N(1) 1.359(13) C(9)— N(3) 1.333(15) C10)—N(3) 1.449(14) C(10)— S(2) 1.784(13) C(11) —S(2)1.786(13) C(17)—Ru(1) 2.139(14) C(18)—Ru(1) 2.174(15) C(19) —Ru(1) 2.187(13) C(20) —Ru(1) 2.179(13) C(21)— Ru(1) 2.151(12) C(22)— Ru(1) 2.173(13) Cl(1)— Ru(1) 2.394(3) N(1)— N(2) 1.313(12) N(1)— Ru(1) 2.091(9) N(2)—N(3) 1.318(12) Ru(1)— S(1) 2.388(2)	N(1)— Ru(1)— C(17) 91.3(5) C(17)— Ru(1)— C(21) 67.2(6) C(17)— Ru(1)— C(22) 37.6(6) N(1)— Ru(1)— C(18) 104.1(6) C(17)— Ru(1)— C(18) 37.1(6) C(17)— Ru(1)— C(19) 67.4(7) N(1)— Ru(1)— S(1) 80.4(3) C(17)— Ru(1)— S(1) 135.4(6) C(21)— Ru(1)— S(1) 92.1(4) C(22)— Ru(1)— S(1) 103.5(5) C(18)— Ru(1)— S(1 170.3(5) C(20)— Ru(1)— S(1)108.1(5) C(19)— Ru(1)— S(1) 141.2(6) N(1)— Ru(1)— Cl(1) 87.2(2) C(17)— Ru(1)— Cl(1) 142.6(6) C(21)— Ru(1)— Cl(1) 130.1(6) C(22)— Ru(1)— Cl(1) 165.6(4) C(18)— Ru(1)— Cl(1) 107.5(6) C(20)— Ru(1)— Cl1) 99.6(5) C(19)— Ru(1)— Cl(1) 88.7(4) S(1)— Ru(1)— Cl(1)– 81.09(10) C(6)— S(1)— C(7) 104.8(5) C(6)— S(1)— Ru(1) 108.3(4) C(7)— S(1)— Ru(1) 99.9(4) C(10)— S(2)— C(11)99.5(6)
2	C(6)— S(1) 1.783(7) C(7)— S(1) 1.834(7) C(8)— N(1) 1.350(9) C(9)— N(3) 1.319(10) C(10)— N(3) 1.450(9) C(10)— Se(1) 1.970(8) C(11)— Se(1) 1.909(9) C(17)—Ru(1) 2.166(9) C(18)— Ru(1) 2.194(9) C(19)— Ru(1) 2.191(9) C(20)— Ru(1) 2.134(9) C(21)— Ru(1) 2.173(9) C(22)— Ru(1) 2.156(8) Cl(1)— Ru(1) 2.399(2) N(1)— N(2)1.304(8) N(1)— Ru(1) 2.104(6) N(2)— N(3) 1.350(8) Ru(1)— S(1) 2.3902(19)	N(1)— Ru(1)— C(20) 140.1(4) N(1)— Ru(1)— C(22) 91.4(3) N(1)— Ru(1)— C(17) 104.8(4) N(1)— Ru(1)— C(21) 106.5(4) N(1)— Ru(1)— C(19) 169.9(3) N(1)— Ru(1)— C(18) 137.7(4) N(1)— Ru(1)— S(1) 80.55(16) C(17) —Ru(1) —C(21) 67.3(4) C(20)— Ru(1)— S(1) 92.4(3) C(22)— Ru(1)— S(1) 135.4(4) C(17)—Ru(1)— S(1) 170.5(3) C(21)— Ru(1)— S(1) 103.8(3) C(19)— Ru(1)— S(1) 107.4(3) C(18)— Ru(1)— S(1) 140.3(4) N(1)— Ru(1)— Cl(1) 87.14(16) C(20)— Ru(1)— Cl(1) 130.7(4) C(22)— Ru(1)— Cl(1) 143.0(4) . C(17)— Ru(1)— Cl(1) 107.0(4) C(21)— Ru(1)— Cl(1) 166.1(3) C(19)— Ru(1)— Cl(1) 100.1(3) C(18)— Ru(1)— Cl(1) 89.5(3) S(1)— Ru(1)— Cl(1) 80.85(7)

		C(6)— S(1)— C(7) 103.9(3) C(11)— Se(1) —C(10)95.9(3)
3	Ru(1)— N(1) 2.092(2) Ru(1)— C(22) 2.168(3) Ru(1)— C(21) 2.169(3) Ru(1)— C(20) 2.181(3) Ru(1)— C(19) 2.184(3) Ru(1)— C(17) 2.186(3) Ru(1)— C(18) 2.196(3) Ru(1)— Cl(1) 2.4032(7) Ru(1)— Se(1) 2.5007(4) Se(1)— C(6) 1.939(3) Se(1)— C(7) 1.969(3) N(1)— N(2) 1.323(3) S(1)— C(11) 1.789(3) S(1)— C(10)1.812(3) N(1)— C(8) 1.360(4) N(3)— C(9) 1.349(4) N(3)— C(10) 1.463(4) N(2)— N(3) 1.333(3)	N(1)—Ru(1)—C(22) 90.26(10) N(1)—Ru(1)—C(21)110.67(10) N(1)—Ru(1)—C(20)147.48(11) N(1)—Ru(1)—C(19)165.43(11) N(1)—Ru(1)—C(17)97.99(10) C(19)—Ru(1)—C(17) 67.92(12) N(1)—Ru(1)—C(18)127.71(11) C(17)—Ru(1)—C18) 37.12(13) N(1)— Ru(1)— Cl(1) 88.93(6) C(22)—Ru(1)—Cl(1) 151.06(10) C(21)— Ru(1)—Cl(1) 160.12(9) C(20)— Ru(1)— Cl(1) 121.86(9) C(19)—Ru(1)—Cl(1) 93.45(9) C(17)— Ru(1)—Cl(1) 113.85(9) C(18)—Ru(1)—Cl(1) 90.14(9) N(1)—Ru(1)—Se(1) 81.03(6) C(22)— Ru(1)—Se(1) 130.18(10) C(21)—Ru(1)—Se(1) 100.97(8) C(20)— Ru(1)—Se(1) 94.42(9) C(19)—Ru(1)—Se(1) 113.53(9) C(17)—Ru(1)—Se(1) 167.96(9) C(18)—Ru(1)—Se(1) 149.14(9) C(l1)—Ru(1)—Se(1) 78.18(2) C(6)—Se(1)—C(7) 101.60(13) C(6)—Se(1)—Ru(1) 108.15(8) C(7)— Se(1)—Ru(1) 95.29(8) N(2)— N(1)—C(8) 110.9(2) N(2)—N(1)—Ru(1) 124.40(17) C(8)—N(1)—Ru(1) 124.30(18) C(11)—S(1)—C(10) 100.03(14) C(12)—C(11)—S(1) 119.8(2) C(16)—C(11)—S(1) 120.2(2) C(8)—C(7)—Se(1) 110.02(19)
4	C(6)—Se(1) 1.946(10) C(7)—Se(1) 1.986(10) C(8)—N(1) 1.404(12) C(9)—N(3) 1.355(14) C(10)—N(3) 1.456(14) C(10)—Se(2) 1.970(11) C(11)—Se(2) 1.952(10) C(17)—Ru(1) 2.175(11) C(18)—Ru(1) 2.184(11) C (19)—Ru(1) 2.196(12) C(20)—Ru(1) 2.188(11) C(21)—Ru(1) 2.204(10) C(22)—Ru(1) 2.193(9) Cl(1)— Ru(1) 2.419(3)	N(1)—C(8)—C9 105.1(9) N(1)—C(8)—C7 121.2(9) N(3)—C(9)—C8 105.5(8) N(3)—C(10)—Se2 112.2(8) N(2)—N(1)—Ru1 126.1(6) C(8)—N(1)—Ru1 123.1(7) N(1)—Ru(1)—C17 90.9(4) N(1)—Ru(1)—C18 99.0(5) C(17)—Ru(1)—C18 38.0(5) N(1)—Ru(1)—C20 166.0(5) C(17)—Ru(1)—C20 79.3(5) C(18)—Ru(1)—C20 67.2(6) N(1)—Ru(1)—C22 110.6(4) N(1)—Ru(1)—C19 129.5(5)

	N(3)—N(2) 1.335(11) N(2)—N(1) 1.316(11) N(1)—Ru(1) 2.096(7) Ru(1)—Se(1) 2.5262(19)	N(1)—Ru(1)—C21 147.3(5) C(17)—Ru(1)—C21 67.2(5) C(18)—Ru(1)—C(21) 78.8(5) N(1)—Ru(1)—Cl(1) 88.2(2) C(17)—Ru(1)—Cl(1) 150.4(4) C(18)—Ru(1)—Cl(1) 113.1(4) C(20)—Ru(1)—Cl(1) 95.4(4) C(22)—Ru(1)—Cl(1) 161.1(3) C(19)—Ru(1)—Cl(1) 90.0(4) C(21)—Ru(1)—Cl(1) 123.0(4) N(1)— Ru(1)—Se(1) 81.5(3) C(17)—Ru(1)—Se(1) 130.7(4) C(18)—Ru(1)—Se(1) 168.4(4) C(20)—Ru(1)—Se(1) 112.5(4) C(22)—Ru(1)—Se(1) 101.8(3) C(19)—Ru(1)—Se(1) 146.9(5) C(21)— Ru(1)—Se(1) 94.5(4) Cl(1)— Ru(1)—Se(1) 78.40(9) C(6)—Se(1)—C(7) 101.7(4) C(6)—Se(1)—Ru(1) 108.0(3) C(7)—Se(1)—Ru(1) 95.1(3) C(11)—Se(2)—C(10) 96.9(5)

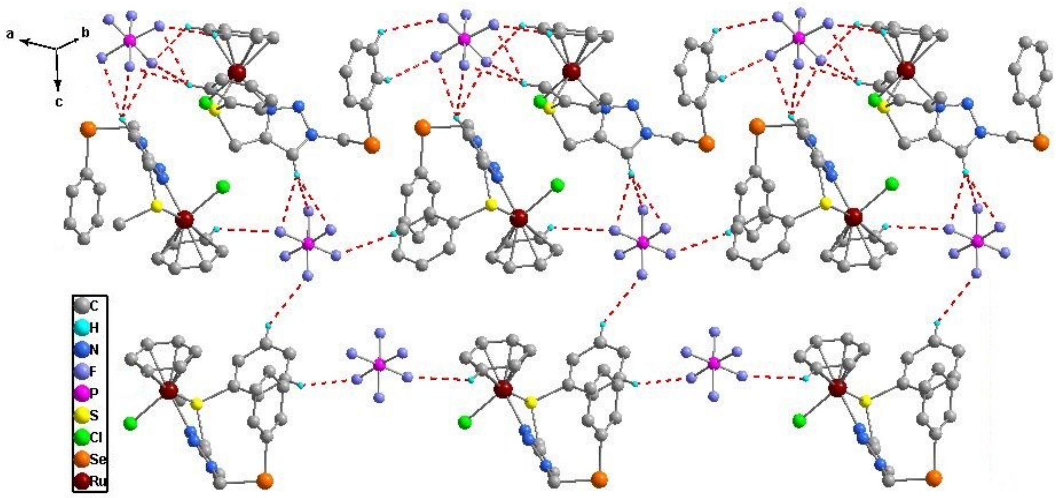


Figure S1. Non-covalent C–H···F interactions in **2**

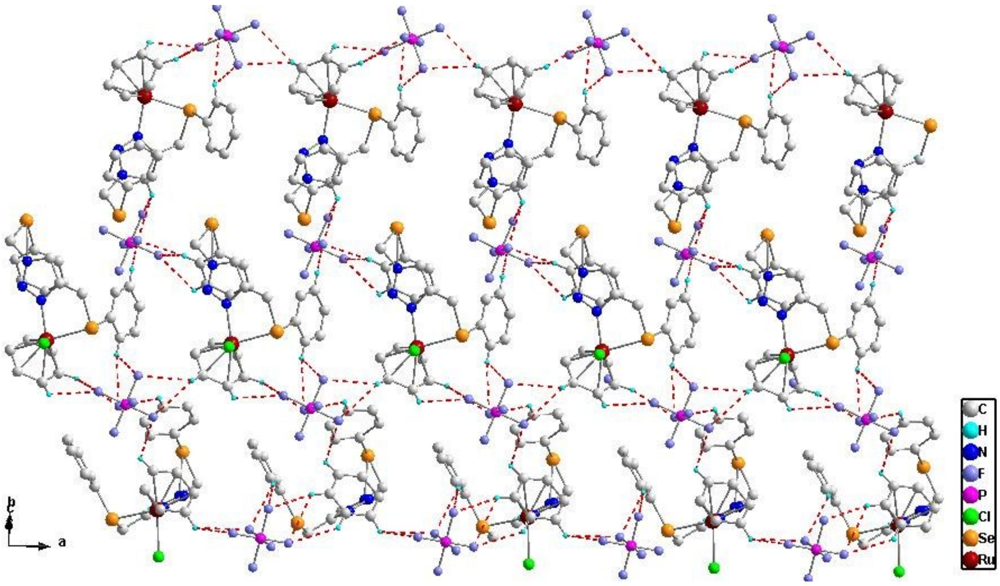


Figure S2. Non-covalent C–H···F interactions in **4**

Table S3 *Non-covalent interactions C–H···F distances[Å] of* **1−4**

1		**2**	
C(13)–H(13)···F(6)	2.763	C(17)–H(17)···F(2)	2.817
C(15) –H(15)···F(4)	2.775	C(2)–H(2)···F(3)	2.420
C(4)–H(4)···F(4)	2.750	C(4)–H(4)···F(4)	2.721
C(5)–H(5)···F(3)	2.719	C(13)–H(13)···F(5)	2.710
C(18)–H(18)···F(3)	2.840	C(9)–H(9)···F(3)	2.790
C(21)–H(21)···F(1)	2.791	C(9)–H(9)···F(1)	3.786
C(5)–H(5)···F(1)	2.589	C(9)–H(9)···F(2)	2.607
C(5)–H(5)···F(2)	2.819	C(17)–H(17)···F(2)	2.817
C(20)–H(20)···F(1)	2.710	C(16)–H(16)···F(3)	2.601
C(16)–H(16)···F(5)	2.583	C(15)–H(15)···F(4)	2.819
C(2)–H(2)···F(5)	2.417	C(5)–H(5)···F(1)	2.607
C(9)–H(9)···F(3)	2.610	C(5)–H(5)···F(2)	2.693
C(10A) –H(10A)···F(1)	2.825	C(5)–H(5)···F(6)	2.861
C(9) –H(9)···F(5)	2.770	C(19)–H(19)···F(1)	2.846
		C(20)–H(20)···F(6)	2.764
3		**4**	
C(16)–H(16)···F(1)	2.693	C(20)–H(20)···F(6)	2.729
C(19)–H(19)···F(5)	2.770	C(21) –H(21)···F(6)	2.798
C(20)–H(20)···F(6)	2.815	C(21)–H(21)···F(1)	2.673
C(21)–H(21)···F(6)	2.736	C(1)–H(1)···F(1)	2.769
C(14)–H(14)···F(4)	2.703	C(1)–H(1)···F(5)	2.687
C(21)–H(21)···F(2)	2.616	C(19)–H(19)···F(5)	2.823
C(18)–H(18)···F(2)	2.482	C(19)–H(19)···F(3)	2.750
C(2)–H(2)···F(1)	2.469	C(14)–H(14)···F(5)	2.816
C(10B)–H(10B)···F(1)	2.812	C(4)–H(4)···F(4)	2.505
C(9)–H(9)···F(1)	2.540	C(12)–H(12)···F(4)	2.606
C(9)–H(9)···F(3)	2.665	C(12)–H(12)···F(3)	2.826
C(16)–H(16)···F(2)	2.705	C(13)–H(13)···F(3)	2.818
C(15)–H(15)···F(2)	2.610		
C(5)–H(5)···F(3)	2.669		
C(20)–H(20)···F(5)	2.791		
C(20)–H(20)···F(4)	2.696		
C(5)–H(5)···F(4)	2.748		
C(21)–H(21)···F(4)	2.741		

Table S4 Comparison of Selected Bond Lengths (Å) and Angles (°) of **1−4** Determined Experimentally and Optimized by DFT

1			**2**		
	Bond length / Angle	**optimized value**		**Bond length / Angle**	**optimized value**
N(1)—Ru(1)	2.091(9)	2.102	Ru(1)—N(1)	2.100(6)	2.098
S(1)—Ru(1)	2.391(3)	2.429	Ru(1)—S(1)	2.386(19)	2.431
Cl(1)—Ru(1)	2.394(3)	2.421	Ru(1)—Cl(1)	2.399(2)	2.416
C —Ru(1)	1.675(1)	1.735	C —Ru(1)	1.679(1)	1.759
N1—Ru1—S1	80.4(3)	80.25	N1—Ru1—S1	80.55(16)	80.32
N1—Ru1—Cl1	87.2(2)	84.15	N1—Ru1—Cl1	87.14(16)	84.40
S1—Ru1—Cl1	81.09(10)	81.77	Cl(1)—Ru1—S1	80.85(7)	81.53
3			**4**		
N(1)—Ru(1)	2.092(2)	2.105	Ru(1)—N(2)	2.096(7)	2.102
Ru(1)—Se(1)	2.5007(4)	2.523	Ru(1)—Cl(1)	2.419(3)	2.419
Cl(1)—Ru(1)	2.4032(7)	2.419	Ru(1)—Se(1)	2.526(19)	2.523
C —Ru(1)	1.666	1.738	C —Ru1	1.687	1.737
N1—Ru1—Se1	81.03(6)	81.25	N1—Ru1—Se1	81.5(3)	81.40
N1—Ru1—Cl1	88.93(6)	84.46	N1—Ru1—Cl1	88.2(2)	84.34
Se1—Ru1—Cl1	81.03(6)	80.25	Cl1—Ru1—Se1	78.40(9)	80.13

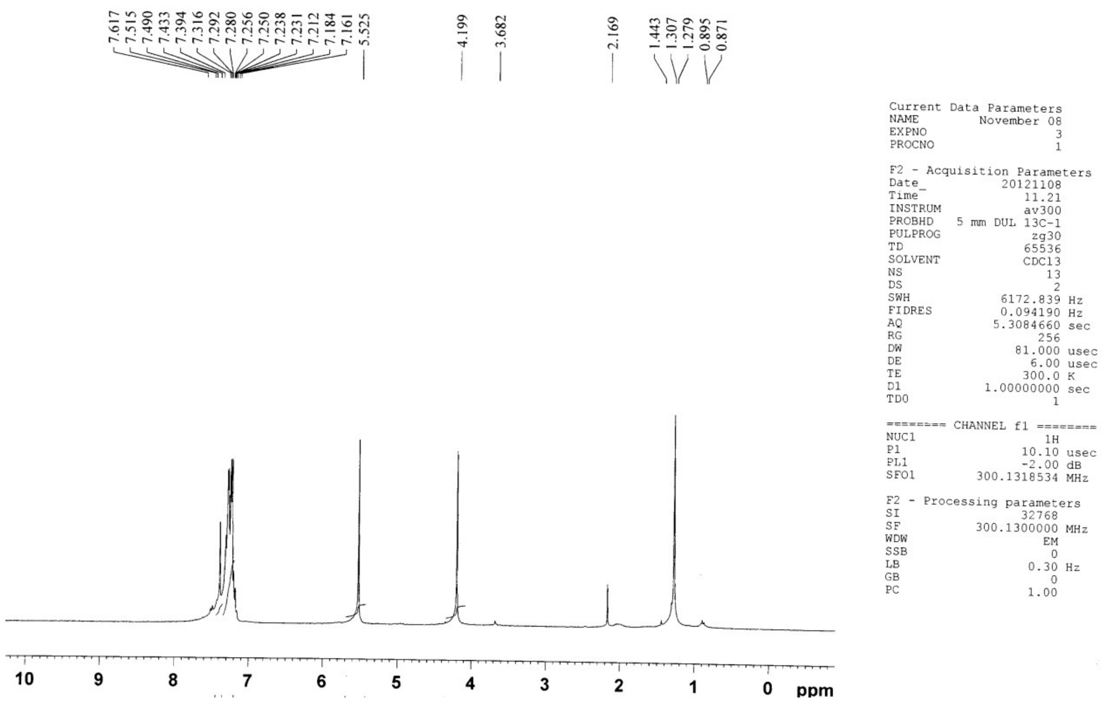


Figure S3 ^{1}H NMR spectrum of **L1**

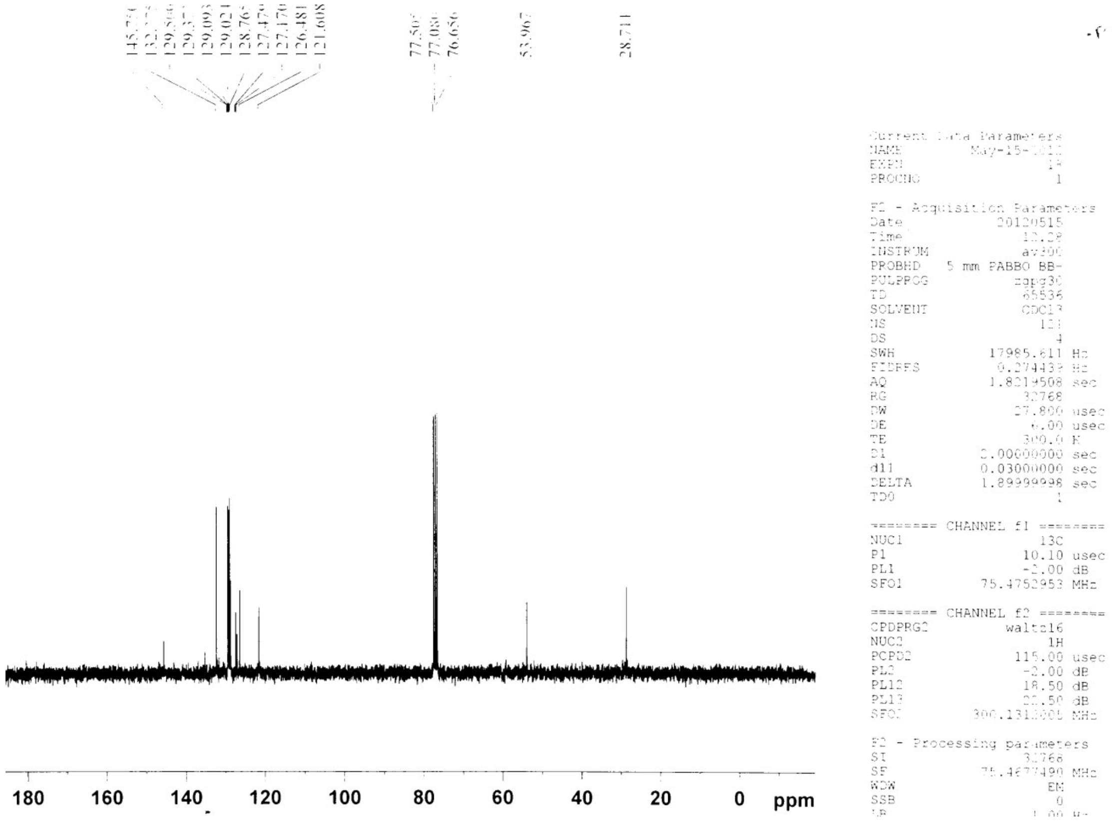


Figure S4 ^{13}C{^{1}H}NMR spectrum of **L1**

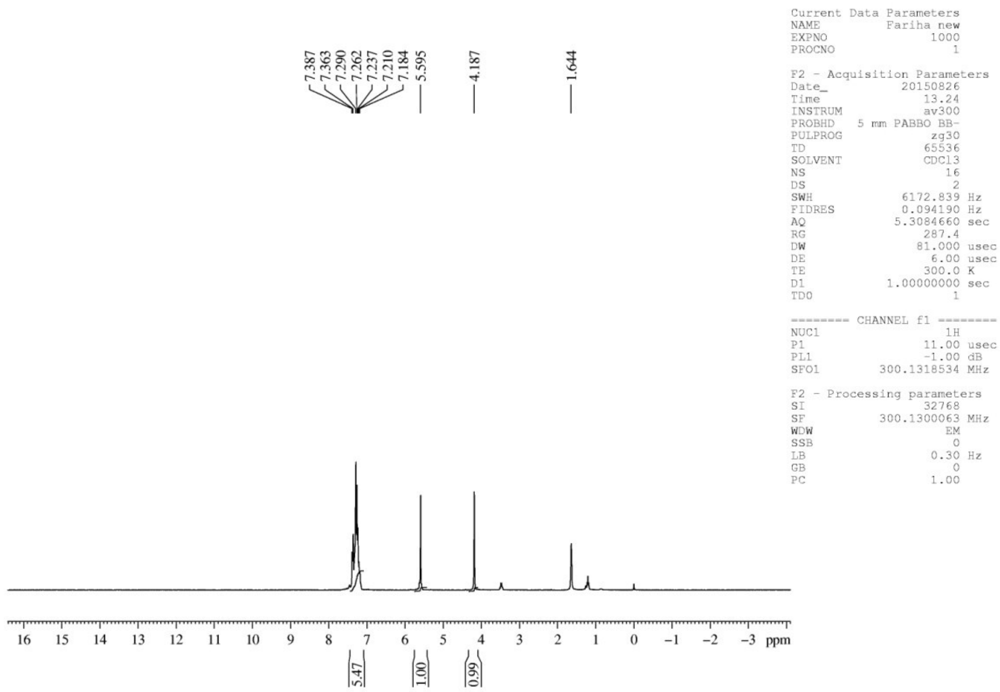


Figure S5 ^{1}H NMR spectrum of **L2**

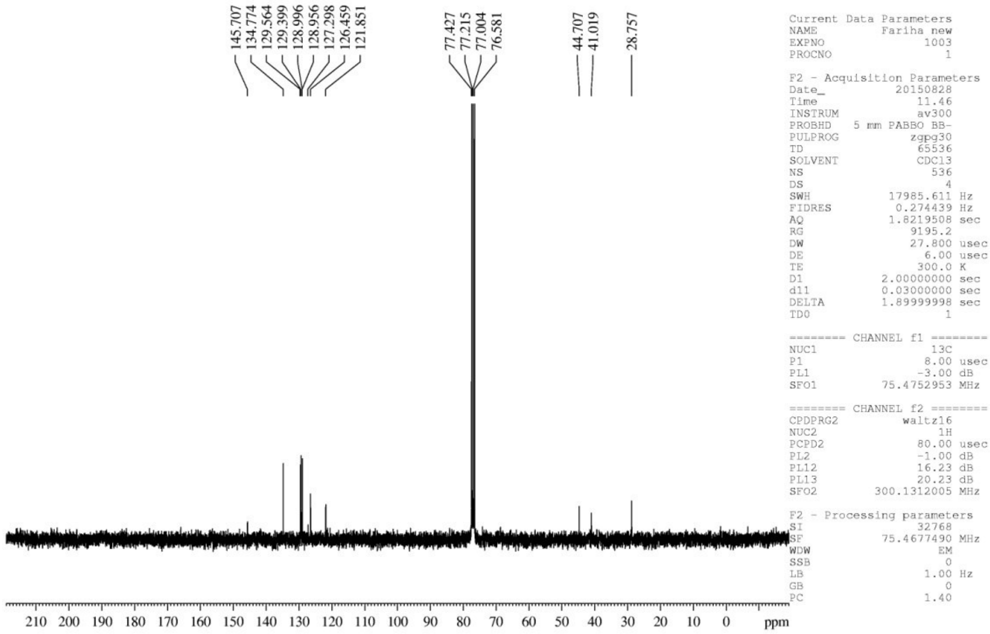


Figure S6 $^{13}C\{^{1}H\}$ NMR spectrum of **L2**

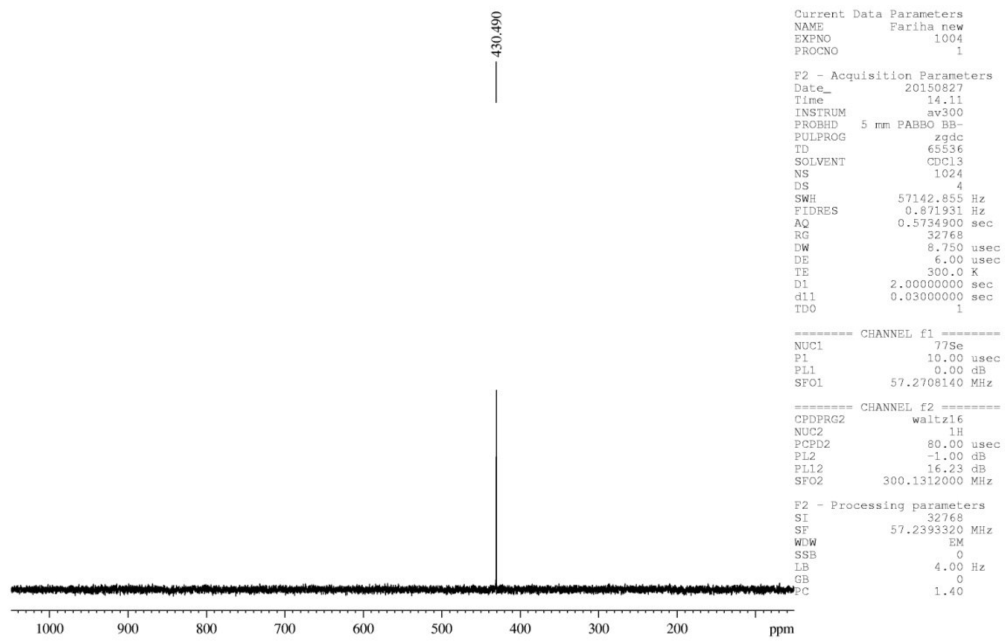


Figure S7 ^{77}Se NMR spectrum of **L2**

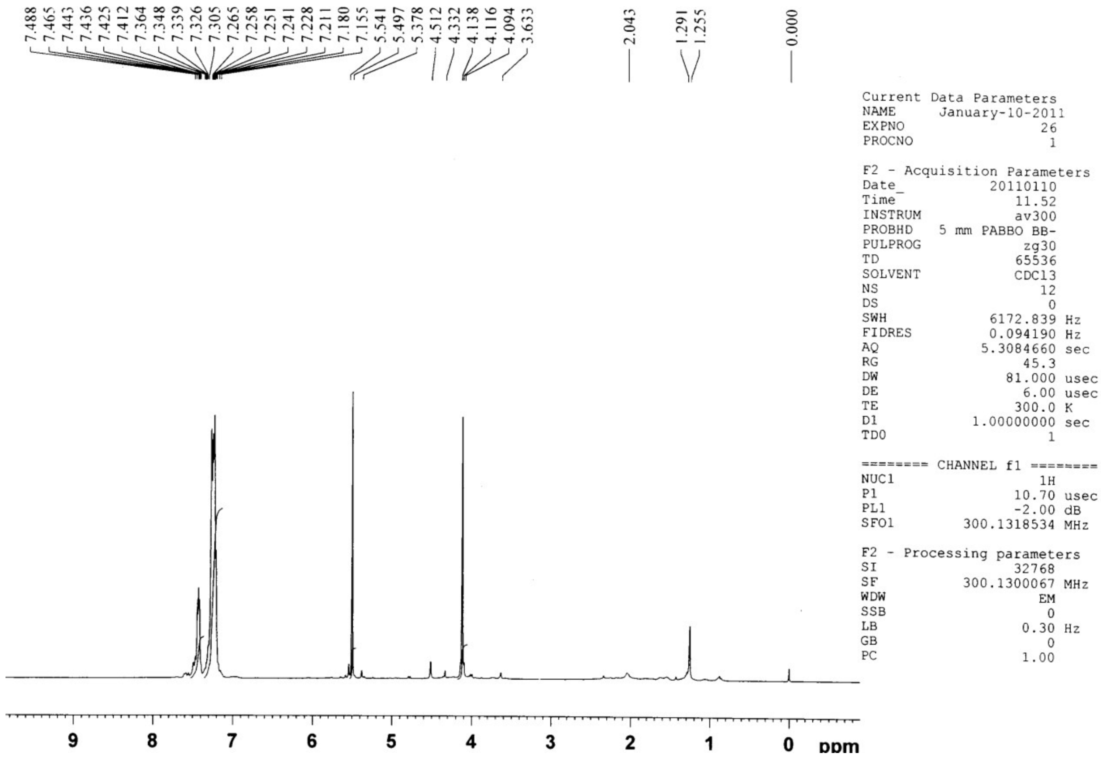


Figure S8 ^{1}H NMR spectrum of **L3**

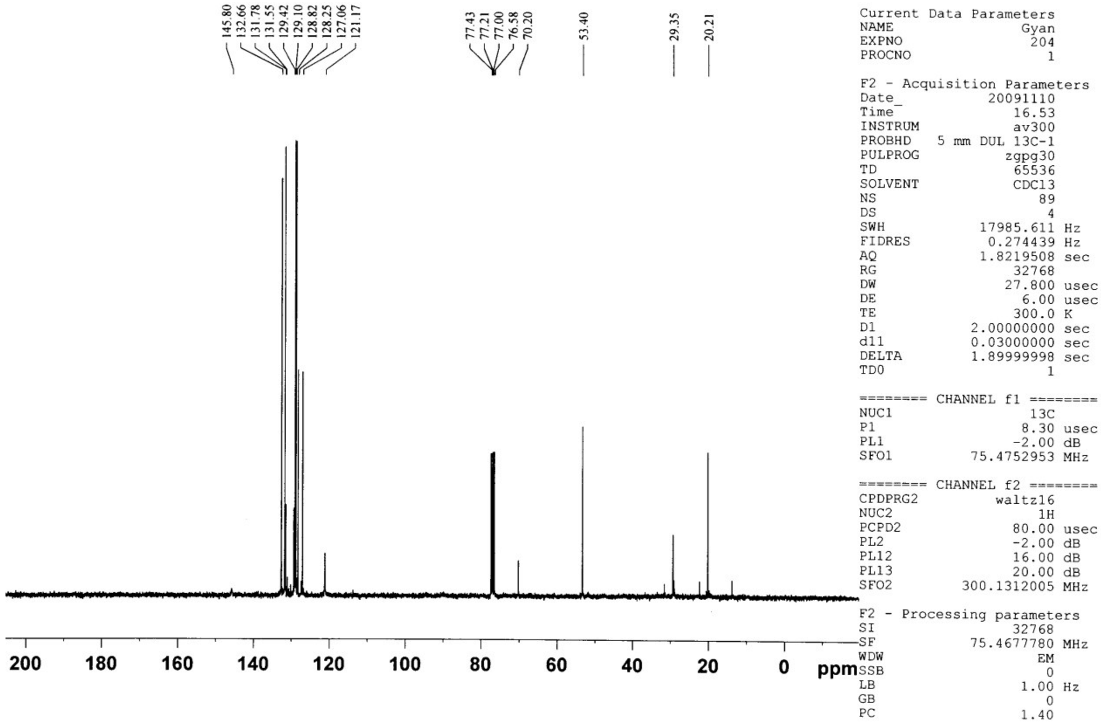


Figure S9 $^{13}C\{^{1}H\}$ NMR spectrum of **L3**

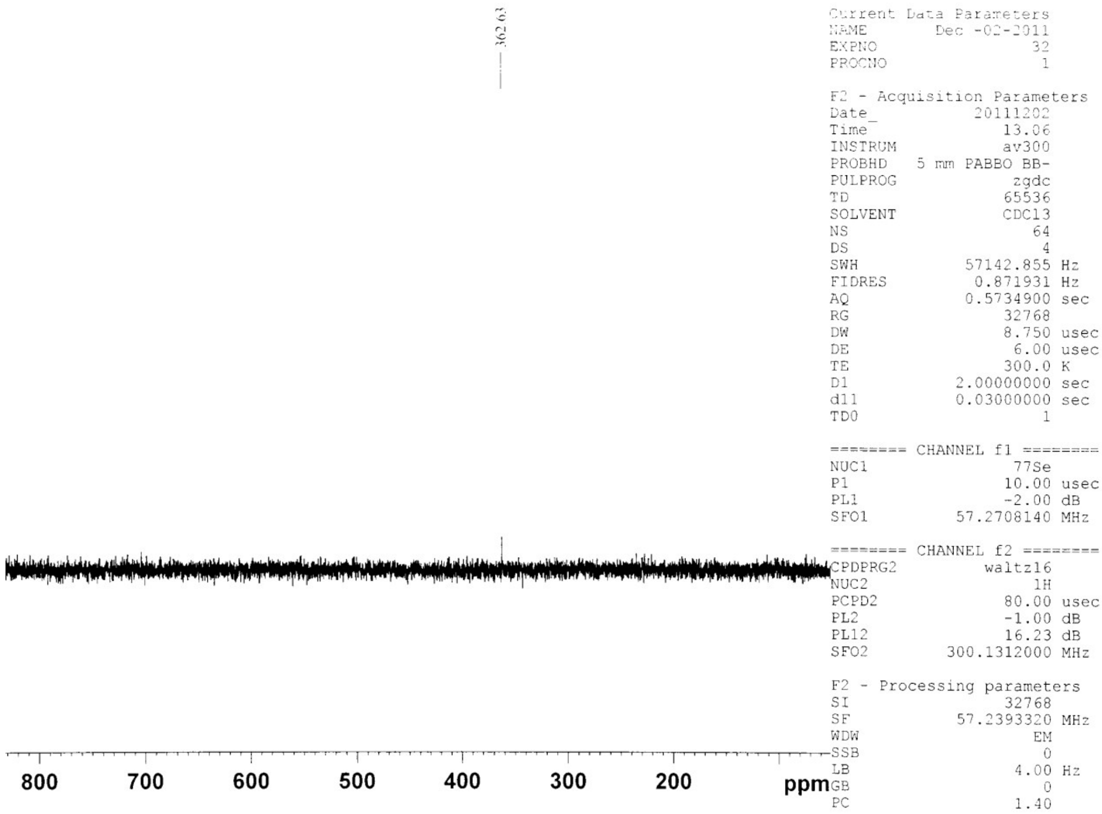


Figure S10 ^{77}Se NMR spectrum of **L3**

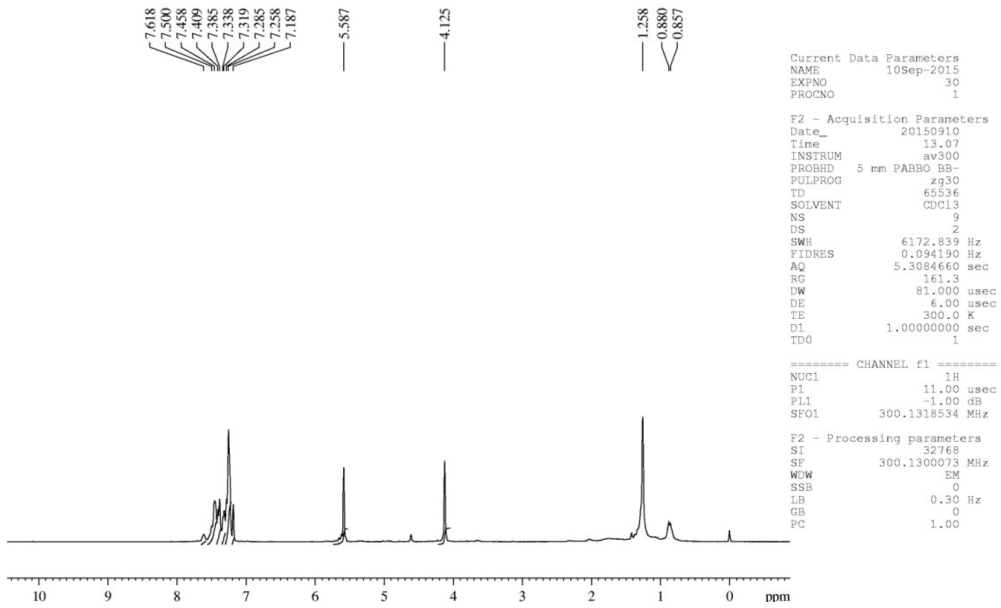


Figure S11 $^{13}C\{^{1}H\}$ NMR spectrum of **L4**

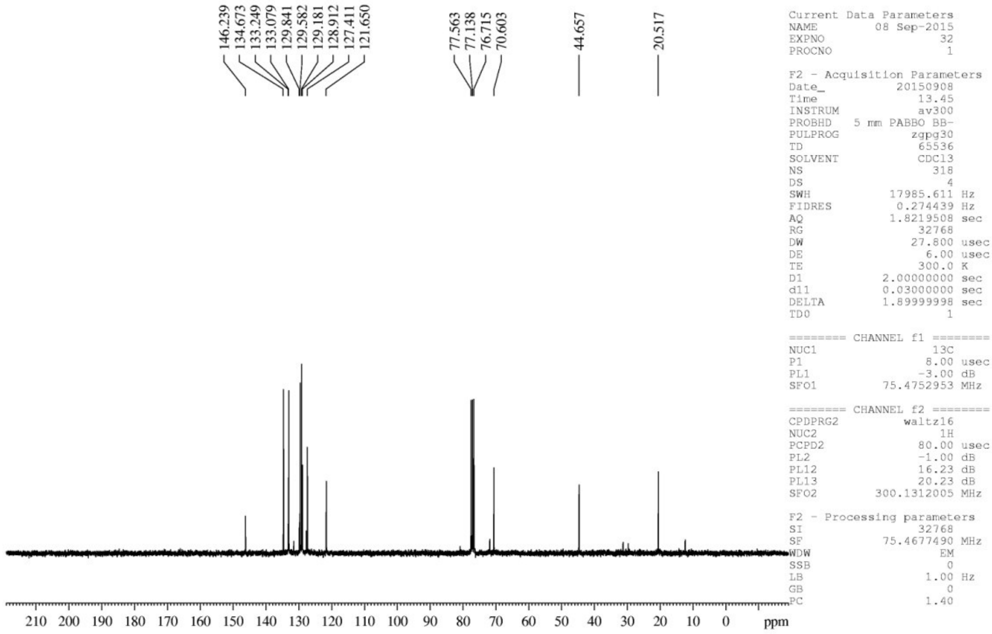


Figure S12 $^{13}C\{^{1}H\}$ NMR spectrum of **L4**

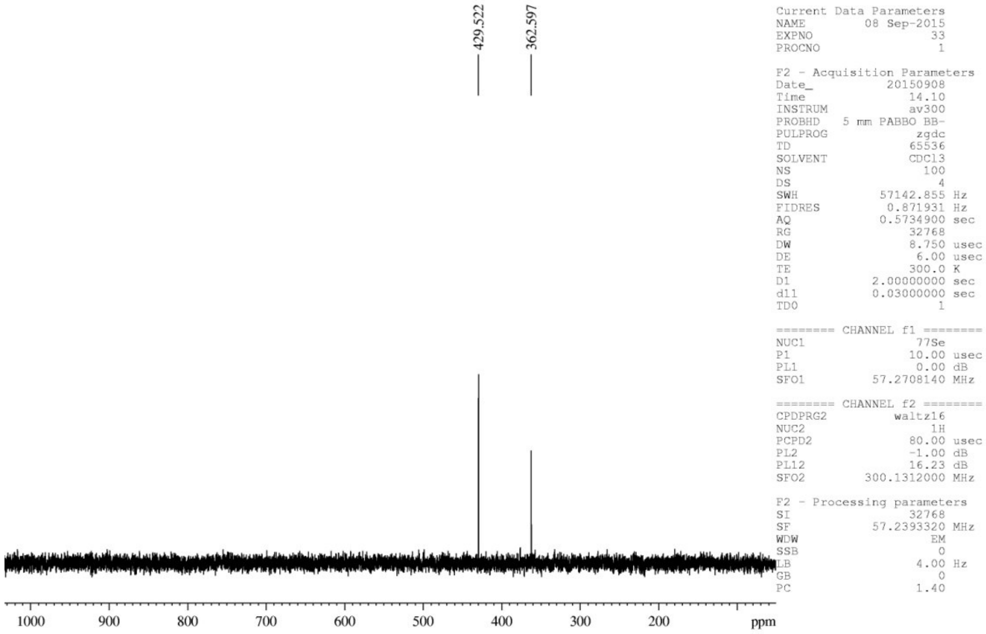


Figure S13 ^{77}Se NMR spectrum of **L4**

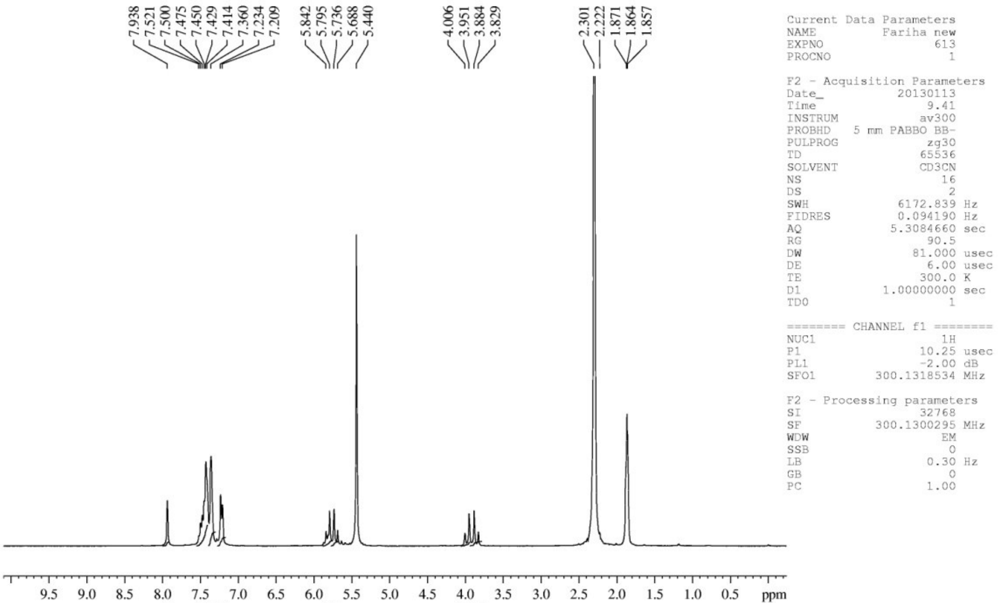


Figure S14 ^{1}H NMR spectrum of **1**

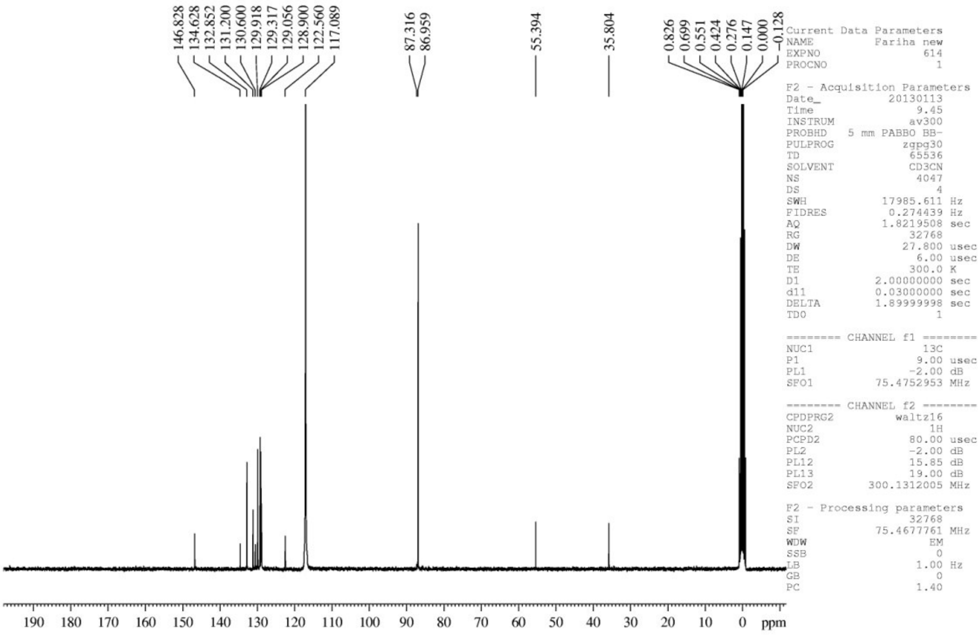


Figure S15 $^{13}C\{^{1}H\}$ NMR spectrum of **1**

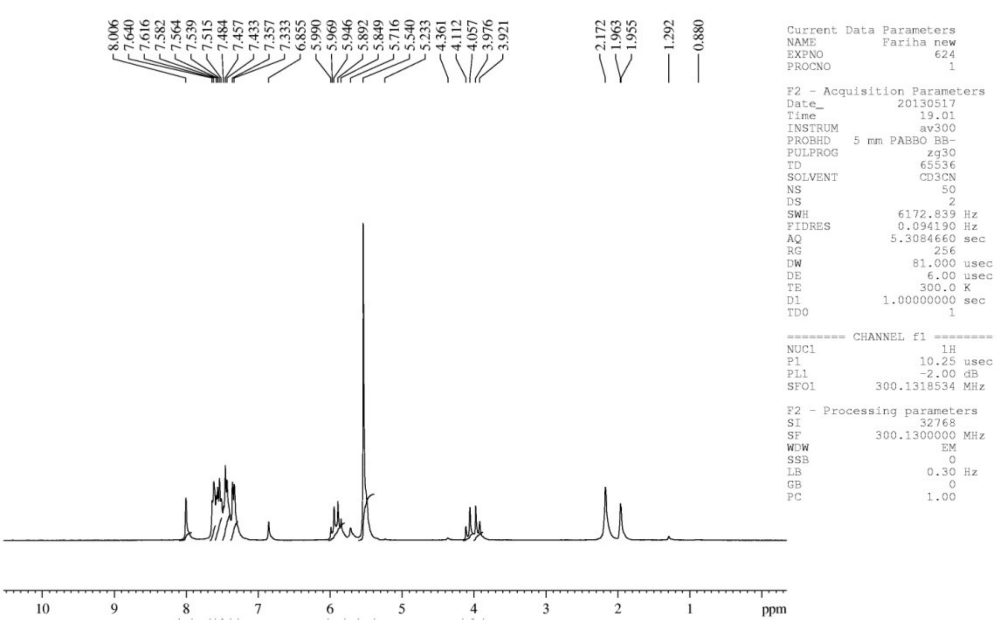


Figure S16 ^{1}H NMR spectrum of **2**

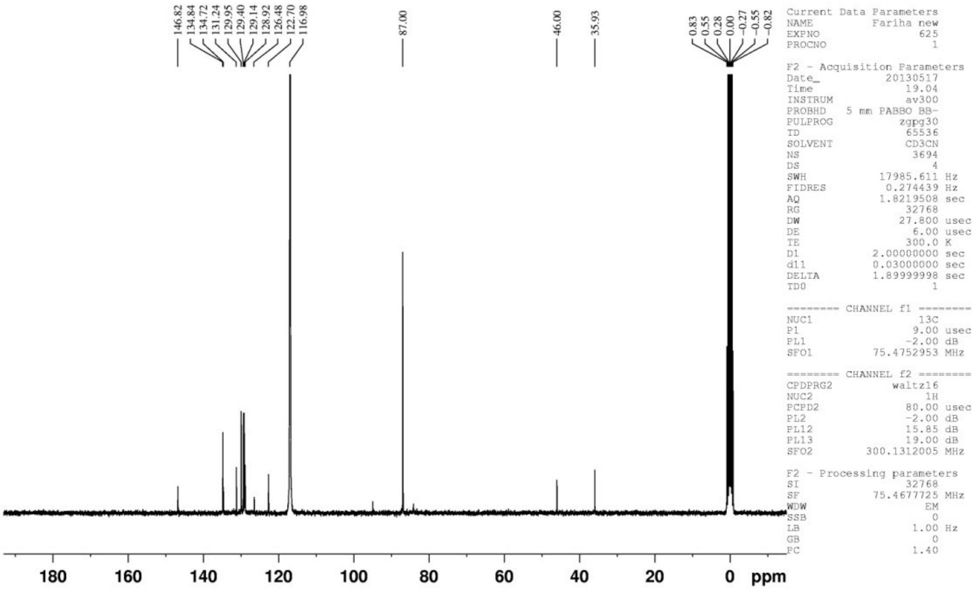


Figure S17 $^{13}C\{^{1}H\}$ NMR spectrum of **2**

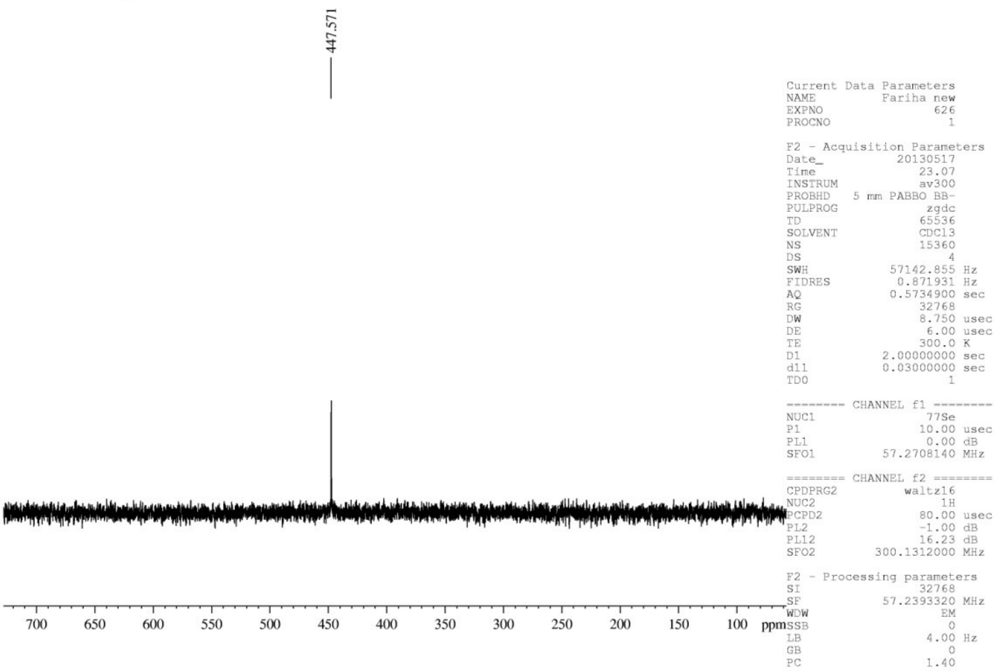


Figure S18 ^{77}Se NMR spectrum of **2**

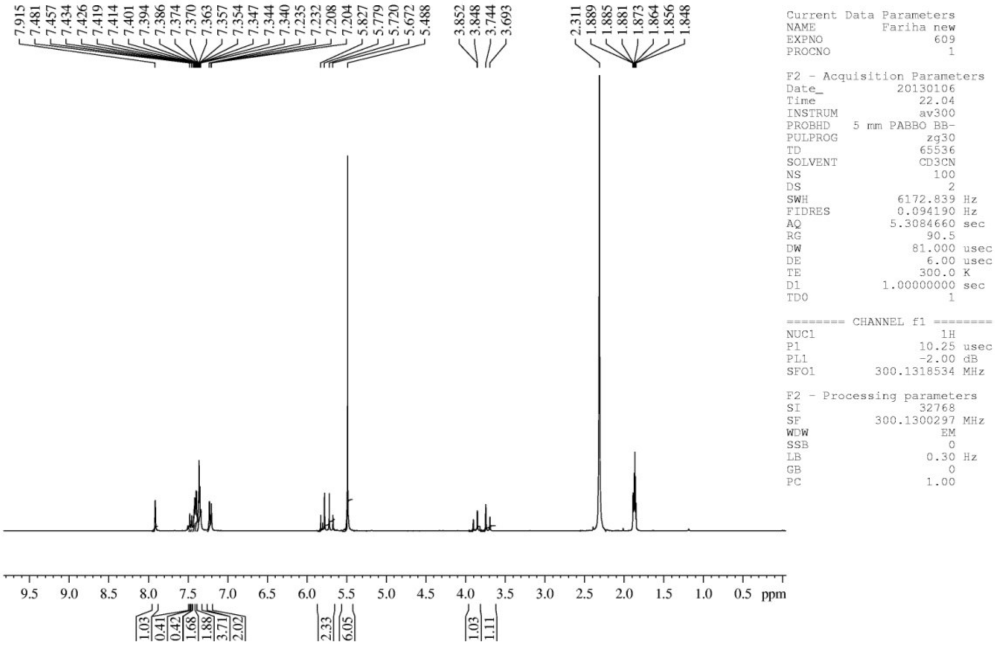


Figure S19 ^{1}H NMR spectrum of **3**

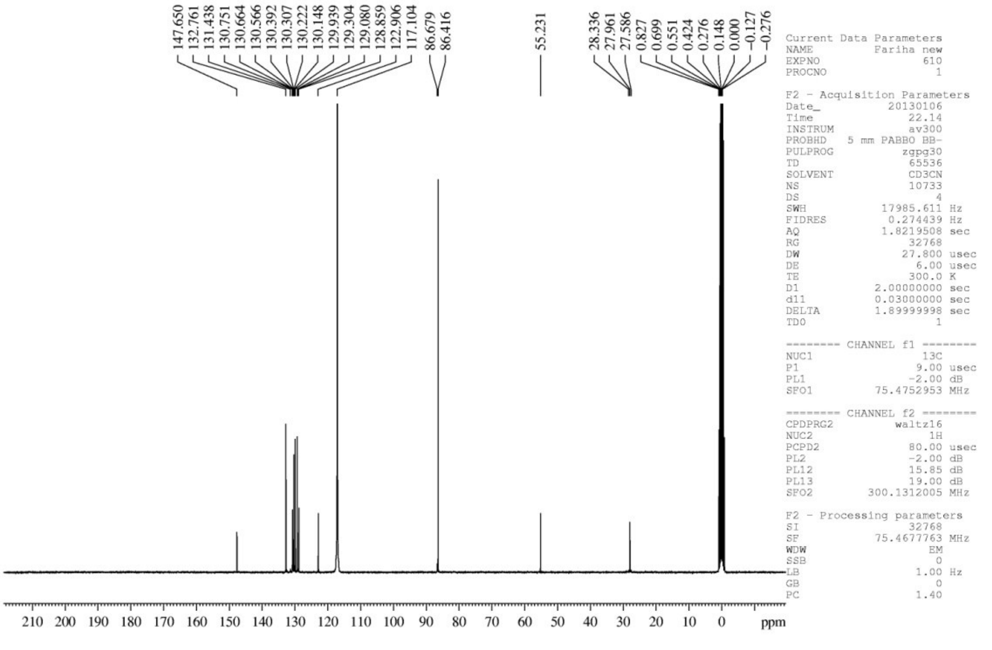


Figure S20 $^{13}C\{^{1}H\}$ NMR spectrum of **3**

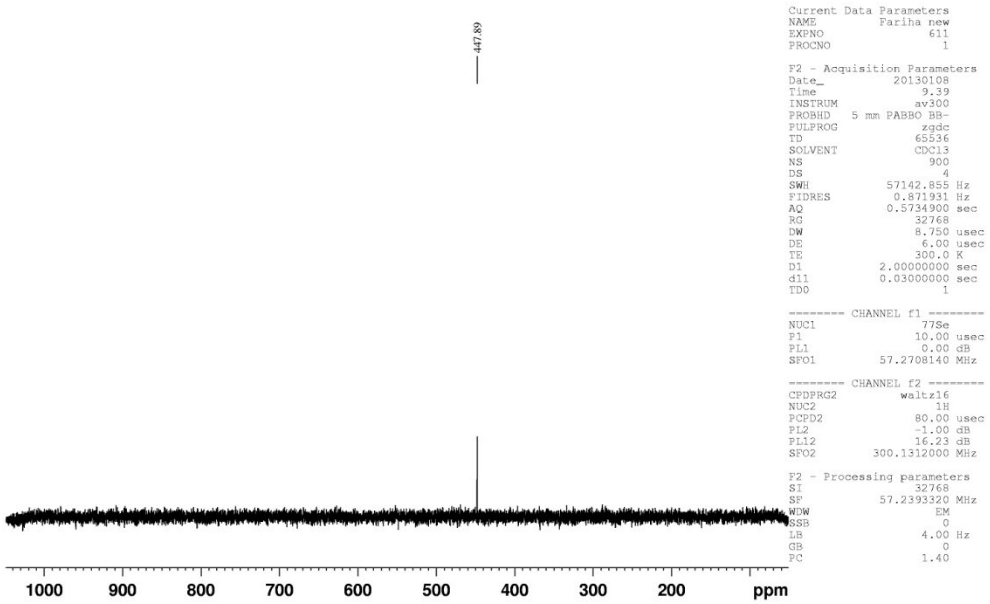


Figure S21 ^{77}Se NMR spectrum of **3**

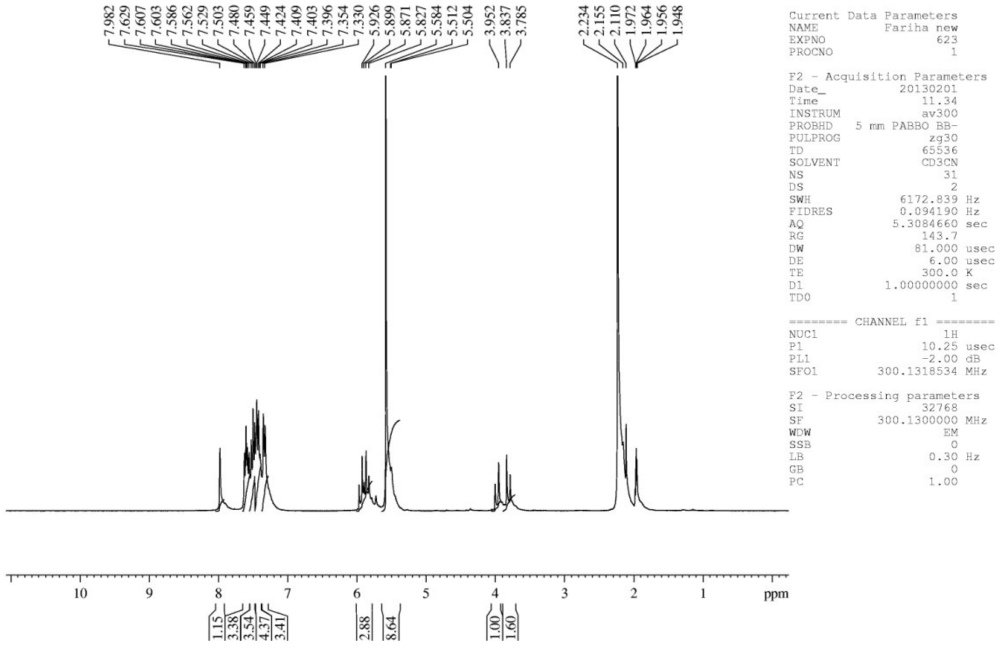


Figure S22 ^{1}H NMR spectrum of **4**

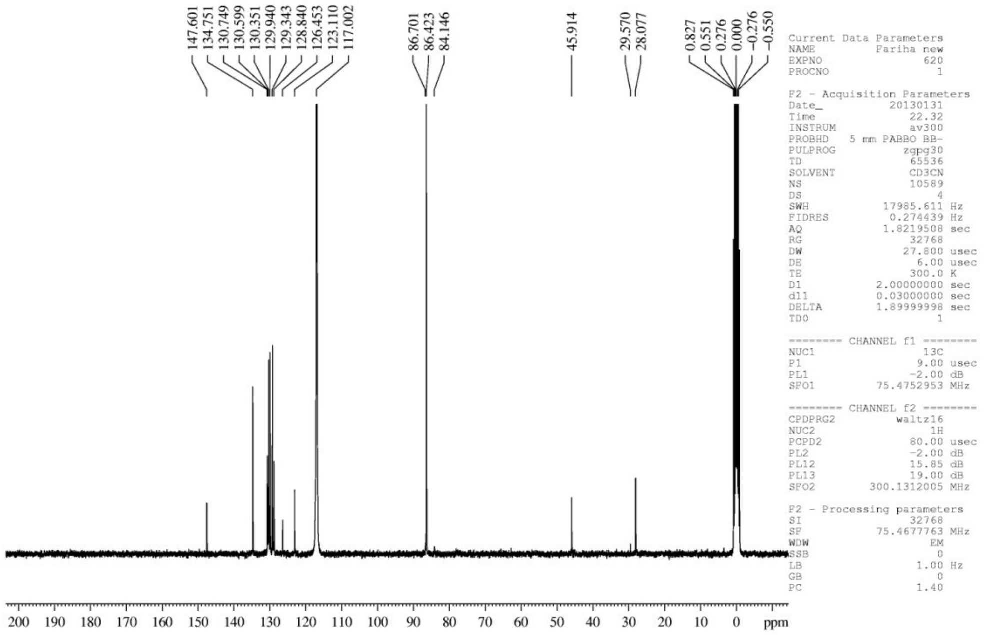


Figure S23 $^{13}C\{^1H\}$ NMR spectrum of **4**

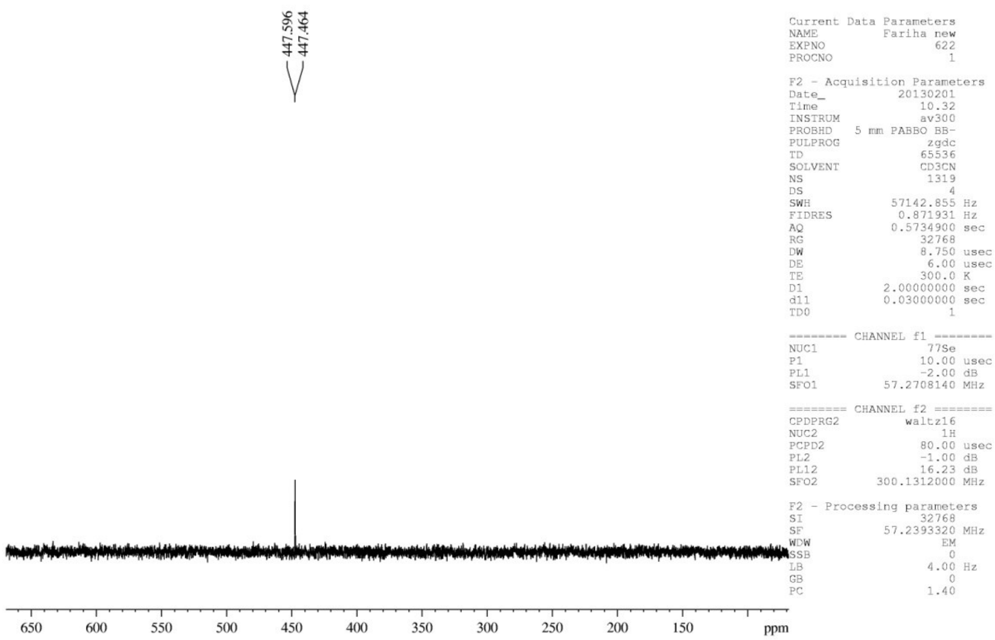


Figure S24 ^{77}Se NMR spectrum of **4**

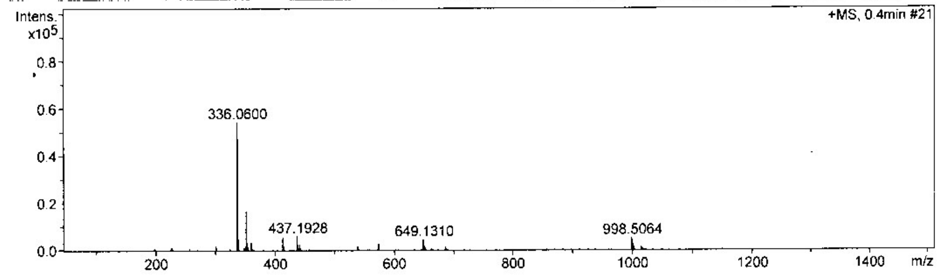
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\NOV_12\f1.d	Acquisition Date	11/6/2012 10:17:52 AM
Method	tune_low.m	Operator	Sharma/Singh
Sample Name	TM 1:100	Instrument / Ser#	micrOTOF-Q II 10262
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	100.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
336.0600	1	C 16 H 15 N 3 Na S 2	100.00	336.0600	-0.0	-0.1	3.5	10.5	even	ok

Figure S25 Mass spectrum of **L1**

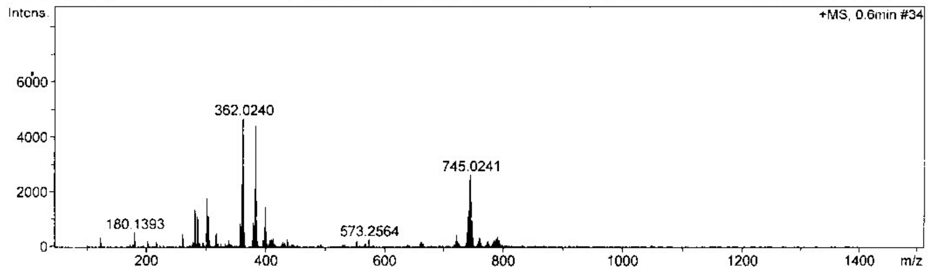
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\MAY_2012\fr2.d	Acquisition Date	5/11/2012 10:52:57 AM
Method	tune_low.m	Operator	Sharma/Singh
Sample Name		Instrument / Ser#	micrOTOF-Q II 10262
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	100.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
362.0240	1	C 16 H 16 N 3 S Se	100.00	362.0224	-1.6	-4.4	12.6	10.5	even	ok

Figure S26 Mass spectrum of **L2**

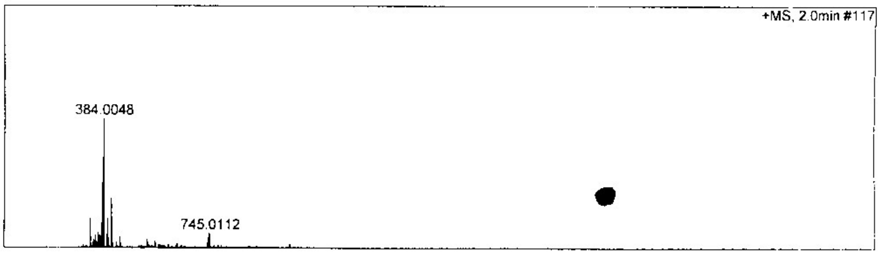
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\JAN_2012\far-4.d	Acquisition Date	1/17/2012 12:12:17 PM
Method	tune_wide.m	Operator	Sharma/Singh
Sample Name		Instrument / Ser#	micrOTOF-Q II 10262
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e^- Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
384.0048	1	C 16 H 15 N 3 Na S Se	384.0044	-1.2	0.3	10.5	ok	even	37.7	52.4	0.6	16.2	0.9	842.7

Figure S27 Mass spectrum of **L3**

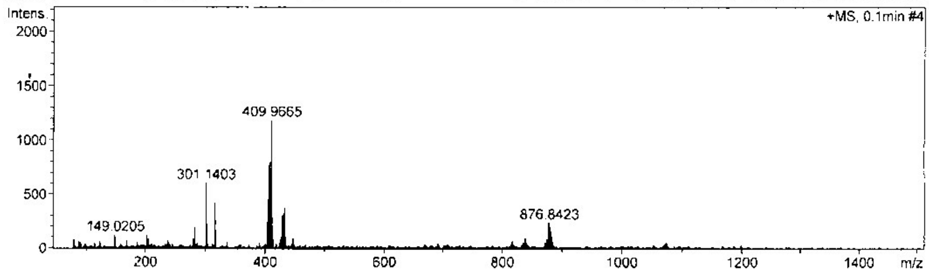
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\Service\fr1.d	Acquisition Date	5/11/2012 10:31:59 AM
Method	tune_low.m	Operator	Sharma/Singh
Sample Name		Instrument / Ser#	micrOTOF-Q II 10262
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	100.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e^- Conf	N-Rule
409.9665	1	C 16 H 16 N 3 Se 2	100.00	409.9672	0.7	1.8	78.6	10.5	even	ok

Figure S28 Mass spectrum of **L4**

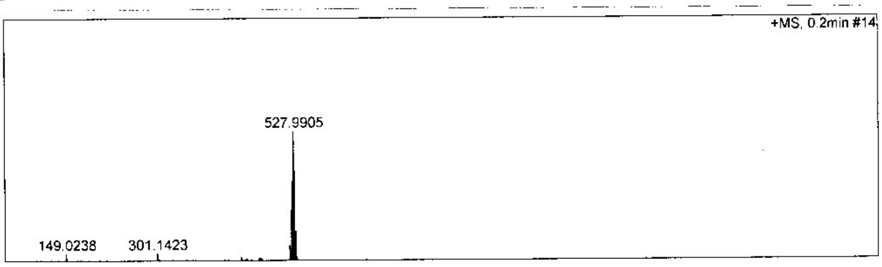
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\NOV_12\F 1.d	Acquisition Date	11/21/2012 10:22:07 AM
Method	tune_low.m	Operator	Sharma/Singh
Sample Name	TM 1:100	Instrument / Ser#	micrOTOF-Q II 10262
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	100.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
527.9905	1	C 22 H 21 Cl N 3 Ru S 2	100.00	527.9905	-0.0	-0.0	8.6	14.0	odd	-

Figure S29 Mass spectrum of **1**

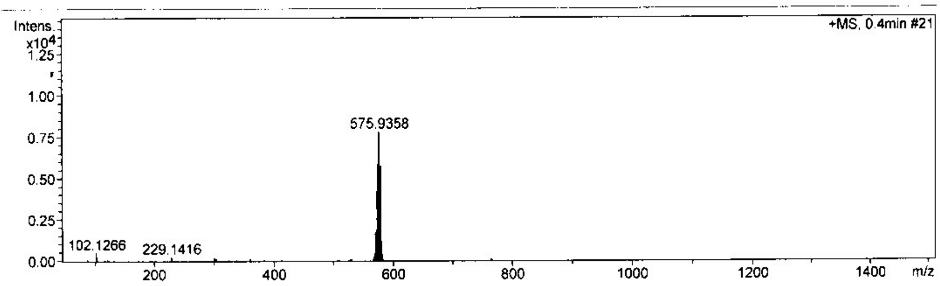
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\MAY_2012\fr3.d	Acquisition Date	5/11/2012 11:39:37 AM
Method	tune_low.m	Operator	Sharma/Singh
Sample Name		Instrument / Ser#	micrOTOF-Q II 10262
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	100.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
575.9358	1	C 22 H 21 Cl N 3 Ru S Se	100.00	575.9352	-0.6	-1.0	15.2	14.0	odd	-

Figure S30 Mass spectrum of **2**

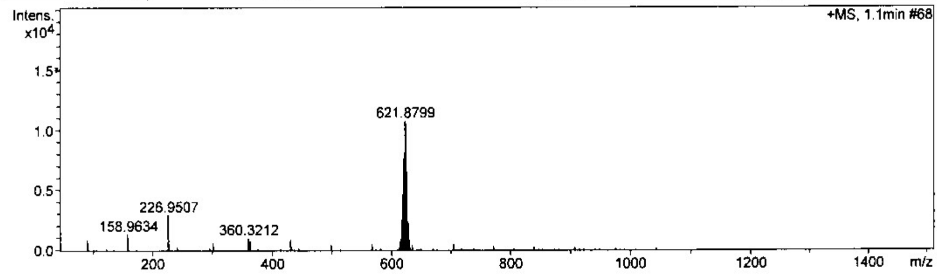
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\March_12\sese-a.d	Acquisition Date	3/30/2012 12:12:37 PM
Method	tune_low.m	Operator	Sharma/Singh
Sample Name		Instrument / Ser#	micrOTOF-Q II 10262
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	100.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
623.8793	1	C 22 H 21 Cl N 3 Ru Se 2	100.00	623.8800	0.8	1.2	12.1	14.0	odd	-

Figure S31 Mass spectrum of **3**

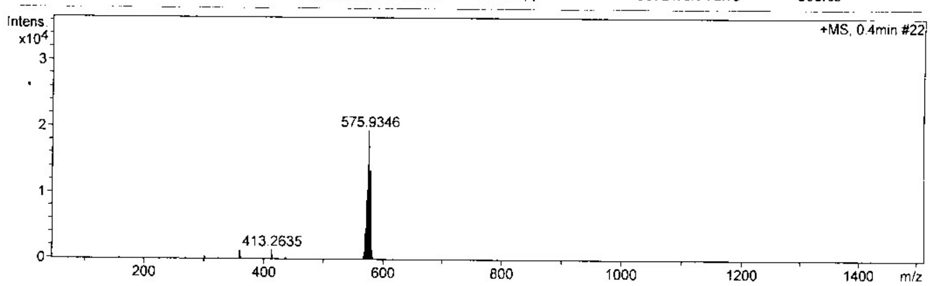
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\March_12\f3.d	Acquisition Date	3/16/2012 11:11:01 AM
Method	tune_low.m	Operator	Sharma/Singh
Sample Name		Instrument / Ser#	micrOTOF-Q II 10262
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	100.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
575.9346	1	C 22 H 21 Cl N 3 Ru S Se	100.00	575.9352	0.6	1.0	13.4	14.0	odd	-

Figure S32 Mass spectrum of **4**

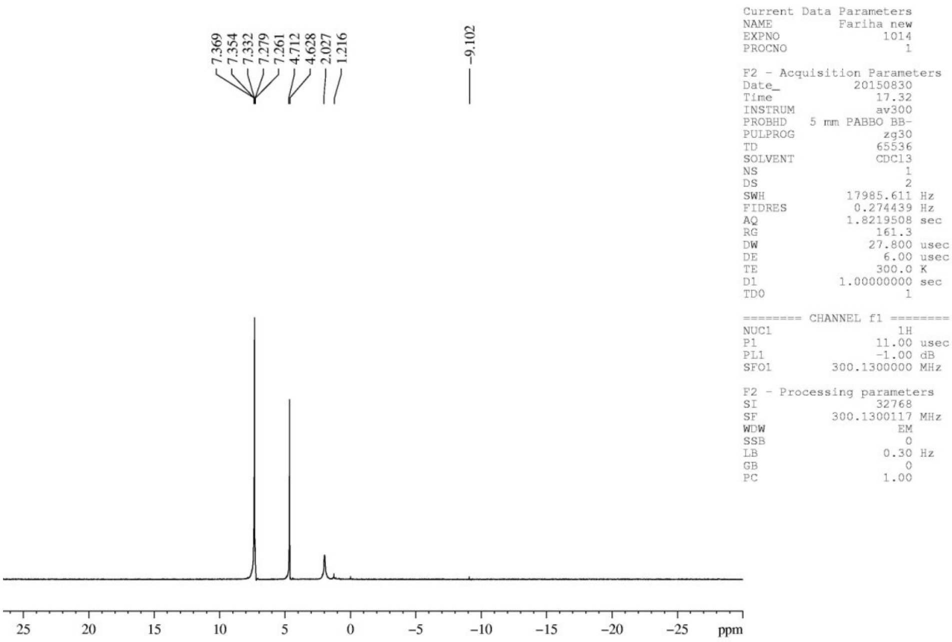


Figure S33 [1]HNMR spectrum of Oppenauer-type oxidation of benzyl alcohol showing M-H bond

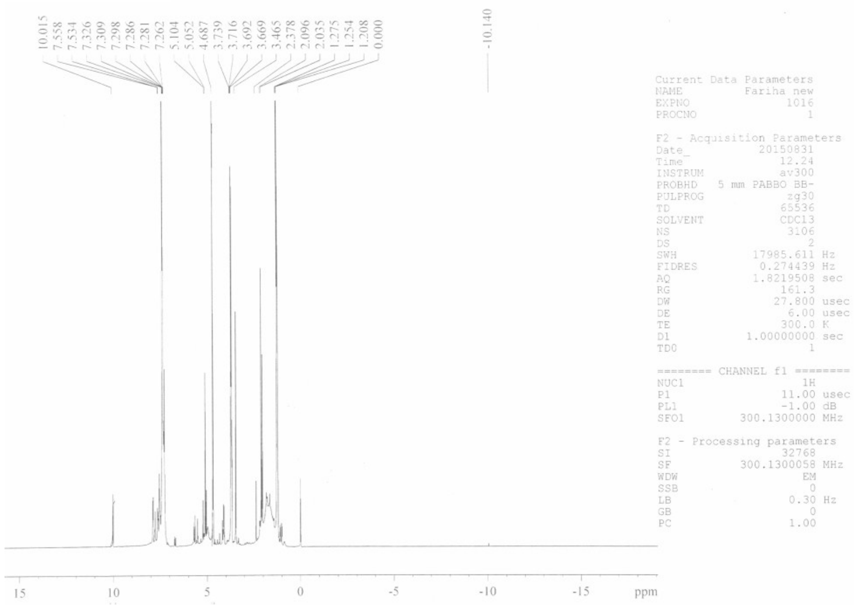


Figure S34 [1]HNMR spectrum of TH of Benzaldehyde showing M-H bond