Electronic Supplementary Material (ESI) for Dalton Transactions


**Supplementary Information**

# Anti-Leishmanial Activity of Heteroleptic Organometallic Sb(V) Compounds

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**Contents:**

**General Synthetic Procedure (GP)**

All reactions were conducted using 5.0 mmol of antimony(V) dibromide precursor and 10.0 mmol of potassium or sodium salt of carboxylic acid. Aryl substituted antimony(V) dibromide was ground together with the chosen carboxylic acid salt and dried in vacuo prior to use. The mixture of reagents were placed in a Schlenk flask with dried toluene (ca 100 mL) and stirred for 12 hours. The salt(s) formed were filtered off and the resulting clear solution was removed under reduced pressure to yield a solid residue.

**Synthesis of bis-(2-thiophenecarboxylato)triphenylantimony(V), [$SbPh_3(C_4H_3SCO_2)_2$], 12**

Reaction of triphenylantimony(V) dibromide (2.56 g, 5 mmol) with the potassium salt of 2-thiophenecarboxylic acid (1.66 g, 10 mmol) was performed and purified according to **GP**, producing a colourless solid. This was identified as **12**. Yield: 84 %. Melting point: 130-131 ˚C. FT-IR (KBr, $cm^{-1}$) 3127 (m), 3055 (m), 1616 (s), 1524 (s), 1478 (m), 1417 (s), 1361 (m), 1300 (s, br), 1170 (w), 1130 (w), 1103 (m), 1020 (w), 854 (m), 807 (s), 763 (m), 688 (m, br), 511 (m, br), 457 (m, br), 419 (s). Elemental Analysis; ($C_{28}H_{21}S_2O_4Sb$), Calc (Found): C 55.37 (55.22), H 3.49 (3.48), S 10.56 (10.55)%. $^1$H-NMR (300MHz, $CDCl_3$, 30 °C) $\delta$ = 8.18 (dd, 6H, $^3J$ = 7.5 Hz, $^4J$ = 4.2 Hz, Ar*H*), 7.64 (dd, 2H, $^3J$ = 3.6 Hz, $^4J$ =1.2 Hz, thiophene-*H*), 7.52-7.57 (m, 9H, Ar*H*), 7.44 (dd, 2H, $^3J$ = 5.1 Hz, $^4J$ = 3.6 Hz, thiophene-*H*), 7.03 (t, 2H, $^3J$ = 4.8 Hz, thiophene-*H*). $^{13}$C-NMR (75 MHz, $CDCl_3$, 30 °C) $\delta$ = 166.7 (*C*=O), 137.9 (Sb-*C*), 136.9 (Ar-*C*), 134.0 (thiopene-*C*), 132.5 (thiopene-*C*), 131.8 (Ar-*C*), 131.1 (thiopene-C), 129.6 (Ar-*C*), 127.5 (Ar-*C*).

**Synthesis of bis-(2-(m-tolyl)acetate)triphenylantimony(V), [$SbPh_3(m\text{-}CH_3C_6H_4CH_2CO_2)_2$], 13**

Reaction of triphenylantimony(V) dibromide (2.56 g, 5 mmol) with potassium salt of 2-(*m*-tolyl)acetic acid (1.88 g, 10 mmol) was performed and purified according to **GP**, producing a white crystalline solid. This was identified as **13**. Yield: 87%. Melting point: 76-77 ˚C. FT-IR (KBr, $cm^{-1}$): 3058 (m), 3010 (w), 2950 (w), 1640 (s), 1502 (m), 1434 (m), 1336 (s, br), 1183 (w), 1133 (m), 1066 (m), 994 (m), 801 (w), 730 (s), 690 (s), 656 (m), 547 (m), 455 (s, br), 323 (m), 282 (m). Elemental Analysis;

($C_{36}H_{33}O_4Sb$), Calc (Found): C 66.35 (66.38), H 5.12 (5.11)%. $^1$H-NMR (300 MHz, $CDCl_3$, 30 °C): $\delta$ = 8.18 (dd, $^3J$ = 7.5 Hz, $^4J$ = 2.4 Hz, 6H, Ar*H*), 7.83-7.85 (m, 4H, Ar*H*), 7.52-7.58 (m, 7H, Ar*H*), 7.26-7.31 (m, 6H, Ar*H*), 3.77 (s, 4H, C$H_2$), 2.39 (s, 6H, C$H_3$). $^{13}$C-NMR (75 MHz, $CDCl_3$, 30 °C): $\delta$ = 170.3 (*C*=O), 138.4 (Sb-*C*), 137.7 (Ar-*C*), 133.8 (Ar-*C*), 132.9 (Ar-*C*), 132.4 (Ar-*C*), 131.2 (Ar-*C*), 130.5 (Ar-*C*), 129.3 (Ar-*C*), 127.8 (Ar-*C*), 127.0 (Ar-*C*), 43.2 (-*C*$H_2$), 21.32 (-*C*$H_3$).

**Synthesis of bis-(2-methoxybenzoato)triphenylantimony(V), [$SbPh_3$(*o*-$OCH_3C_6H_4CO_2$)$_2$], 14**

Reaction of triphenylantimony(V) dibromide (2.56 g, 5 mmol) with potassium salt of 2-methoxybenzoic acid (1.90 g, 10 mmol) was performed and purified according to **GP**, producing a white crystalline solid. This was identified as **14**. Yield: 85%. Melting point: 90-93˚C. FT-IR (KBr, cm$^{-1}$): 3054 (m), 2987 (m), 2832 (m), 1595 (s), 1576 (sh), 1462 (m), 1346 (s, br), 1256 (s, br), 1143 (w), 1018 (w), 858 (m), 742 (m), 692 (m), 615 (w), 557 (w), 452 (s, br), 268 (m). Elemental Analysis; ($C_{34}H_{29}O_6Sb$), Calc (Found): C 62.31 (62.27), H 4.46 (4.45)%. $^1$H-NMR (300 MHz, $CDCl_3$, 30 °C) $\delta$ = 8.26 (dd, 6H, $^3J$ = 7.2 Hz, $^4J$ = 3.3 Hz, Ar*H*), 7.66 (dd, 2H, $^3J$ = 7.5 Hz, $^4J$ = 1.5 Hz, Ar*H*), 7.46-7.52 (m, 9H, Ar*H*), 7.34-7.37 (m, 4H, Ar*H*), 6.90 (d, 2H, $^3J$ = 7.5 Hz, Ar*H*), 3.85 (s, 6H, OC$H_3$). $^{13}$C-NMR (75 MHz, $CDCl_3$, 30 °C) $\delta$ = 170.1 (*C*=O), 158.7 (*C*$OCH_3$), 138.0 (Sb-*C*), 136.2 (Ar-*C*), 134.2 (Ar-*C*), 132.2 (Ar-*C*), 131.8 (Ar-*C*), 130.9 (Ar-*C*), 129.2 (Ar-*C*), 120.0 (Ar-*C*), 112.0 (Ar-*C*), 55.3 (O*C*$H_3$).

**Synthesis of bis-(phenoxyacetato)triphenylantimony(V), [$SbPh_3$($C_6H_5OCH_2CO_2$)$_2$], 15**

Reaction of triphenylantimony(V)dibromide (2.56 g, 5 mmol) with potassium salt of phenoxyacetic acid (1.90 g, 10 mmol) was performed and purified according to **GP**, producing a colorless solid. This was identified as **15**. Yield: 86%. Melting point: 70-71 ˚C. FT-IR (KBr, cm$^{-1}$): 3053 (m), 2915 (m), 2675 (m), 1668 (s), 1596 (s), 1490 (s), 1431 (s), 1316 (s, br), 1255 (w), 1216 (m), 1068 (m, br), 895 (m, br), 748 (m), 689 (m), 595 (w), 453 (m), 412 (m), 292 (m), 260 (m). Elemental Analysis; ($C_{34}H_{29}O_6Sb$), Calc (Found): C 62.31 (62.27), H 4.46 (4.45)%. $^1$H-NMR (300 MHz, $CDCl_3$, 30 °C) $\delta$ = 7.94 (dd, 6H, $^3J$ = 7.5 Hz, $^4J$ = 1.2 Hz, Ar*H*), 7.48-7.57 (m, 10H, Ar*H*), 7.35-7.40

(m, 7H, Ar*H*), 7.20 (t, 2H, $^{3}J$ = 7.5 Hz, Ar*H*), 4.14 (s, 4H, C$H_2$). $^{13}$C-NMR (75MHz, $CDCl_3$, 30 °C) $\delta$ =172.3 (*C*=O), 157.9 (*C*O$CH_2$), 136.2 (Ar-*C*), 134.1 (Ar-*C*), 131.6 (Ar-*C*), 129.4 (Ar-*C*), 128.8 (Ar-*C*), 128.5 (Ar-*C*), 114.4 (Ar-*C*), 65.8 (*C*$H_2$).

**Synthesis of bis-(furan-2-carboxylato)triphenylantimony(V), [$SbPh_3(C_4H_3OCO_2)_2$], 16**

Reaction of triphenylantimony(V) dibromide (2.56 g, 5 mmol) with potassium salt of furan-2-carboxylic acid (1.50 g, 10 mmol) was performed and purified according to **GP**, producing a white crystalline solid. This was identified as **16**. Yield: 91%. Melting point: 189-190 ˚C. FT-IR (KBr, $cm^{-1}$): 3125 (m), 3057 (m), 1639 (s), 1578 (w, sh), 1479 (s), 1433 (m), 1341 (s, br), 1182 (s), 1132 (m), 1068 (m), 1014 (m, br), 929 (m), 812 (s), 769 (m), 735 (m), 685 (m, br), 609 (w), 550 (m), 453 (s, br), 331 (w), 302 (w), 269 (m). Elemental Analysis; ($C_{28}H_{21}O_6Sb$), Calc (Found): C 58.44 (58.46), H 3.67 (3.68)%. $^{1}$H-NMR (300 MHz, $CDCl_3$, 30 °C): $\delta$ = 8.17 (dd, $^{3}J$ = 7.5 Hz, $^{4}J$ = 4.2 Hz, 6H, Ar*H*), 7.50-7.55 (m, 9H, Ar*H*), 7.45 (d, $^{3}J$ = 3.4 Hz, 2H, furyl-*H*), 7.02 (d, $^{3}J$ = 3.3 Hz, $^{4}J$ = 1.8 Hz, 2H, furyl-*H*), 6.39 (dd, $^{3}J$ = 3.3 Hz, $^{4}J$ = 1.8 Hz, 2H, furyl-*H*). $^{13}$C-NMR (75 MHz, $CDCl_3$, 30 °C): $\delta$ = 161.8 (*C*=O), 146.9 (furyl-*C*), 145.3 (*C*-COO), 136.9 (Ar-*C*), 134.1 (Ar-*C*), 131.4 (Ar-*C*), 129.5 (Ar-*C*), 116.6 (furyl-*C*), 114.4 (furyl-*C*).

**Reaction of bis-(3-phenyl-2-propenato)triphenylantimony(V), [$SbPh_3(C_6H_5CH{=}CHCO_2)_2$], 17**

Reaction of triphenylantimony(V) dibromide (2.56 g, 5 mmol) with potassium salt of cinnamic acid (1.86 g, 10 mmol) was performed and purified according to GP, producing a colourless solid. This was identified as **17**. Yield: 73%. Melting point: 160-163 ˚C. FT-IR (KBr, $cm^{-1}$): 3050 (m), 1641 (s), 1566 (s), 1482 (m), 1437 (m), 1363 (s, br), 1196 (m), 1068 (m), 969 (m), 869 (m), 744 (s), 686 (s), 587 (m), 540 (w), 458 (s, br), 362 (m), 318 (m). Elemental Analysis; ($C_{36}H_{29}O_4Sb$), Calc (Found): C 66.79 (66.71), H 4.52 (4.50)%. $^{1}$H-NMR (300 MHz, $CDCl_3$, 30 °C) $\delta$ = 8.16 (dd, 6H, $^{3}J$ = 7.5 Hz, $^{4}J$ = 3.2 Hz, Ar*H*), 7.54-7.58 (m, 10H, Ar*H*), 7.45-7.50 (m, 6H, Ar*H*, -C*H*=CH-), 7.34-7.37 (m, 5H, Ar*H*), 6.39 (d, 2H, $^{3}J$ = 7.5 Hz, -CH=C*H*). $^{13}$C-NMR (75MHz, $CDCl_3$, 30 °C) $\delta$ = 170.9 (*C*=O), 143.5 (-*C*H=CH),

138.7 (Ar-*C*), 134.9 (Ar-*C*), 133.9 (Ar-*C*), 131.1 (Ar-*C*), 129.8 (Ar-*C*), 129.4 (Ar-*C*), 128.7 (Ar-*C*), 127.9 (Ar-*C*), 120.9 (-CH=*C*H).

**Synthesis of bis-(2-methylbenzoato)triphenylantimony(V), [$SbPh_3$(*o*-C $H_3C_6H_4CO_2$)$_2$], 18**

Reaction of triphenylantimony(V) dibromide (2.56 g, 5 mmol) with potassium salt of 2-methylbenzoic acid (1.74 g, 10 mmol) was performed and purified according to **GP**, producing a colourless solid. This was identified as **18**. Yield: 89%. Melting point: 71-72 ˚C. FT-IR (KBr, $cm^{-1}$): 3057 (m), 2966 (m), 1637 (s, br), 1478 (m), 1433 (s), 1317 (s, br), 1275 (w), 1145 (m), 1084 (w), 994 (w), 858 (m), 788 (m), 736 (s), 690 (m), 567 (s), 451 (m), 301 (m). Elemental Analysis; ($C_{36}H_{29}O_4Sb$), Calc (Found): C 65.61 (65.51), H 4.69 (4.67)%. $^1$H-NMR (300MHz, $CDCl_3$, 30 ˚C) $\delta$ = 8.20 (dd, 6H, $^3J$ = 6.9 Hz, $^4J$ = 3.4 Hz, Ar*H*), 7.80 (d, 2H, $^3J$ = 7.2 Hz, Ar*H*), 7.51-7.53 (m, 9H, Ar*H*), 7.32 (t, 2H, $^3J$ = 7.5 Hz, Ar*H*), 7.15-7.22 (m, 4H, Ar*H*), 2.42 (s, 6H, -C$H_3$). $^{13}$C-NMR (75 MHz, $CDCl_3$, 30 ˚C) $\delta$ = 172.6 (*C*=O), 139.5 (*C*-$CH_3$), 134.0 (Ar-*C*), 132.4 (Ar-*C*), 131.2 (Ar-*C*), 131.0 (Ar-*C*), 130.6 (Ar-***C***), 130.2 (Ar-*C*), 129.3 (Ar-*C*), 128.3 (Ar-*C*), 125.4 (Ar-*C*), 21.62 (-*C*$H_3$).

**Synthesis of bis-(4-methoxybenzoato)tribenzylantimony(V), [$Sb(C_6H_5CH_2)_3$(*p*-$OCH_3C_6H_4CO_2$)$_2$], 19**

Reaction of tribenzylantimony(V)dibromide (2.78 g, 5 mmol) with potassium salt of 4-methoxybenzoic acid (1.90 g, 10 mmol) was performed and purified according to **GP**, producing a white solid. This was identified as **19**. Yield: 89%. Melting point: 126-129 ˚C. FT-IR (KBr, $cm^{-1}$): 3046 (m), 2991 (m), 2832 (m), 1637 (s), 1591 (s), 1569 (w), 1467 (m), 1353 (s, br), 1241 (s, br), 1141 (w), 1013 (w), 852 (m), 741 (m), 689 (m), 615 (w), 565 (w), 452 (s, br), 262 (m). Elemental Analysis; ($C_{37}H_{35}O_6Sb$), Calc (Found): C 63.72 (63.58), H 5.06 (5.05)%. $^1$H-NMR (300 MHz, $CDCl_3$, 30 ˚C) $\delta$ = 8.10 (d, 4H, $^3J$ = 6.9 Hz, Ar*H*), 7.29-7.34 (m, 6H, Ar*H*) 7.20-7.24 (m, 9H, Ar*H*), 6.97 (d, 4H, $^3J$ = 6.9 Hz, Ar*H*), 3.90 (s, 6H, -O$CH_3$), 2.95 (s, 6H, -$CH_2$-). $^{13}$C-NMR (75MHz, $CDCl_3$, 30 ˚C) $\delta$ = 163.4 (*C*=O), 141.8 (*C*$OCH_3$), 132.3 (Ar-*C*), 129.1 (Ar-*C*), 128.4 (Ar-*C*), 128.3 (Ar-*C*), 128.1 (Ar-*C*), 125.9 (Ar-*C*), 121.7 (Ar-*C*), 55.5 (-O*C*$H_3$), 37.9 (-*C*$H_2$).

**Synthesis of bis-(2-methoxybenzoato)tris-(o-tolyl)antimony(V), [Sb(*o*-$CH_3C_6H_4$)$_3$(*o*-$OCH_3C_6H_4CO_2$)$_2$], 20**

Reaction of *tris*-(*o*-tolyl)antimony(V)dibromide (2.78 g, 5 mmol) with potassium salt of 2-methoxybenzoic acid (1.90 g, 10 mmol) was performed and purified according to **GP**, producing a white crystalline solid. This was identified as **20**. Yield: 84%. Melting point: 174-175 ˚C. FT-IR (KBr, $cm^{-1}$) 3054 (m), 2934 (m), 2892 (m), 1639 (s), 1595 (m), 1462 (s, br), 1321 (s), 1248 (m), 1165 (m), 1134 (m), 1095 (w), 1019 (m), 845 (m), 750 (s), 704 (w), 657 (m), 568 (m), 436 (s), 280 (m). Elemental Analysis; ($C_{37}H_{35}O_6Sb$), Calc (Found): C 63.72 (63.61), H 5.06 (5.06)%. $^1$H-NMR (300 MHz, $CDCl_3$, 30 ˚C) $\delta$ = 8.47 (dd, 3H, $^3J$ = 7.2 Hz, $^4J$ =1.2 Hz, Ar*H*), 7.26-7.47 (m, 13H, Ar*H*), 6.78-6.83 (m, 4H, Ar*H*), 3.61 (s, 6H, -OC$H_3$), 2.60 (s, 9H, -C$H_3$). $^{13}$C-NMR (75 MHz, $CDCl_3$, 30 ˚C) $\delta$ 169.3 (*C*=O), 158.4 (2C), 142.1 (3C), 138.8 (3C), 135.1 (2C), 134.9 (3C), 131.8 (3C), 131.3 (3C), 131.1 (2C), 128.9 (2C), 126.8 (3C), 122.3 (2C), 119.7 (2C), 55.4 (-O*C*$H_3$), 23.5 (-*C*$H_3$).

**Synthesis of bis-(4-methoxybenzoato)tris-(o-tolyl)antimony(V), [Sb(*o*-$CH_3C_6H_4$)$_3$(*p*-$OCH_3C_6H_4CO_2$)$_2$], 21**

Reaction of *tris*-(*o*-tolyl)antimony(V)dibromide (2.78 g, 5 mmol) with potassium salt of 4-methoxybenzoic acid (1.90 g, 10 mmol) was performed and purified according to **GP**, producing a white crystalline solid. This was identified as **21**. Yield: 84%. Melting point: 190-193 ˚C. FT-IR (KBr, $cm^{-1}$): 3048 (m), 2931 (m), 2889 (m), 1647 (s), 1901 (s), 1507 (m), 1461 (m), 1314 (s), 1255 (s), 1161(s), 1121 (m), 1027 (s), 850 (m), 751(s), 696 (m), 616 (m), 558 (m), 441 (m), 376 (w), 292 (w), 266 (m). Elemental Analysis; ($C_{37}H_{35}O_6Sb$), Calc (Found): C 63.72 (63.67), H 5.06 (5.03)%. $^1$H-NMR (300 MHz, $CDCl_3$, 30 ˚C) $\delta$ = 8.46 (d, 3H, $^3J$ = 7.5 Hz, Ar*H*), 7.74 (d, 4H, $^3J$ = 6.9 Hz, Ar*H*), 7.34-7.46 (m, 9H, Ar*H*), 6.79 (d, 4H, $^3J$ = 7.5 Hz, Ar*H*), 3.80 (s, 6H, -OC$H_3$), 2.60 (s, 9H, -C$H_3$). $^{13}$C-NMR (75 MHz, $CDCl_3$, 30 ˚C) $\delta$ = 168.2 (*C*=O), 162.2 (*C*$OCH_3$), 141.9 (Sb-*C*), 139.4 (*C*-$CH_3$), 134.9 (Ar--*C*), 131.6 (Ar-*C*), 131.4 (Ar-*C*), 131.0 (Ar-*C*), 126.7 (Ar-*C*), 126.2 (Ar-*C*), 113.0 (Ar-*C*), 55.3 (-O*C*$H_3$), 23.5 (-*C*$H_3$).

**Synthesis of bis-(2-phenylacetato)tris-(o-tolyl)antimony(V),**

**[Sb(*o*-$CH_3C_6H_4$)$_3$($C_6H_5CH_2CO_2$)$_2$], 22**

Reaction of *tris*-(*o*-tolyl)antimony(V)dibromide (2.78 g, 5 mmol) with potassium salt of phenylacetic acid (1.74 g, 10 mmol) was performed and purified according to **GP**, producing a colourless solid. This was identified as **22**. Yield: 86%. Melting point: 158-160 ˚C. FT-IR (KBr, $cm^{-1}$): 3050 (m), 2934 (m), 2897 (m), 1656 (s), 1448 (s, br), 1307 (s, br), 1130 (s), 934 (m), 751 (s), 728 (s), 697 (m), 650 (s), 516 (m), 439 (w), 341 (m), 317 (m), 262 (m). Elemental Analysis; ($C_{37}H_{35}O_4Sb$), Calc (Found): C 66.78 (66.61), H 5.30 (5.29)%. $^1$H-NMR (300 MHz, $CDCl_3$, 30 ˚C) $\delta$ = 7.98 (d, 3H, $^3J$ = 7.5 Hz, Ar*H*), 7.41 (t, 2H, $^3J$ = 7.5 Hz, Ar*H*), 7.24-7.29 (m, 6H, Ar*H*), 7.10-7.19 (m, 7H, Ar*H*), 6.92 (d, 4H, $^3J$ = 6.9 Hz, Ar*H*), 3.31 (s, 4H, -C$H_2$-), 2.34 (s, 9H, -C$H_3$). $^{13}$C-NMR (75 MHz, $CDCl_3$, 30 ˚C) $\delta$ = 173.4 (*C*=O), 142.0 (Sb-*C*), 138.9 (*C*-$CH_3$), 135.8 (Ar-*C*), 134.6 (Ar-*C*), 131.5 (Ar-*C*), 130.9 (Ar-*C*), 129.3 (Ar-*C*), 128.0 (Ar-*C*), 126.4 (Ar-*C*), 126.2 (Ar-*C*), 44.0 (-*C*$H_2$), 23.3 (-*C*$H_3$).

**Synthesis of bis-[2-(2,3-dimethylphenyl)aminobenzoato)tris-(o-tolyl)antimony(V),**

**[Sb(*o*-$CH_3C_6H_4$)$_3${$C_6H_3(CH_3)_2NHC_6H_4CO_2$}$_2$], 23**

Reaction of *tris*-(*o*-tolyl)antimony(V)dibromide (2.78 g, 5 mmol) with potassium salt of 2-(2,3-dimethylphenyl)aminobenzoic acid (2.80 g, 10 mmol) was performed and purified according to **GP**, producing a white crystalline solid. This was identifies as **23**. Yield: 84%. Melting point: 172-174 ˚C. FT-IR (KBr, $cm^{-1}$): 3420 (m, br), 3271 (m), 3090 (m), 2932 (m), 1630 (s), 1577 (s), 1505 (s), 1450 (m), 1334 (m), 1255 (s, br), 1154 (m), 1081 (w), 847 (w), 746 (s), 568 (m), 448 (s), 345 (m), 323 (m), 264 (m). Elemental Analysis; ($C_{51}H_{49}N_2O_4Sb$), Calc (Found): C 69.95 (69.87), H 5.60 (5.59), N 3.20 (3.11)%. $^1$H-NMR (300 MHz, $CDCl_3$, 30 ˚C) $\delta$ = 9.34 (s, 2H, -N*H*). 8.58 (d, 3H, $^3J$ = 7.5 Hz, Ar*H*), 7.83 (d, 2H, $^3J$ = 7.5 Hz, Ar*H*), 7.38-7.48 (m, 9H, Ar*H*), 7.01-7.21 (m, 8H, Ar*H*), 6.73 (d, 2H, $^3J$ = 7.4 Hz, Ar*H*), 6.62 (t, 2H, $^3J$ = 7.2 Hz, Ar*H*), 2.71 (s, 9H, -C$H_3$), 2.36 (s, 6H, -C$H_3$), 2.01 (s, 6H, -C$H_3$). $^{13}$C-NMR (75MHz, $CDCl_3$, 30 ˚C) $\delta$ = 170.8 (*C*=O), 149.1 (*C*-COO), 142.1 (Sb-*C*), 139.6 (*C*-NH), 139.4 (*C*-NH), 137.9 (*C*-$CH_3$), 134.9 (*C*-$CH_3$), 132.9 (*C*-$CH_3$), 132.4 (Ar-*C*), 132.2 (Ar-*C*), 131.8 (Ar-*C*), 131.1 (Ar-*C*), 126.7 (Ar-*C*), 126.3 (Ar-*C*), 125.7 (Ar-*C*), 123.2 (Ar-*C*), 115.6 (Ar-*C*), 114.5 (Ar-*C*), 113.1 (Ar-*C*), 23.7 (-*C*$H_3$), 20.7 (-*C*$H_3$), 13.9 (-*C*$H_3$)

**Synthesis of bis-(4-bromobenzoato)tris-(o-tolyl)antimony(V),**

**[Sb(*o*-$CH_3C_6H_4$)$_3$(*p*-$BrC_6H_4CO_2$)$_2$], 24**

Reaction of *tris*-(*o*-tolyl)antimony(V)dibromide (2.78 g, 5 mmol) with sodium salt of 3-bromophenylacetic acid (2.37 g, 10 mmol) was performed and purified according to **GP**, producing a brownish solid. This was identified as **25**. Yield: 79%. Melting point: 236-237 ˚C. FT-IR (KBr, $cm^{-1}$): 3048 (m), 2930 (m), 2899 (m), 1633 (s), 1581 (m), 1444 (s, br), 1349 (w), 1271 (m), 1199 (m), 1117 (m), 1027 (m), 743 (s), 634 (s, br), 561 (m), 468 (m), 453 (s), 394 (m), 293 (m). Elemental Analysis; ($C_{37}H_{33}Br_2O_4Sb$), Calc (Found): C 53.98 (53.81), H 4.04 (4.04) %. $^1$H-NMR (300 MHz, $CDCl_3$, 30 ˚C) $\delta$ = 8.39 (d, 3H, $^3J$ = 7.5 Hz, Ar*H*), 7.31-7.59 (m, 13H, Ar*H*), 6.83 (d, 4H, $^3J$ = 7.5 Hz, Ar*H*), 3.28 (s, 4H, -C$H_2$-), 2.60 (s, 9H, -C$H_3$). $^{13}$C-NMR (75 MHz, $CDCl_3$, 30 ˚C) $\delta$ = 164.7 (*C*=O), 146.4 (***C***-Br), 139.4 (Sb-*C*), 137.4 (Ar-C), 134.1 (Ar-C), 131.9 (***C***-$CH_2$), 131.4 (Ar-*C*), 130.2 (Ar-*C*), 128.4 (Ar-*C*), 124.1 (Ar-*C*), 112.7 (Ar-*C*), 45.7 (-*C*$H_2$), 21.7 (-*C*$H_3$).

**Synthesis of triphenylantimony(V) dibromide,**

**[$SbPh_3Br_2$], 25**

Compound **26** was prepared according to a literature procedure.[1] Yield: 85%. Melting point: 218-219 ˚C; **FT-IR** (KBr, $cm^{-1}$): 3066 (m), 1471 (m), 1430 (s, br), 1325 (m), 1150 (w), 1020 (m), 725 (s), 676 (s, br), 447 (s), 352 (m), 328 (m), 299 (m). Elemental Analysis; ($C_{18}H_{15}Br_2Sb$), Calc (Found): C 42.15 (42.11), H 2.95 (2.94)%. $^1$H-NMR (300 MHz, $CDCl_3$, 30 ˚C) $\delta$ = 8.21 (dd, 6H, $^3J$ = 7.2 Hz, $^4J$ = 3.3 Hz, Ar*H*), 7.53-7.64 (m, 9H, Ar*H*). $^{13}$C-NMR (75MHz, $CDCl_3$, 30 ˚C) $\delta$ = 141.0 (Sb-*C*), 133.7 (Ar-*C*), 131.7 (Ar-*C*), 129.0 (Ar-*C*).

***Synthesis of tris-(o-tolyl)antimony(V) dibromide,***

**[Sb(*o*-$CH_3C_6H_4$)$_3$$Br_2$], 26**

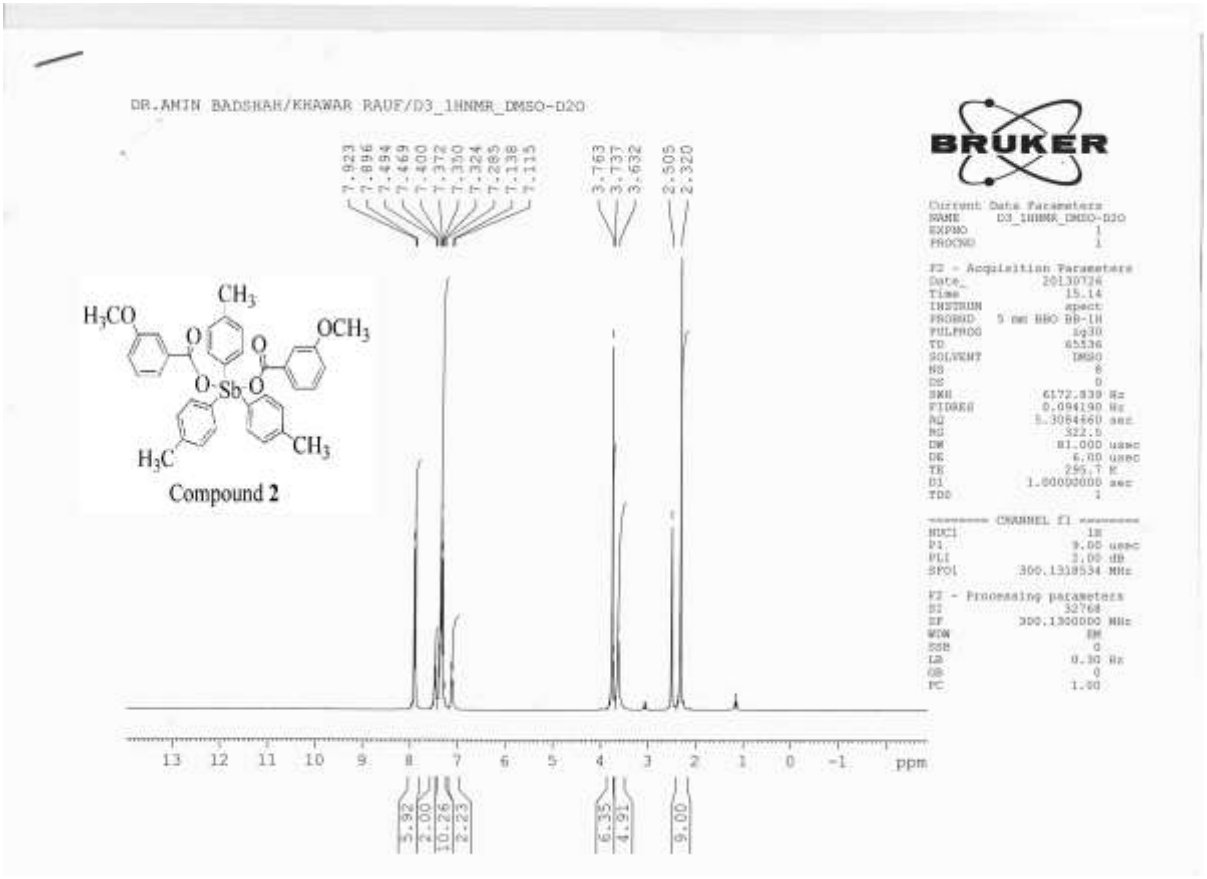
Compound **27** was prepared according to a literature procedure.[1] Yield: 85%; Melting point: 229-230 ˚C. FT-IR (KBr, $cm^{-1}$): 3029 (m), 2926 (m), 1585 (m), 1445 (s, br), 1381 (m), 1303 (w), 1276 (m), 1201 (m), 1021 (m), 748 (s), 555 (m),

435 (s), 365 (w), 344 (m), 293 (m). Elemental Analysis; ($C_{21}H_{21}Br_2Sb$), Calc (Found): C 45.45 (45.44), H 3.81 (3.80)%. $^{1}$H-NMR (300 MHz, $CDCl_3$, 30 ˚C) $\delta$ = 8.02 (d, 3H, $^{3}J$ = 7.5 Hz, Ar*H*), 7.39-7.51 (m, 9H, Ar*H*), 2.77 (s, 9H, -C*H*$_3$). $^{13}$C-NMR (75 MHz, $CDCl_3$, 30 ˚C) $\delta$ = 143.4 (Sb-*C*), 140.7 (*C*-$CH_3$), 134.7 (Ar-*C*) 132.4 (Ar-*C*), 131.6 (Ar-*C*), 126.7 (Ar-*C*), 24.5 (-*C*$H_3$).

## Reference

1. P. L. Millington and D. B. Sowerby, *J. Organomet. Chem.*, 1994, **48**, 227-234.

**Figure S1** $^{1}$H NMR spectra for compound **2** in DMSO/$D_2O$ taken at T = 0



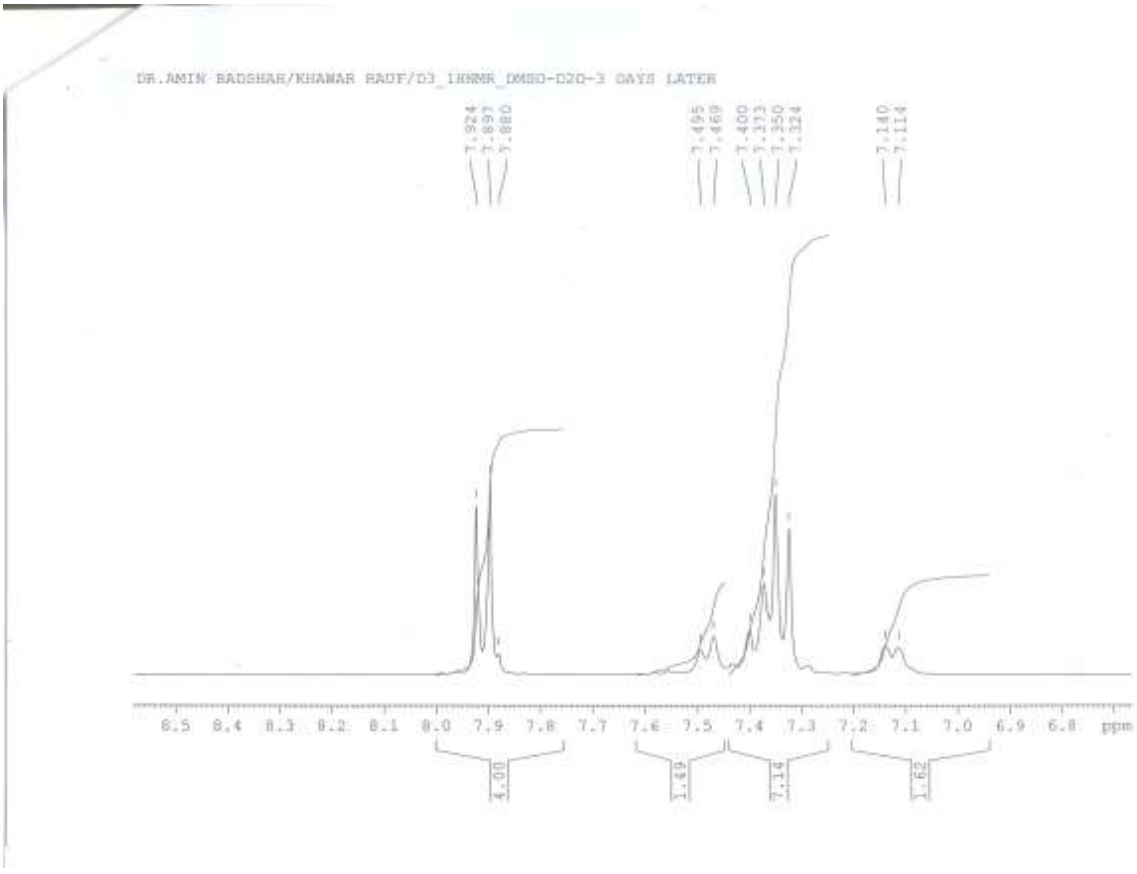
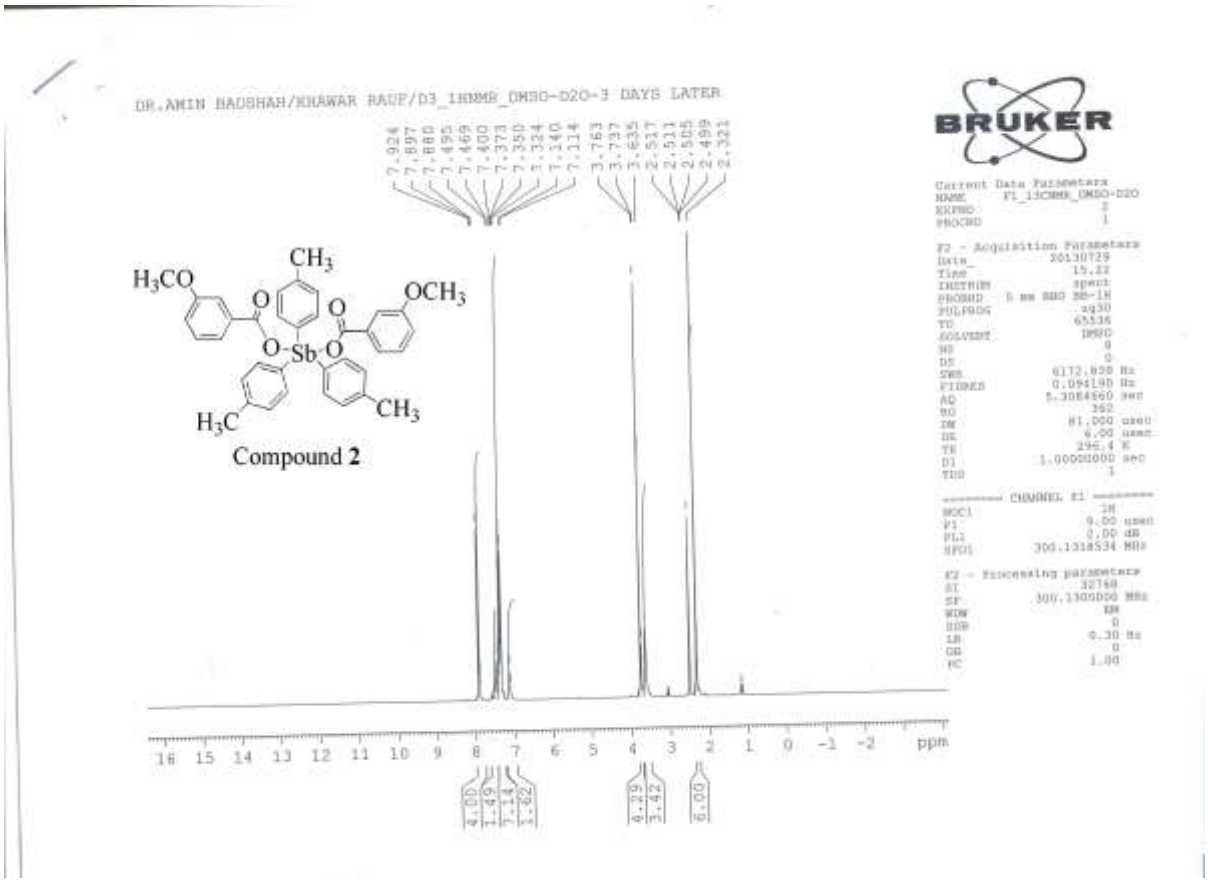



**Figure S2** $^{1}$H NMR spectra for compound **2** in DMSO/$D_2O$ taken at T = 3 days.



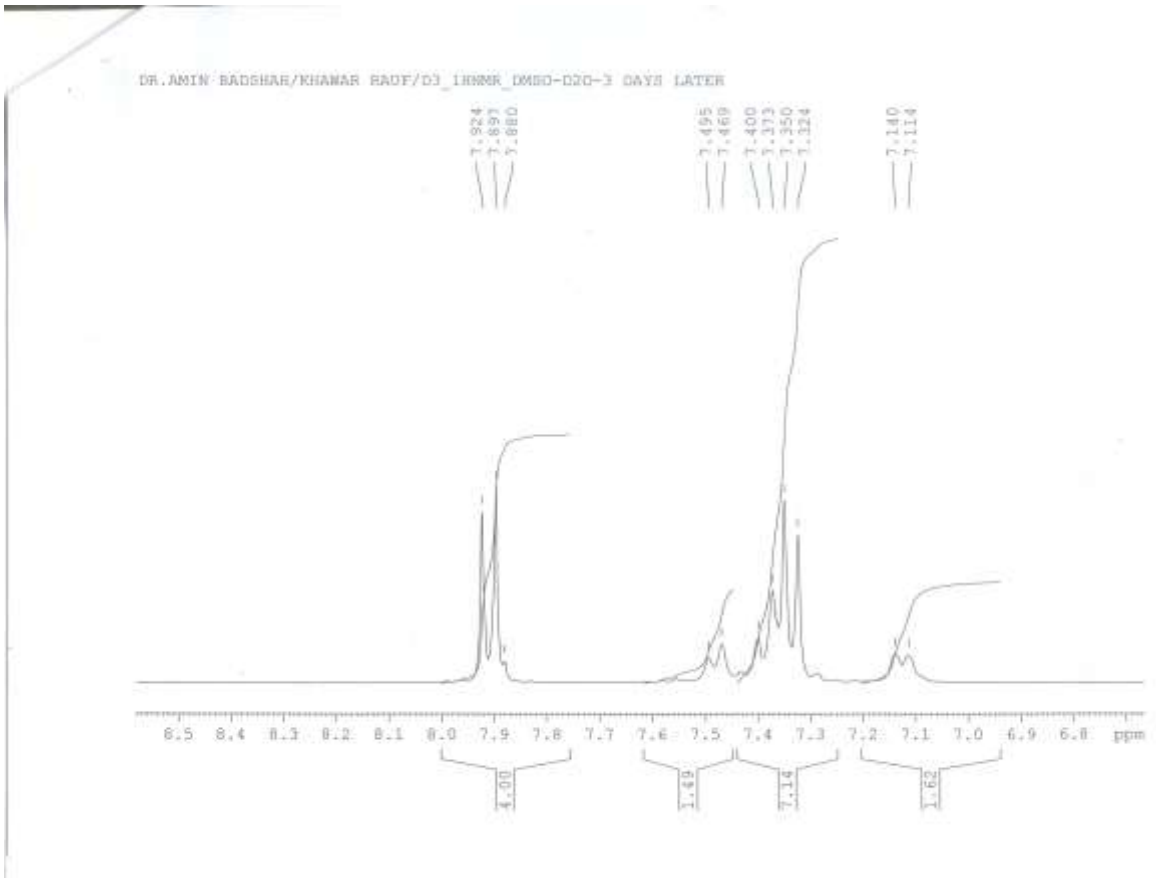



**Figure S3** $^{1}$H NMR spectrum of Sb(*p*-Tolyl)$_3$Br$_2$ in D$_6$-DMSO

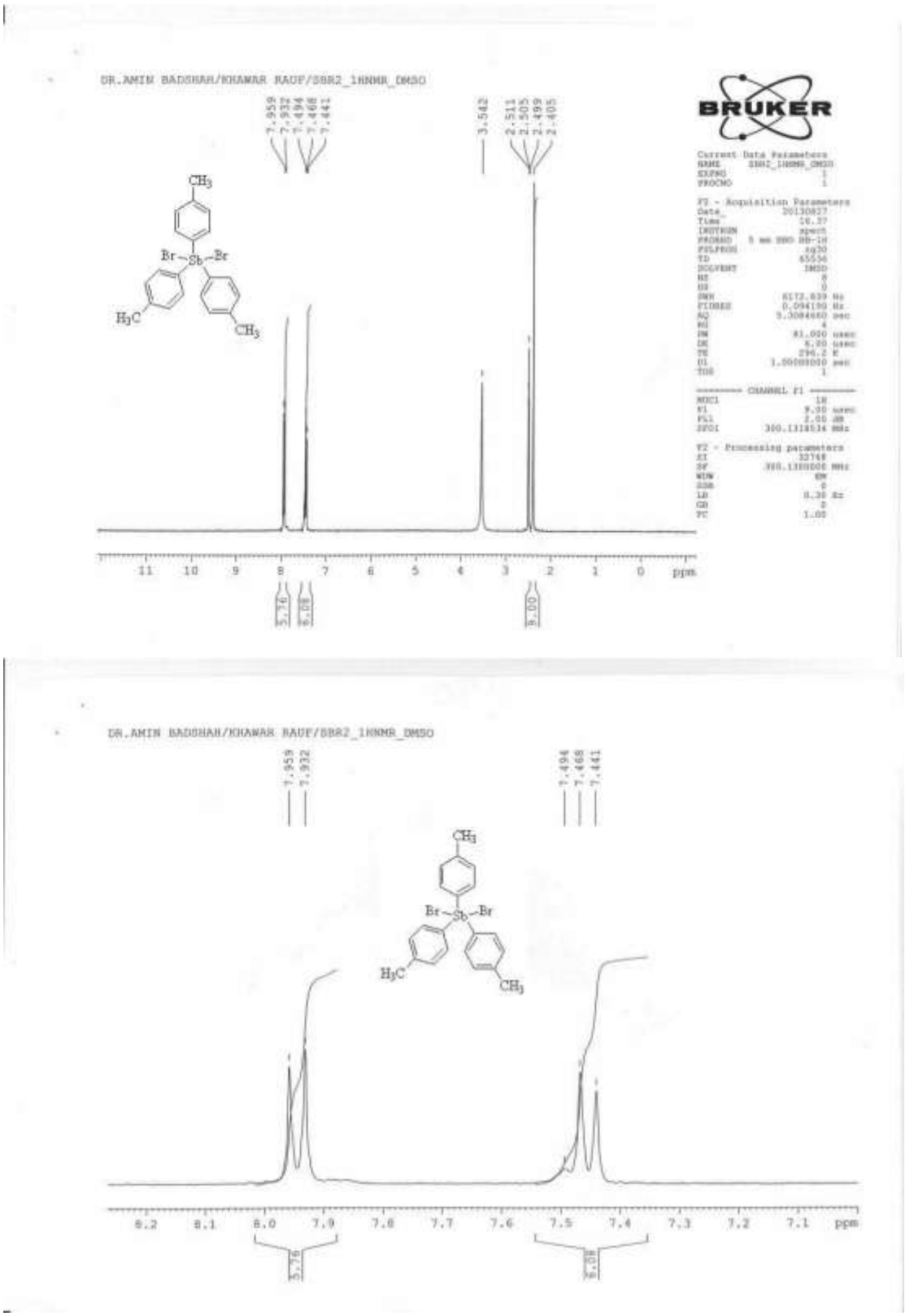


**Figure S4** $^{1}$H NMR spectrum of *m*-methoxybenzoic acid in $D_6$-DMSO

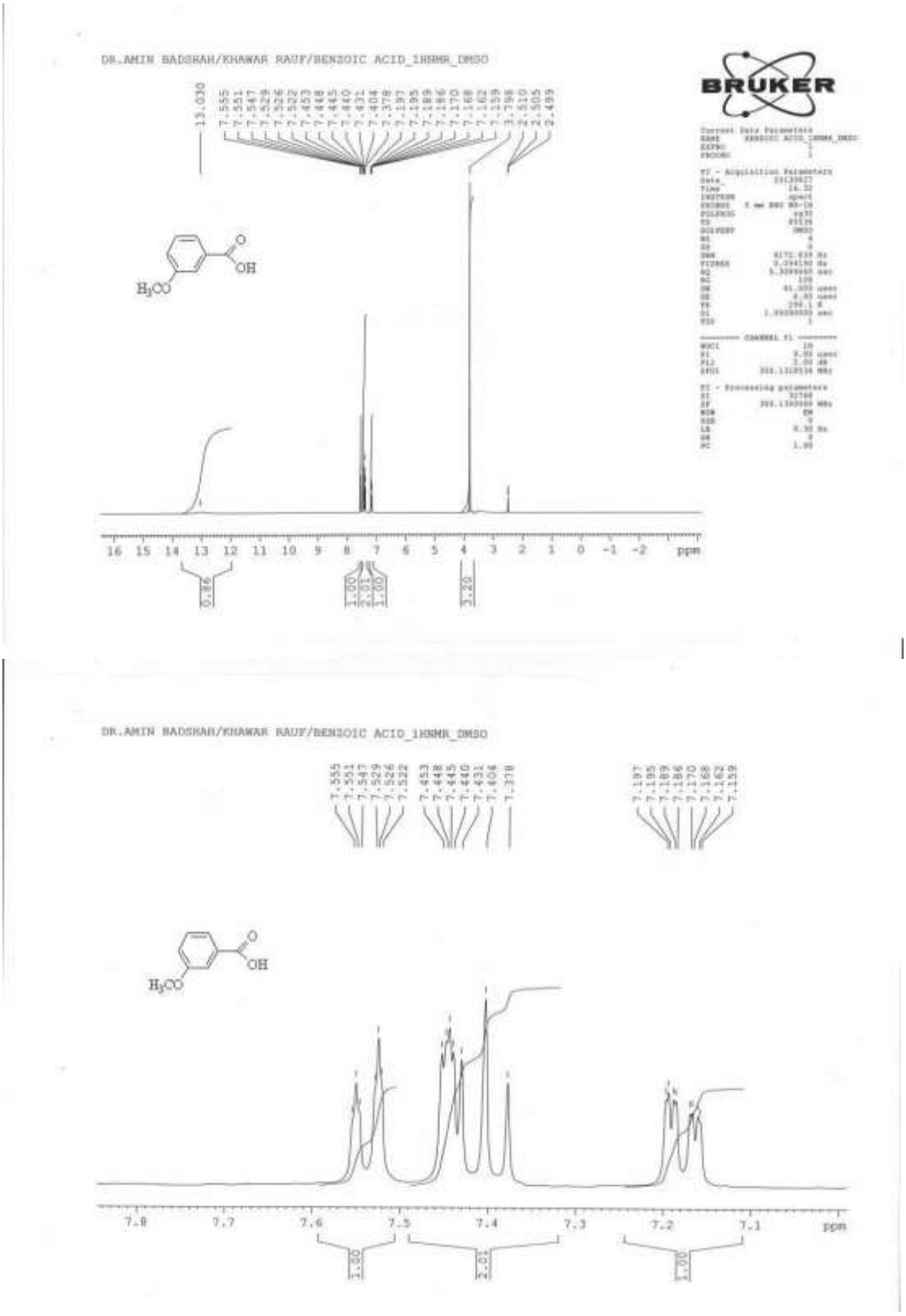
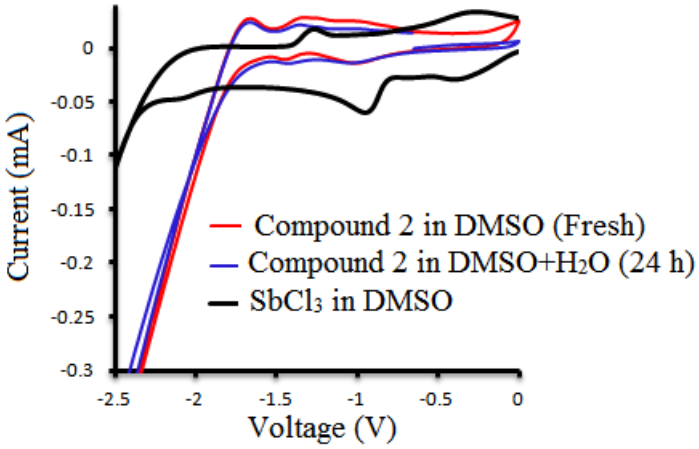


**Figure S5** Cyclic voltammetry study on compound **2**.




Cyclic voltammograms of $SbCl_3$ (black), compound 2 in DMSO fresh (red) and compound 2 in DMSO+$H_2O$ after 24 hours (blue). Concentration of each sample is 5 mM in solvent + 0.1 M TBAP. GC is used as working electrode against SCE as reference.

Cyclic voltammetric measurements were performed using Biolog SP 300 Potentiostat. Tetrabutylammoniumperchlorate (TBAP) having 99% purity, supplied by Fluka was used as an electrolyte. Measurements were carried out in a single compartment cell with a three electrode configuration, consisting of Ag/AgCl as a reference electrode, a thin Pt wire of thickness 0.5 mm with an exposed end of 10 mm as the counter electrode and a platinum disc as working electrode. All the measurements were carried out in DMSO (99.5%, Riedel-de Haen) and distilled water using 0.1 M Tetrabutylammonium perchlorate (TBAP ≥98%, Fluka) at 25 ± 1 °C. Samples concentration was kept 5 mM in each case.

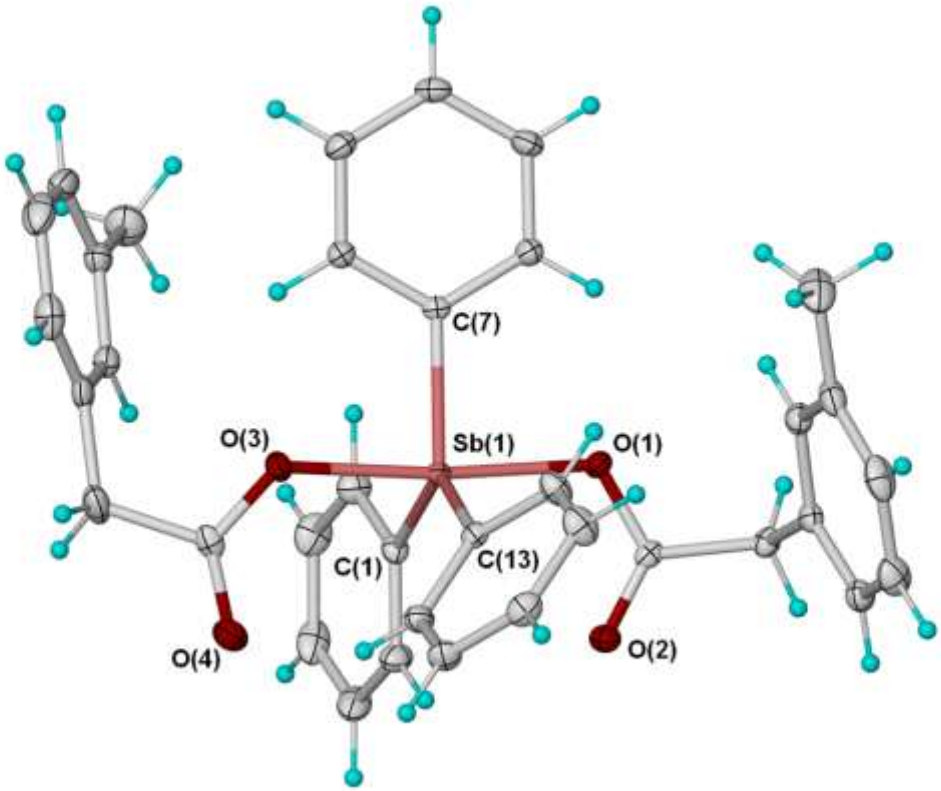
Figure S2 presents the cyclic voltammograms of $SbCl_3$ (black), compound **2** in DMSO fresh (red) and compound 2 in DMSO + $H_2O$ (75:25) after 24 hours (blue). Here $SbCl_3$ is taken as a reference to investigate the possible state of Sb(III) in the synthesized complexes in solution phase over time. The voltammograms show quasireversible to irreversible electrochemical behavior for the system studied, in the potential range of -2.300 to 0.022 V. The overlay of the cyclic voltammograms ruled out the presence of Sb(III) state, and consequently the synthesized antimonials are in pentavalent form.

**Table S1** Calculated CLogP values for compounds **1** – **26.**

| Compound | | Calculated CLogP Value[a] |
|---|---|---|
| **1** | [Sb(*p*-$CH_3C_6H_4$)$_3$($C_6H_5CH_2CO_2$)$_2$], | 11.5 |
| **2** | [Sb(p-$CH_3C_6H_4$)$_3$)(*m*-$OCH_3C_6H_4CO_2$)$_2$], | 10.7 |
| **3** | [Sb(*p*-$CH_3C_6H_4$)$_3$(3,4,5-$(OCH_3)_3C_6H_2CO_2$)$_2$] | 9.5 |
| **4** | [Sb(*p*-$CH_3C_6H_4$)$_3$(*o*-$BrC_6H_4CO_2$)$_2$], | 12.6 |
| **5** | [$SbPh_3$(4-$NH_2C_3H_6CO_2$)$_2$], | 6.9 |
| **6** | [Sb(*m*-$CH_3C_6H_4$)$_3$(*o*-$OCH_3C_6H_4CO_2$)$_2$], | 10.7 |
| **7** | [Sb(*m*-$CH_3C_6H_4$)$_3$(3,4,5-$(OCH_3)_3C_6H_2CO_2$)$_2$], | 9.5 |
| **8** | [Sb(*m*-$CH_3C_6H_4$)$_3$(*m*-$CH_3C_6H_4CO_2$)$_2$], | 11.9 |
| **9** | [Sb(*m*-$CH_3C_6H_4$)$_3$($C_6H_5CH$=$CHCO_2$)$_2$], 9 | 13.8 |
| **10** | [Sb(*p*-$CH_3C_6H_4$)$_3Br_2$], 10 | 6.5 |
| **11** | [Sb(*m*-$CH_3C_6H_4$)$_3Br_2$], 11 | 6.5 |
| **12** | [$SbPh_3$($C_4H_3SCO_2$)$_2$] | 8.7 |
| **13** | [$SbPh_3$(*m*-$CH_3C_6H_4CH_2CO_2$)$_2$] | 11.0 |
| **14** | [$SbPh_3$(*o*-$OCH_3C_6H_4CO_2$)$_2$] | 9.2 |
| **15** | [$SbPh_3$($C_6H_5$ $OCH_2CO_2$)$_2$] | 9.4 |
| **16** | [$SbPh_3$($C_4$ $H_3OCO_2$)$_2$] | 7.7 |
| **17** | [$SbPh_3$($C_6$ $H_5CH$=$CHCO_2$)$_2$] | 11.3 |
| **18** | [$SbPh_3$(*o*-C $H_3C_6H_4CO_2$)$_2$] | 10.4 |
| **19** | [Sb($C_6H_5CH_2$)$_3$(*p*-$OCH_3C_6H_4CO_2$)$_2$] | 10.6 |
| **20** | [Sb(*o*-$CH_3C_6H_4$)$_3$(*o*-$OCH_3C_6H_4CO_2$)$_2$] | 10.7 |
| **21** | [Sb(*o*-$CH_3C_6H_4$)$_3$(*p*-$OCH_3C_6H_4CO_2$)$_2$] | 10.7 |
| **22** | [Sb(*o*-$CH_3C_6H_4$)$_3$($C_6H_5$ $CH_2CO_2$)$_2$] | 12.4 |
| **23** | [Sb(*o*-$CH_3C_6H_4$)$_3${$C_6H_3(CH_3)_2NHC_6H_4CO_2$}$_2$] | 15.6 |
| **24** | [Sb(*o*-$CH_3C_6H_4$)$_3$(*p*-$BrC_6H_4CO_2$)$_2$] | 13.3 |
| **25** | [$SbPh_3Br_2$] | 5.0 |
| **26** | [Sb(*o*-$CH_3C_6H_4$)$_3Br_2$] | 6.5 |

[a] CLogP values calculated using the function in ChemBioDraw 13.0, CambridgeSoft, Perkin Elmer Informatics.

**Figure S6.** Molecular diagram of [$SbPh_3$(m-$CH_3C_6H_4CH_2CO_2)_2$], **13**. Non-hydrogen atoms represented by 50% thermal ellipsoids and hydrogen atoms as spheres of arbitrary size. Selected bond lengths (Å) and angles (o) : Sb(1)-O(1) 2.0880(9); Sb(1)-C(1) 2.0949(14); Sb(1)-C(13) 2.0974(14); Sb(1)-C(7) 2.1105(13); Sb(1)-O(3) 2.1108(10); O(1)-C(19) 1.3170(16); O(2)-C(19) 1.2191(17); O(1)-Sb(1)-C(1) 95.36(5); O(1)-Sb(1)-C(13) 90.81(4); C(1)-Sb(1)-C(13) 130.18(5); O(1)-Sb(1)-C(7) 87.14(4); C(1)-Sb(1)-C(7) 114.55(5); C(13)-Sb(1)-C(7) 115.11(5); O(1)-Sb(1)-O(3) 174.48(4); C(1)-Sb(1)-O(3) 87.92(5).




**Summary of crystallographic data for compound 13**

$C_{36}H_{33}O_4Sb$, $M$ = 651.37, 0.25 x 0.20 x 0.13 mm, triclinic, space group $P$-1, 10.4324(7), b = 11.6012(7), c = 13.6076(8) Å, α = 68.481(2)°, β = 72.324(3)°, γ= 82.668(3)°, V = 1459.53(16) $Å^3$, Z = 2, $\rho_{calc}$ = 1.482 g $cm^{-3}$, $\mu$ = 0.985 $mm^{-1}$, $F_{000}$ = 664, $T$ = 123(2) K, $2\theta_{max}$ = 59.80°, 26389 reflections collected, 8253 unique ($R_{int}$ = 0.0240). Final GooF = 1.054, $R_1$ = 0.021 for observed data, w$R_2$ = 0.049 for all data.

**Figure S7.** Effects of compounds **1 - 26** on *L. major* promastigotes (closed circles) and human fibroblasts (open circles). Dose response curves were generated over a range of concentrations from 48 nM to 1 00 μM in culture media from 10 mM DMSO stock. All readings were compared to non-treated control and percent growth inhibition calculated. A range of DMSO concentrations (0.0048 - 1.0 %) was also included (data not shown). Data shown are mean from duplicate values.