Electronic Supplementary Information (ESI)

Nanostructured films of *in situ* deprotected thioacetyl-functionalized C60-fullerenes on gold surface

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Electronic Supplementary Information includes:

synthesis details, ESI-MS, IR and 1H NMR spectra for new coumponds, voltammetric data including voltammograms, orbital energies from CV experiments, XPS spectra of fullerene derivative films on gold surface, and absolute energies and Cartesian coordinates for compounds A1-A3, I-VI and coresponding ylides from DFT//B3LYP/6-31G(d) calculations.

Synthesis of compounds 1-6

To a well stirred solution of corresponding dibromoalkane (26,32mmol) and potassium carbonate (1,28g, 9.2mmol) in DMF (30mL) at 80oC, a solution of vanillin (1.0g, 6,58mmol) in DMF (10mL) was added dropwise. Reaction was kept at 80oC for 1h, then cooled to 0oC on an ice bath and quenched with 1N HCl. The mixture was extracted with ethyl acetate and the organic layer was dried over anhydrous sodium sulfate. After removing the solvent under reduced pressure the purification was accomplished by means of flash column chromatography (3:1 n-hexane- ethyl acetate) to give compounds 1-6 as white solids.

4-(2-Bromoethoxy)-3-methoxybenzaldehyde (1): Yield: 68%, mp 70.2-71.1 ^{o}C, the mass spectrum (ESI-MS) showed a $[M,^{79}Br+Na]^{+}$ peak at 280.7 and $[M,^{81}Br+Na]^{+}$ peak at 282,7 see Figure S1; IR (KBr disk) $\nu_{max}(cm^{-1})$ 2845.1, 2756.4, 1683.9, 1585.5, 1506.5, 1464.0, 1427.4, 1396.5, 1269.2, 1234.5, 1136.1, 1016.5, 864.1, 812.1, 733.0, 680.9, 632.7, 569.0, see Figure S2; δ^{1}H (200 MHz; $CDCl_3$; TMS) 3.68-3.73 (2H, t), 3.94 (3H, s), 4.39-4.46 (2H, t), 6.97-7.01 (1H, d), 7.43-7.47 (2H, d), 9.87 (1H, s) ppm, see Figure S3.

4-(2-Bromobutoxy)-3-methoxybenzaldehyde (2): Yield: 95%, mp 54.6-55.7 ^{o}C, the mass spectrum (ESI-MS) showed a $[M,^{79}Br+H]^{+}$ peak at 287,0 and $[M,^{81}Br+H]^{+}$ peak at 289,0 see Figure S4; IR (KBr disk) $\nu_{max}(cm^{-1})$ 2951.2, 2875.0, 2822.0, 2727.4, 1683.9, 1674.3, 1585.5, 1506.4, 1471.7, 1456.3, 1417.7, 1398.4, 1352.1, 1280.8, 1261.5, 1234.5, 1159.3, 1134.2, 1026.2, 864.1, 814.0, 727.2, 653.9, 630.7, see Figure S5; δ^{1}H (200 MHz; $CDCl_3$; TMS) 2.02-2.11 (4H, m), 3.48-3.55 (2H, t), 3.93 (3H, s), 4.12-4.17 (2H, t) 6.95-6.99 (1H, d), 7.44-7.48 (2H, d), 9.85 (1H, s) ppm, see Figure S6.

4-(2-Bromohexoxy)-3-methoxybenzaldehyde (3): Yield: 98%, mp 49.6-50.3 ^{o}C, the mass spectrum (ESI-MS) showed a $[M,^{79}Br+Na]^{+}$ peak at 337,1 and $[M,^{81}Br+Na]^{+}$ peak at 339,1 see Figure S7; IR (KBr disk) $\nu_{max}(cm^{-1})$ 2937.7, 2860.5, 2725.5, 1670.4, 1583.6, 1506.4, 1456.9, 1419.7, 1257.7, 1134.2, 1026.2, 1003.0, 864.1, 802.4, 729.1, 653.9, 572.9, 474.5, see Figure S8; δ^{1}H (200 MHz; $CDCl_3$; TMS) 1.50-1.57 (4H, m), 1.87-1.95 (4H, m), 3.40-3.46 (2H, t), 3.93 (3H, s), 4.06-4.15(2H, t) 6.95-6.99 (1H, d), 7.42-7.46 (2H, d), 9.85 (1H, s) ppm, see Figure S9.

4-(2-Bromooctoxy)-3-methoxybenzaldehyde (4): Yield: 92%, mp 46.6-47.8 ^{o}C, the mass spectrum (ESI-MS) showed a $[M,^{79}Br+Na]^{+}$ peak at 364,9 and $[M,^{81}Br+Na]^{+}$ peak at 366,9 see Figure S10; IR (KBr disk) $\nu_{max}(cm^{-1})$ 2991.7, 2920.3, 2837.4, 1683.9, 1581.7, 1506.5, 1456.3, 1423.5, 1398.4, 1269.2, 1242.2, 1134.2, 1018.4, 993.4, 860.3, 819.8, 777.3, 731.0, 655.8, 592.2, 559.4, see Figure S11;δ^{1}H (200 MHz; $CDCl_3$; TMS) 1.39-1.52 (8H, m), 1.87-1.96 (4H, m), 3.38-3.45 (2H, t), 3.93 (3H, s), 4.07-4.14(2H, t) 6.95-6.99 (1H, d), 7.42-7.46 (2H, dd), 9.85 (1H, s) ppm, see Figure S12.

4-(2-Bromodecoxy)-3-methoxybenzaldehyde (5): Yield: 87%, mp 45.2-45.9 ^{o}C, the mass spectrum (ESI-MS) showed a $[M,^{79}Br+Na]^{+}$ peak at 393,1 and $[M,^{81}Br+Na]^{+}$ peak at 395,1 see Figure S13; IR (KBr disk) $\nu_{max}(cm^{-1})$ 2925.3, 2852.8, 1687.8, 1593.3, 1581.7, 1506.5, 1464.8, 1421.6, 1265.3, 1242.2, 1157.3, 1132.2, 1032.0, 1004.9, 866.1, 808.2, 731.0, 644.2, 561.3, see Figure S14;δ^{1}H (200 MHz; $CDCl_3$; TMS) 1.30-1.46 (8H, m), 1.78-1.92 (8H, m), 3.37-3.44 (2H, t), 3.93 (3H, s), 4.07-4.13(2H, t) 6.95-6.99 (1H, d), 7.41-7.46 (2H, dd), 9.85 (1H, s) ppm, see Figure S15.

4-(2-Bromododecoxy)-3-methoxybenzaldehyde (6): Yield: 99%, mp 39.8-40.4 ^{o}C, the mass spectrum (ESI-MS) showed a $[M,^{79}Br+H]^{+}$ peak at 399,2 and $[M,^{81}Br+H]^{+}$ peak at 401,2 see Figure S16; IR (KBr disk) $\nu_{max}(cm^{-1})$ 2922.3, 2850.9, 1683.9, 1651.1, 1583.6, 1508.4, 1464,0, 1413.9, 1267.3, 1128.4, 1022.4, 864.1, 866.3, 725.3, 642.3, see Figure S17; δ^{1}H (200 MHz; $CDCl_3$; TMS) 1.28-1.46 (8H, m), 1.78-1.92 (12H, m), 3.38-3.45 (2H, t), 3.93 (3H, s), 4.07-4.14(2H, t) 6.95-6.99 (1H, d), 7.42-7.46 (2H, dd), 9.85 (1H, s) ppm, see Figure S18.

Synthesis of compounds 7-12

Potassium thioacetate (228 mg, 2 mmol) was added to a stirred solution of corresponding 4-(2-Bromoalkyloxy)-3-methoxybenzaldehyde (1-6) (1 mmol) in dry DMF (15 mL) at room temperature. After stirring for 8 h at room temperature under nitrogen atmosphere, the reaction mixture was diluted with diethyl ether. Formed precipitate was removed by filtration, then the organic portion was washed with water (3x10 mL). Ethereal solution was dried over anhydrous sodium sulfate, filtered and the solvent was removed at reduced pressure. Purification of the product was accomplished by the means of flash column chromatography (3:1 n-hexane- diethyl ether) to give compounds 7-12 as white solids.

4-(S-acetylthioethoxy)-3-methoxybenzaldehyde (7): Yield: 96%, mp 56.9-57.7 oC, the mass spectrum (ESI-MS) showed a [M+Na]+ peak at 277.2 see Figure S19; IR (KBr disk) vmax(cm-1) 2958.5, 2937.7, 2850.9, 1631.6, 1681.9, 1585.5, 1506.4, 1460.2, 1417.7, 1398.4, 1279.2, 1236.4, 1157.3, 1132.2, 1026.2, 1010.7, 966.4, 869.9, 819.1, 729.1, 650.3, 626.9, 590.2, see Figure S20; δ1H (200 MHz; CDCl3; TMS) 2.39 (3H, s) 3.30-3.37 (2H, t), 3.96 (3H, s), 4.20-4.27 (2H, t), 7.05-7.09 (1H, d), 7.42-7.48 (1H, d), 8.02 (1H, s), 9.86 (1H, s) ppm, see Figure S21.

4-(S-acetylthiobutoxy)-3-methoxybenzaldehyde (8): Yield: 99%, mp 55.4-56.0 oC, the mass spectrum (ESI-MS) showed a [M+Na]+ peak at 305.1 see Figure S22; IR (KBr disk) νmax(cm-1) 2930.0, 2820.1, 2723.6, 1697.4, 1680.0, 1585.5, 1598.5, 1466.0, 1423.5, 1265.3, 1236.4, 1140.0, 1130.9, 1026.2, 995.1, 929.7, 864.1, 812.0, 729.1, 655.8, 636.5, 592.2, 553.6, see Figure S23; δ1H (200 MHz; CDCl3; TMS) 1.71-1.86 (2H, m), 1.89-2.03 (2H, m), 2.34 (3H, s) 2.93-3.00 (2H, t), 3.92 (3H, s), 4.08-4.15 (2H, t), 6.94-6.98 (1H, d), 7.40-7.45 (2H, d), 9.85 (1H, s) ppm, see Figure S24.

4-(S-acetylthiohexoxy)-3-methoxybenzaldehyde (9): Yield: 95%, mp 52.9-54.0 oC, the mass spectrum (ESI-MS) showed a [M+Na]+ peak at 333.1 see Figure S25; IR (KBr disk) νmax(cm-1) 2985.9, 2928.0, 2854.7, 1709.0, 1683.9, 1585.5, 1506.45, 1464.0, 1423.5, 1352.1, 1265.3, 1134.2, 1026.2, 991.4, 943.2, 868.0, 812.0, 729.1, 630.7, 574.8, see Figure S26; δ1H (200 MHz; CDCl3; TMS) 1.41-1.65 (6H, m), 1.82-1.95 (2H, m), 2.33 (3H, s) 2.84-2.91 (2H, t), 3.93 (3H, s), 4.06-4.13 (2H, t), 6.94-6.98 (1H, d), 7.43-7.47 (2H, d), 9.85 (1H, s) ppm, see Figure S27.

4-(S-acetylthiooctoxy)-3-methoxybenzaldehyde (10): Yield: 96%, mp 64.7-65.1 oC, the mass spectrum (ESI-MS) showed a [M+Na]+ peak at 360.8 see Figure S28; IR (KBr disk) νmax(cm-1) 2926.1, 2852.8, 2712.0, 1680.0, 1674.3, 1585.5, 1581.6, 1516.1, 1506.5, 1471.7, 1456.3, 1423.5, 1400.4, 1384.9, 1338.6, 1280.8, 1246.0, 1193.9, 1174.7, 1124.5, 1035.8, 1016.5, 983.7, 945.1, 885.4, 817.8, 783.1, 723.3, 636.7, 586.4, see Figure S29; δ1H (200 MHz; CDCl3; TMS) 1.41-1.65 (10H, m), 1.81-1.95 (2H, m), 2.33 (3H, s) 2.83-2.90 (2H, t), 3.93 (3H, s), 4.07-4.13 (2H, t), 6.95-6.99 (1H, d), 7.42-7.46 (2H, d), 9.85 (1H, s) ppm, see Figure S30.

4-(S-acetylthiodecoxy)-3-methoxybenzaldehyde (11): Yield: 89%, mp 46.3-48.1 oC, the mass spectrum (ESI-MS) showed a [M+Na]+ peak at 388.8 see Figure S31; IR (KBr disk) νmax(cm-1) 2924.2, 2850.9, 1682.0, 1691.6, 1581.7, 1506.5, 1471.7, 1423.5, 1398.4, 1338.6, 1265.3, 1242.2, 1155.4, 1132.2, 1033.9, 1001.1, 945.1, 887.3, 867.9, 808.2, 781.2, 729.1, 636.5, 592.2, see Figure S32; δ1H(200 MHz; CDCl3; TMS) 1.30-1.64 (14H, m), 1.81-1.95 (2H, m), 2.32 (3H, s) 2.82-2.90 (2H, t), 3.93 (3H, s), 4.07-4.13 (2H, t), 6.95-6.99 (1H, d), 7.42-7.46 (2H, d), 9.85 (1H, s) ppm, see Figure S33.

4-(S-acetylthiododecoxy)-3-methoxybenzaldehyde (12): Yield: 92%, mp 65.5-65.9 oC, the mass spectrum (ESI-MS) showed a [M+Na]+ peak at 417.2 see Figure S34; IR (KBr disk) νmax(cm-1) 2920.3, 2845.1, 1680.0, 1668.5, 1585.5, 1506.5, 1454.4, 1402.3, 1336.7, 1261.5, 1118.8, 1008.8, 867.0, 790.8, 719.6, 632.7, 577.8, see Figure S35;δ1H (200 MHz; CDCl3; TMS) 1.41-1.65 (18H, m), 1.40-1.63 (2H, m), 2.32 (3H, s) 2.83-2.90 (2H, t), 3.93 (3H, s), 4.07-4.14 (2H, t), 6.95-6.99 (1H, d), 7.42-7.47 (2H, d), 9.85 (1H, s) ppm, see Figure S36.

Preparation of compounds I-VI

A stirred solution of C_{60} fullerene (144 mg, 0.2 mmol), corresponding 4-(S-acetylthioalkyloxy)-3-methoxybenzaldehyde (7-12) (0.2 mmol) and N-methylglycine (89 mg, 1 mmol) in dry toluene (130 mL) was heated at 110 ^{o}C under nitrogen atmosphere for 8 h. The reaction mixture was then cooled, filtered and the solvent was removed under reduced pressure. The residue was chromatographed (2:1 n-hexane- toluene) to give compounds (I-VI) as dark brown powders.

Fullerene thioacetate I: Yield: 42%, the mass spectrum (ESI-MS) showed a [M+Na]+ peak at 1024.0, see Figure S37; IR (KBr disk) νmax(cm-1) 2945.4, 2846.0, 2777.5, 1695.4, 1515.1, 1462.2, 1422.9, 1384.1, 1268.1, 1230.9, 1178.8, 1131.4, 1028.6, 769.9, 623.3, 526.3, see Figure S38; δ1H (200 MHz; CDCl3; TMS) 2.36 (3H, s), 2.82 (3H, s), 3.27-3.34 (2H, t), 3.89 (3H, s), 4.11-4.18 (2H, t), 4.23-4.28 (1H, d), 4.91 (1H, s), 4.96-5.01 (1H, d), 6.94-6.98 (1H, d), 7.20-7.23 (1H, m), 7.36-7.39 (1H, m) ppm, see Figure S39.

Fullerene thioacetate II: Yield: 44%, the mass spectrum (ESI-MS) showed a [M+Na]+ peak at 1052.5, see Figure S40; IR (KBr disk) νmax(cm-1) 2946.2, 2927.4, 2838.2, 2771.7, 1689.8, 1513.8, 1461.7, 1424.2, 1331.6, 1264.6, 1230.4, 1133.9, 1107.9, 1032.7, 803.7, 769.5, 668.9, 626.8, 526.5, see Figure S41; δ1H (200 MHz; CDCl3; TMS) 1.73-1.91 (4H, m), 2.31 (3H, s), 2.82 (3H, s), 2.91-2.98 (2H, t), 3.88 (3H, s), 3.99-4.05 (2H, t), 4.23-4.29 (1H, d), 4.87 (1H, s), 4.96-5.02 (1H, d), 6.86-6.90 (1H, d), 7.34-7.39 (2H, m) ppm, see Figure S42.

Fullerene thioacetate III: Yield: 35%, the mass spectrum (ESI-MS) showed a [M+Na]+ peak at 1080.2, see Figure S43; IR (KBr disk) νmax(cm-1) 2929.8, 2852.3, 2777.3, 1689.4, 1513.4, 1462.3, 1423.4, 1331.7, 1265.5, 1230.9, 1179.4, 1162.8, 1131.7, 1031.1, 954.3, 769.4, 626.7, 526.5, see Figure S44; δ1H (200 MHz; CDCl3; TMS) 1.43-1.61 (4H, m), 1.80-1.86 (4H, m), 2.32 (3H, s), 2.82 (3H, s), 2.84-2.90 (2H, t), 3.88 (3H, s), 3.97-4.03 (2H, t), 4.23-4.28 (1H, d), 4.87 (1H, s), 4.96-5.01 (1H, d), 6.87-6.91 (1H, d), 7.24-7.40 (2H, m) ppm, see Figure S45.

Fullerene thioacetate IV: Yield: 28%, the mass spectrum (ESI-MS) showed a [M+Na]+ peak at 1107.6, see Figure S46; IR (KBr disk) νmax(cm-1) 2920.2, 2848.4, 2771.2, 1685.0, 1582.3, 1511.9, 1460.3, 1423.3,

1329.7, 1263.2, 1228.9, 1128.6, 1028.0, 795.0, 769.5, 626.3, 526.8, see Figure S47; δ1H (200 MHz; CDCl3; TMS) 1.25-1.77 (10H, m), 1.81-1.90 (2H, m), 2.32 (3H, s), 2.82 (3H, s), 2.83-2.89 (2H, t), 3.88 (3H, s), 3.97-4.03 (2H, t), 4.23-4.28 (1H, d), 4.87 (1H, s), 4.96-5.01 (1H, d), 6.87-6.91 (1H, d), 7.39-7.42 (2H, m) ppm, see Figure S48.

Fullerene thioacetate V: Yield: 27%,the mass spectrum (ESI-MS) showed a [M+Na]+ peak at 1135.7, see Figure S49; IR (KBr disk) νmax(cm-1) 2921.2, 2846.9, 2772.2, 1686.9, 1514.4, 1462.3, 1423.3, 1330.2, 1262.7, 1230.0, 1131.6, 1028.4, 769.0, 625.9, 526.5, see Figure S50; δ1H (200 MHz; CDCl3; TMS) 1.24-1.59 (4H, m), 1.75-1.90 (4H, m), 2.32 (3H, s), 2.82 (3H, s), 2.82-2.89 (2H, t), 3.88 (3H, s), 3.97-4.04 (2H, t), 4.23-4.28 (1H, d), 4.87 (1H, s), 4.97-5.01 (1H, d), 6.87-6.91 (1H, d), 7.36-7.43 (2H, m) ppm, see Figure S51.

Fullerene thioacetate VI: Yield: 34%, the mass spectrum (ESI-MS) showed a [M+Na]+ peak at 1165.4, see Figure S52; IR (KBr disk) νmax(cm-1) 2922.8, 2850.0, 2777.9, 1689.9, 1514.3, 1462.5, 1423.3, 1331.7, 1265.7, 1230.9, 1179.1, 1162.8, 1131.4, 1032.9, 955.5, 769.5, 626.4, 526.5, see Figure S53; δ1H (200 MHz; CDCl3; TMS) 1.40-1.76 (16H, m), 1.80-1.90 (4H, m), 2.32 (3H, s), 2.82 (3H, s), 2.82-2.89 (2H, t), 3.88 (3H, s), 3.97-4.04 (2H, t), 4.23-4.27 (1H, d), 4.87 (1H, s), 4.96-5.01 (1H, d), 6.87-6.91 (1H, d), 7.23-7.39 (2H, m) ppm, see Figure S54.

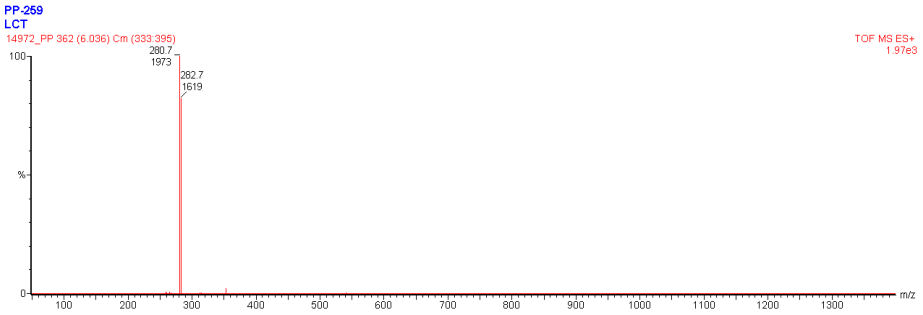


Figure S1. ESI-MS spectrum of 4-(2-bromoethoxy)-3-methoxybenzaldehyde **1**

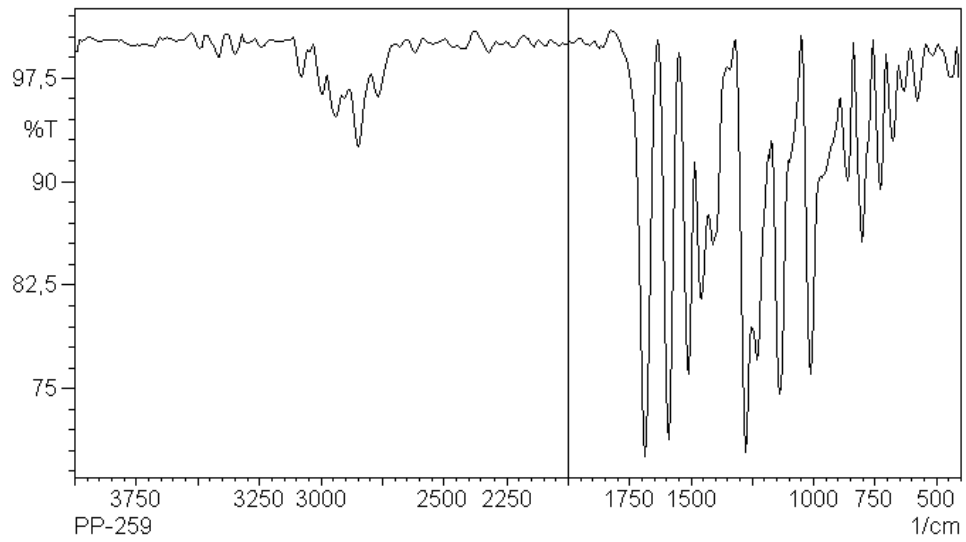


Figure S2. IR spectrum of 4-(2-bromoethoxy)-3-methoxybenzaldehyde **1** (KBr disk)

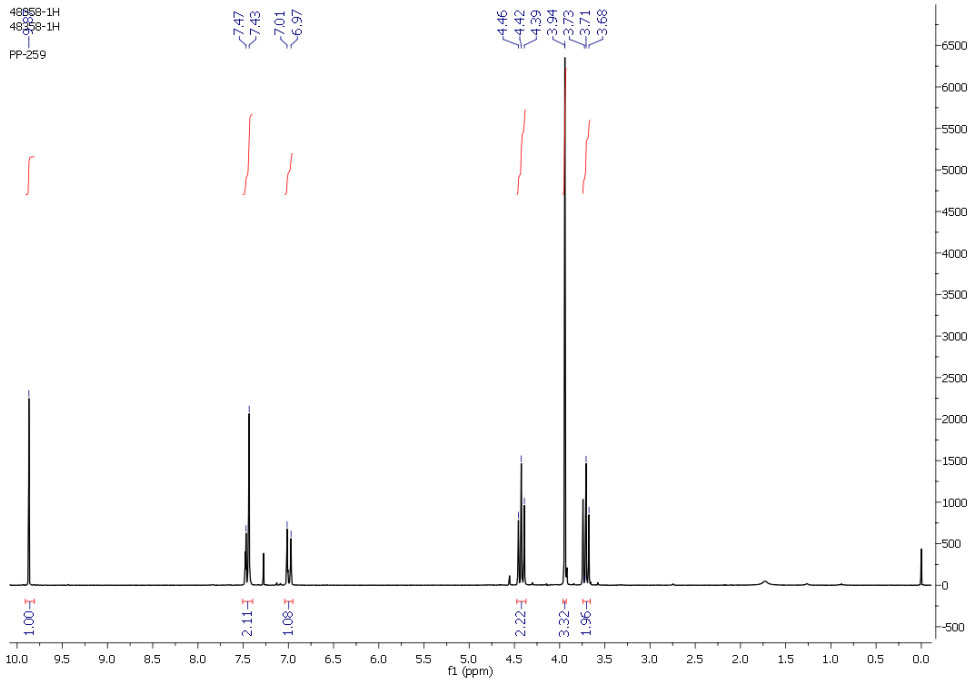


Figure S3. ^{1}H NMR spectrum of 4-(2-bromoethoxy)-3-methoxybenzaldehyde **1**

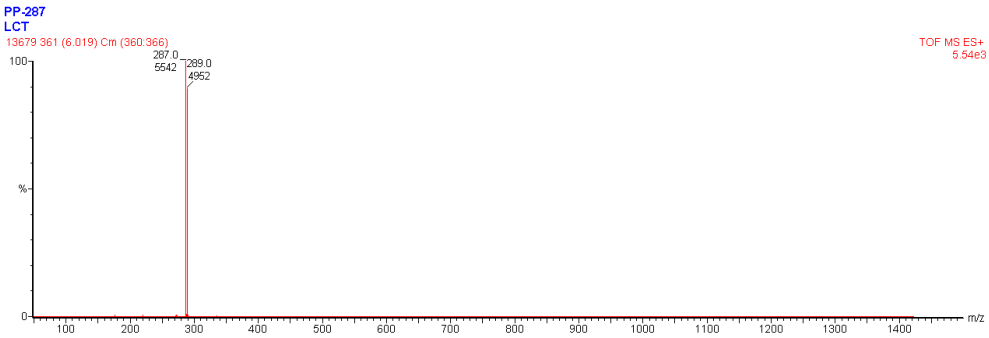


Figure S4. ESI-MS spectrum of 4-(2-bromobutoxy)-3-methoxybenzaldehyde **2**

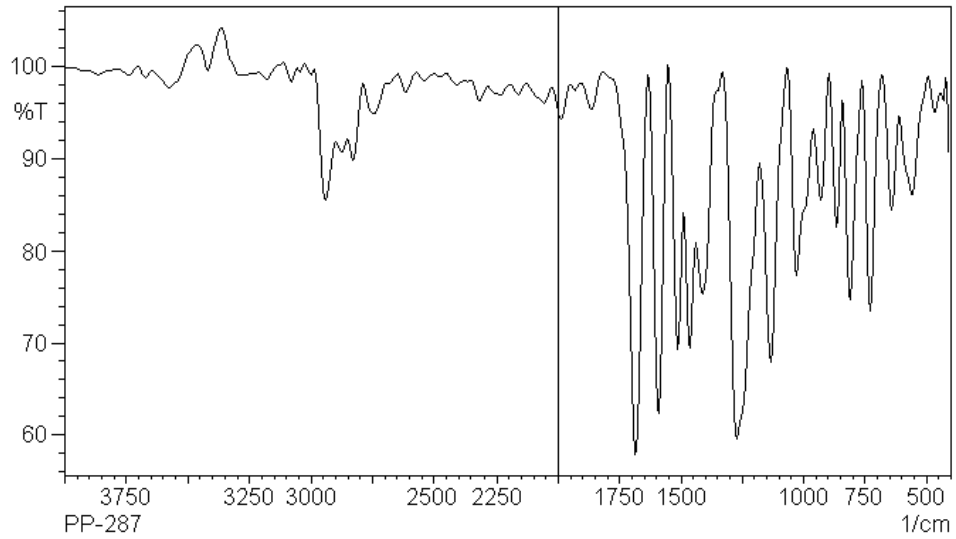


Figure S5. IR spectrum of 4-(2-bromobutoxy)-3-methoxybenzaldehyde **2** (KBr disk)

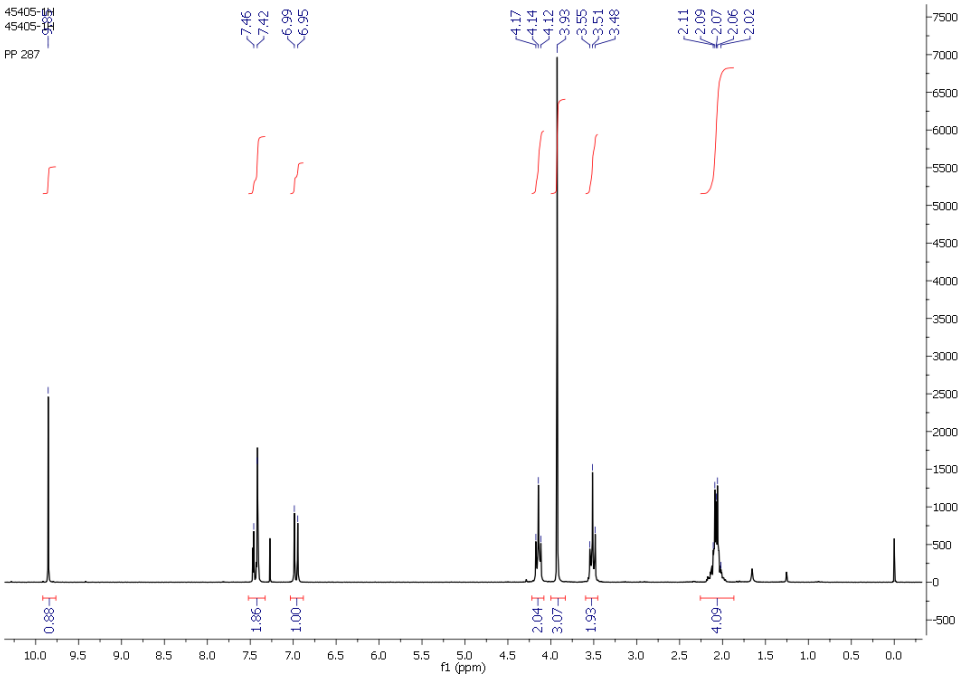


Figure S6. ^{1}H NMR spectrum of 4-(2-bromobutoxy)-3-methoxybenzaldehyde **2**

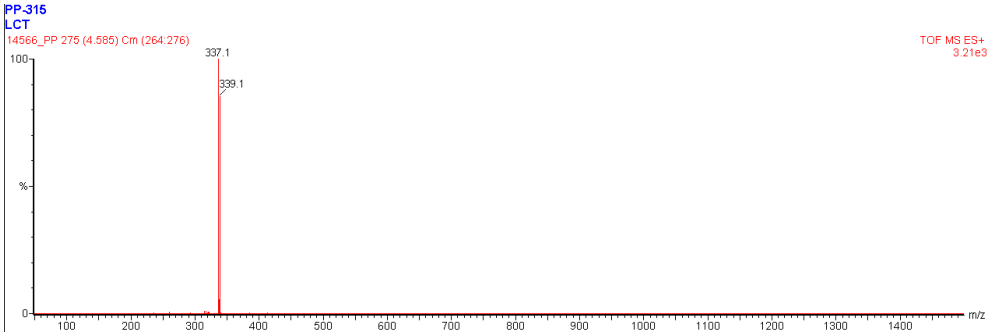


Figure S7. ESI-MS spectrum of 4-(2-bromohexoxy)-3-methoxybenzaldehyde **3**

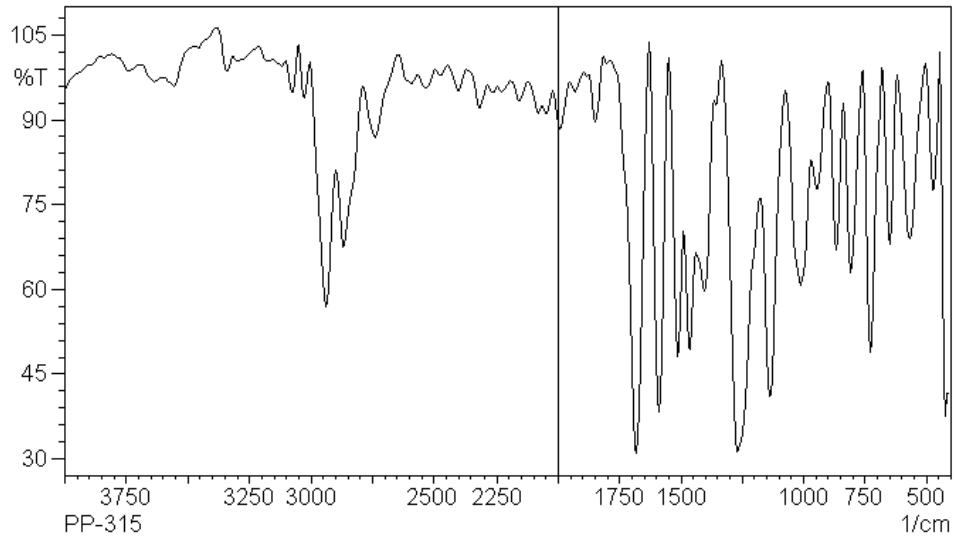


Figure S8. IR spectrum of 4-(2-bromohexoxy)-3-methoxybenzaldehyde **3** (KBr disk)

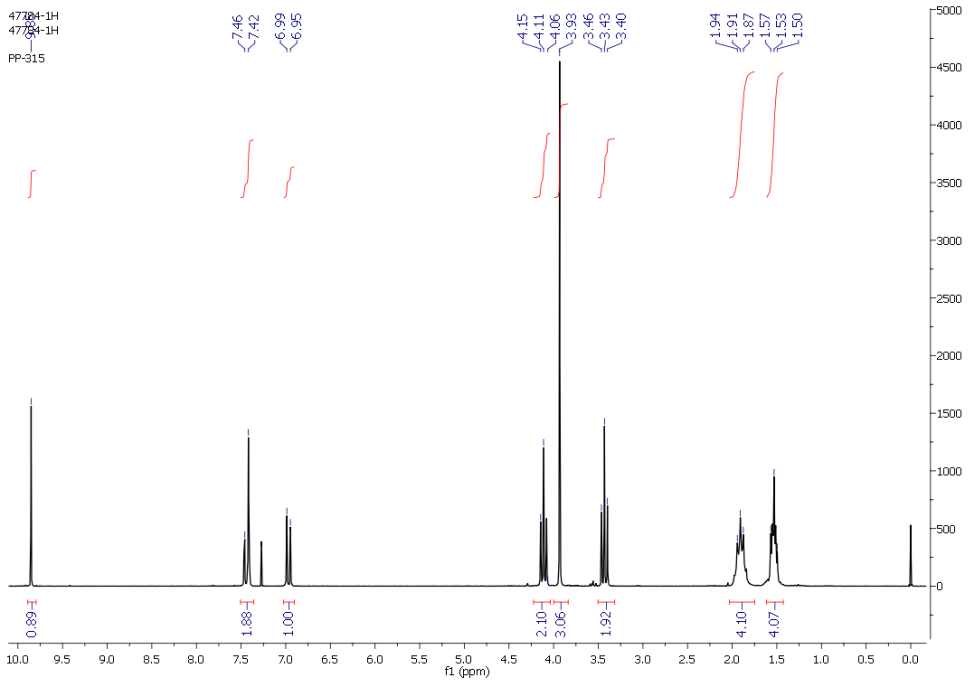


Figure S9. ^{1}H NMR spectrum of 4-(2-bromohexoxy)-3-methoxybenzaldehyde **3**

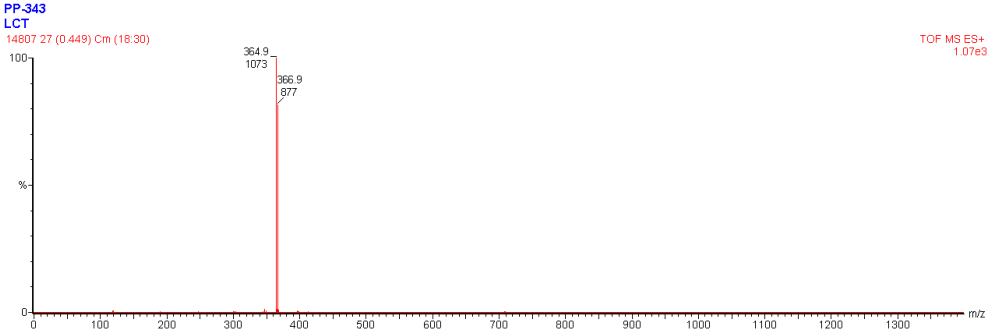


Figure S10. ESI-MS spectrum of 4-(2-bromooctoxy)-3-methoxybenzaldehyde **4**

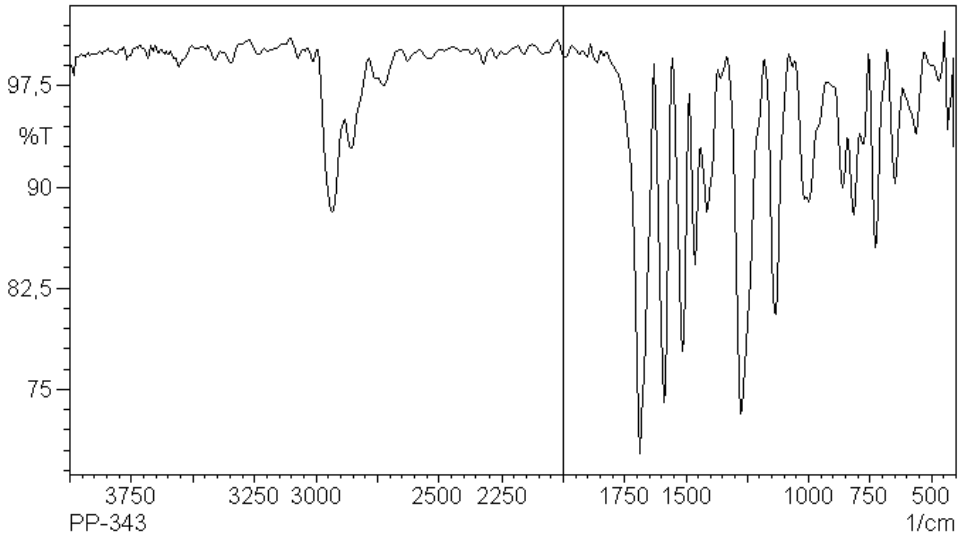


Figure S11. IR spectrum of 4-(2-bromooctoxy)-3-methoxybenzaldehyde **4** (KBr disk)

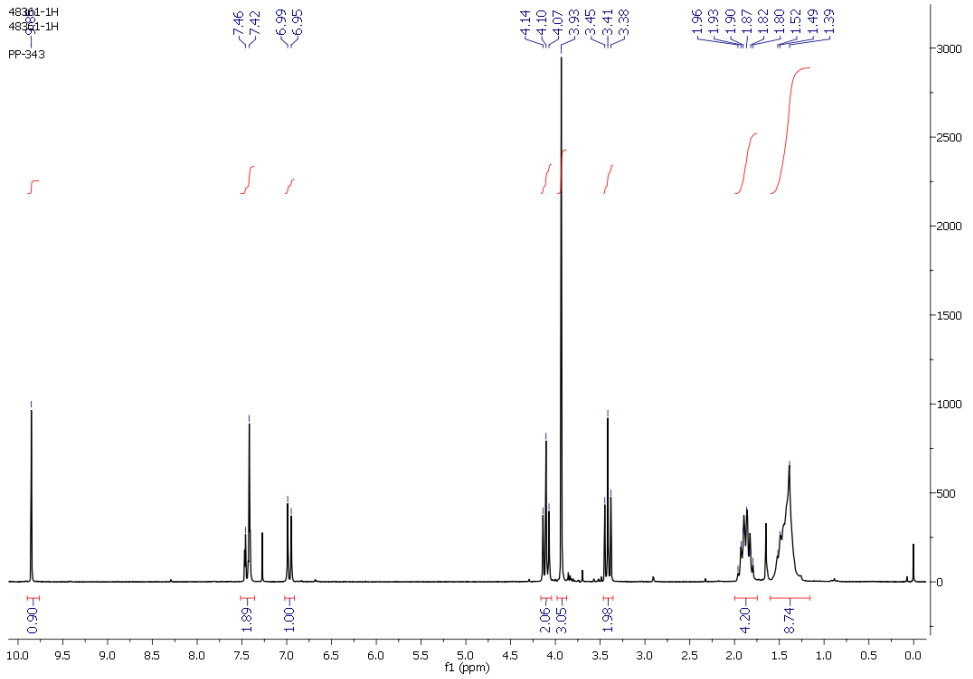


Figure 12. ^{1}H NMR spectrum of 4-(2-bromobutoxy)-3-methoxybenzaldehyde **4**

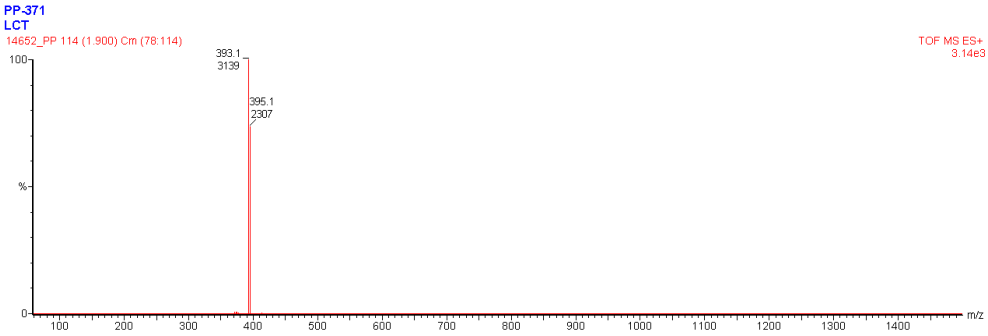


Figure S13. ESI-MS spectrum of 4-(2-bromodecoxy)-3-methoxybenzaldehyde **5**

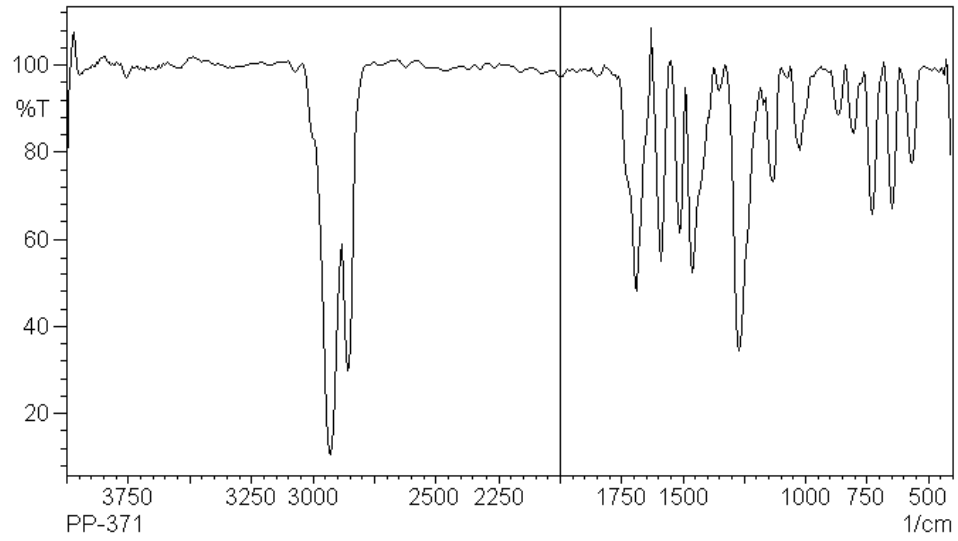


Figure S14. IR spectrum of 4-(2-bromodecoxy)-3-methoxybenzaldehyde **5** (KBr disk)

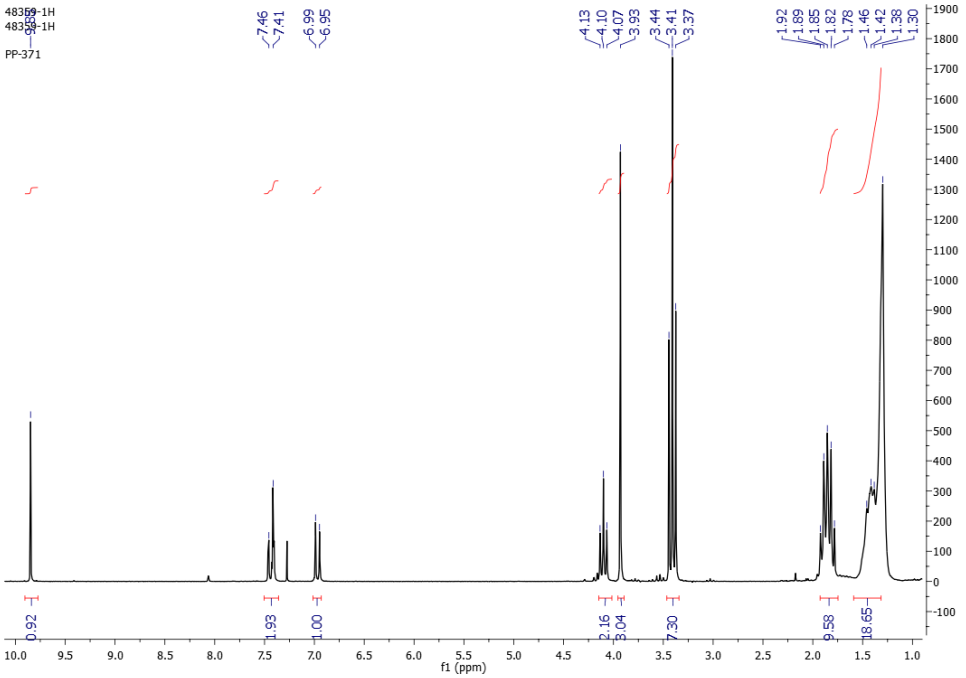


Figure S15. ^{1}H NMR spectrum of 4-(2-bromodecoxy)-3-methoxybenzaldehyde **5**

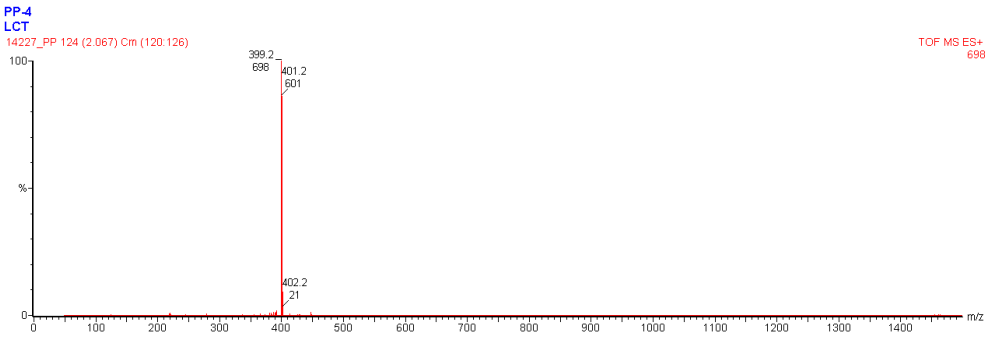


Figure S16. ESI-MS spectrum of 4-(2-bromododecoxy)-3-methoxybenzaldehyde **6**

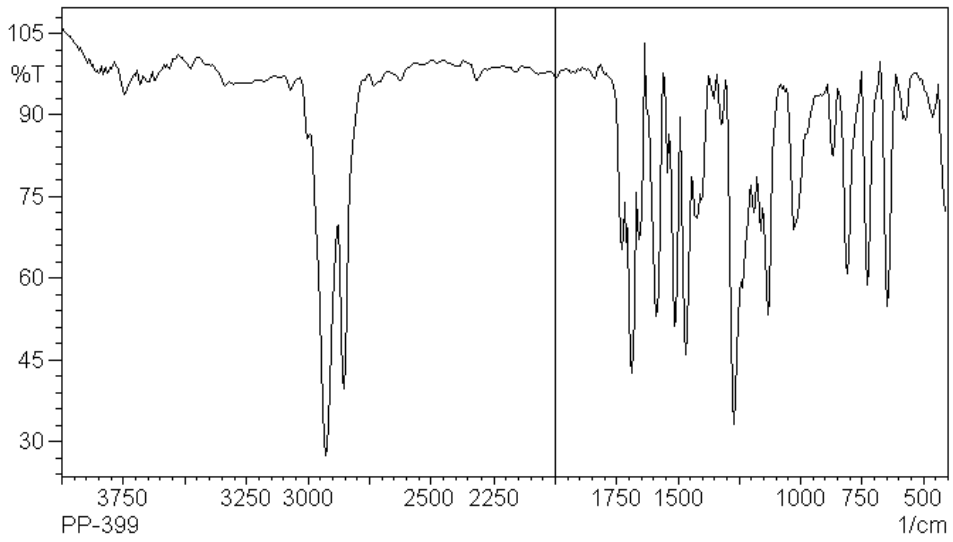


Figure S17. IR spectrum of 4-(2-bromododecoxy)-3-methoxybenzaldehyde **6** (KBr disk)

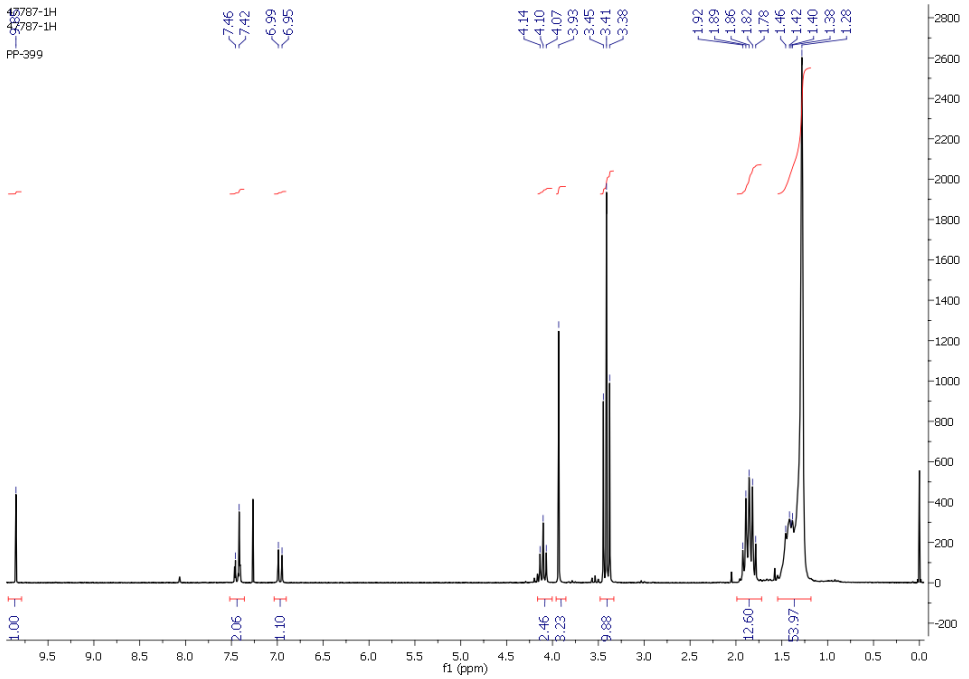


Figure S18. ^{1}H NMR spectrum of 4-(2-bromododecoxy)-3-methoxybenzaldehyde **6**

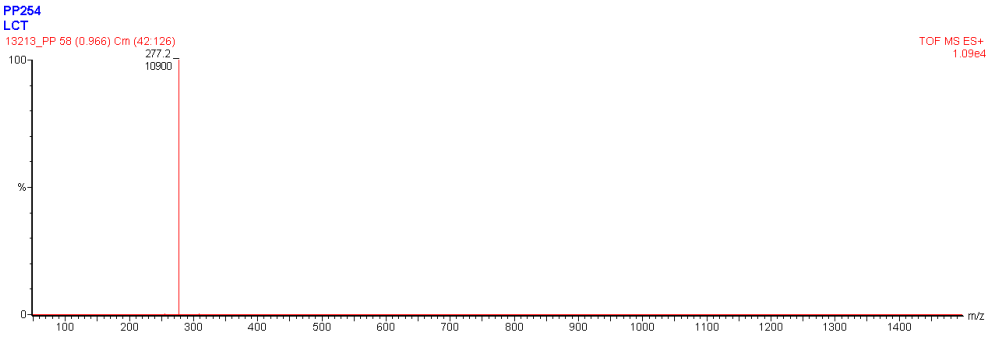


Figure S19. ESI-MS spectrum of 4-(S-acetylthioethoxy)-3-methoxybenzaldehyde **7**

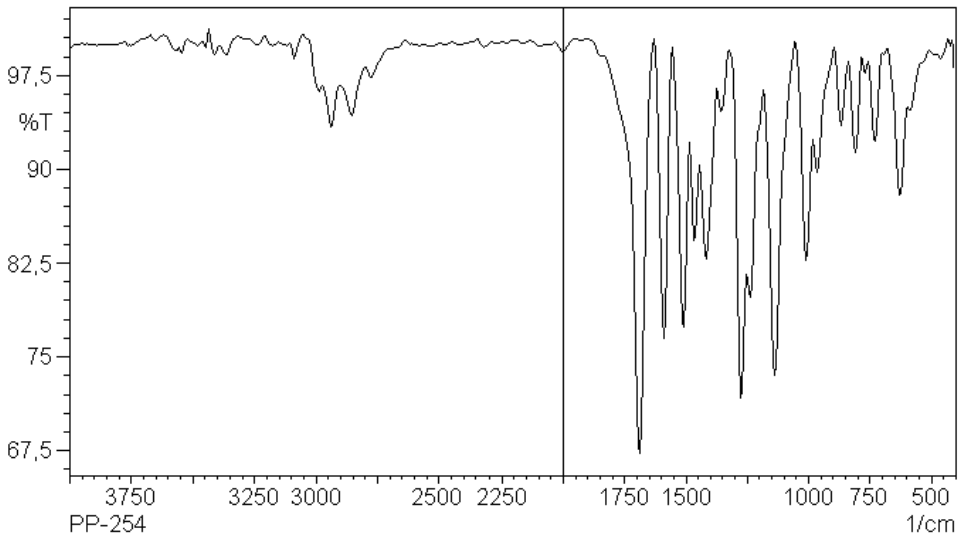


Figure S20. IR spectrum of 4-(S-acetylthioethoxy)-3-methoxybenzaldehyde **7** (KBr disk)

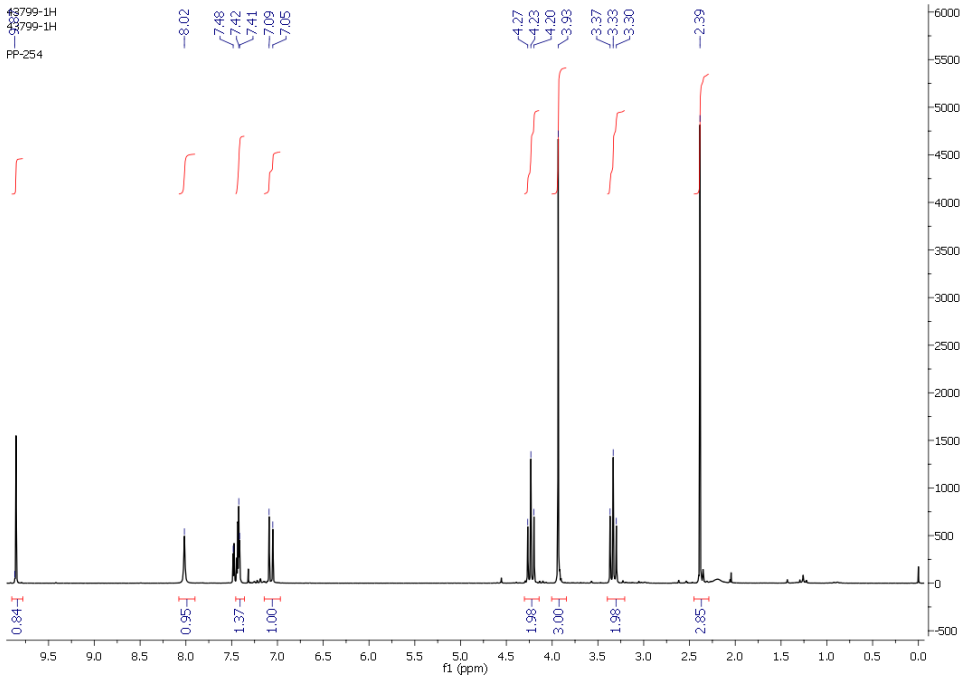


Figure S21. ^{1}H NMR spectrum of 4-(S-acetylthioethoxy)-3-methoxybenzaldehyde **7**

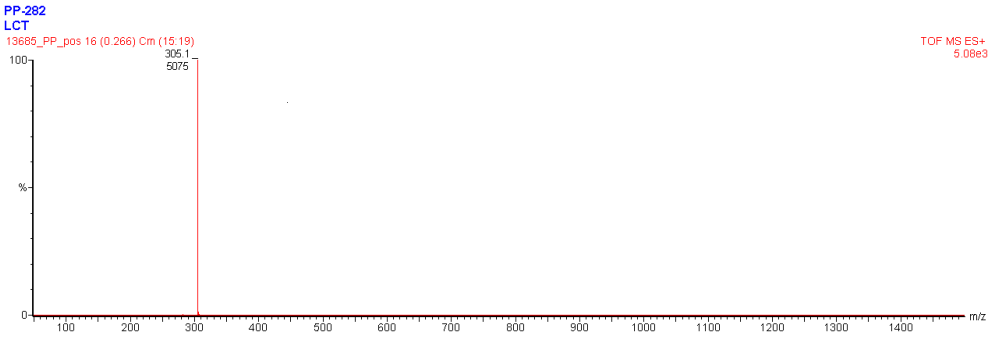


Figure S22. ESI-MS spectrum of 4-(S-acetylthiobutoxy)-3-methoxybenzaldehyde **8**

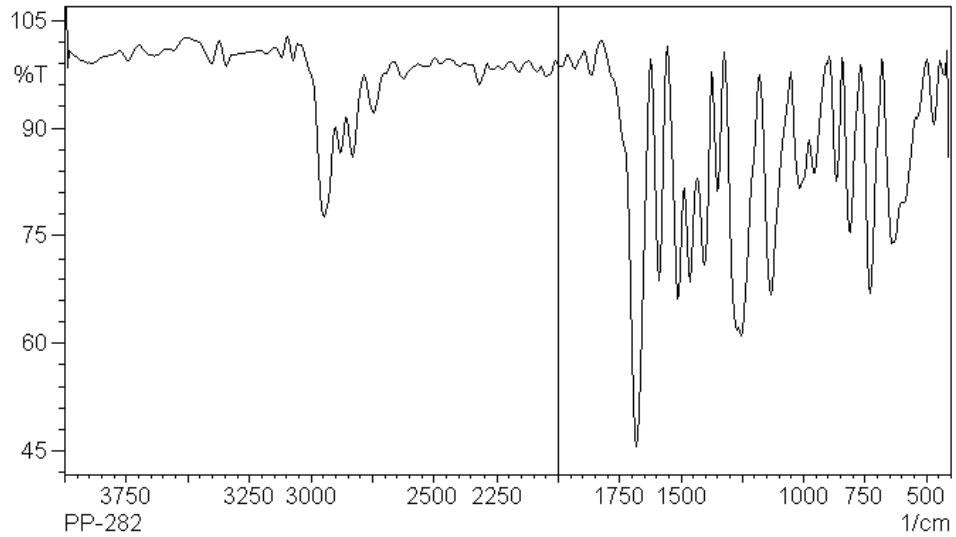


Figure S23. IR spectrum of 4-(S-acetylthiobutoxy)-3-methoxybenzaldehyde **8** (KBr disk)

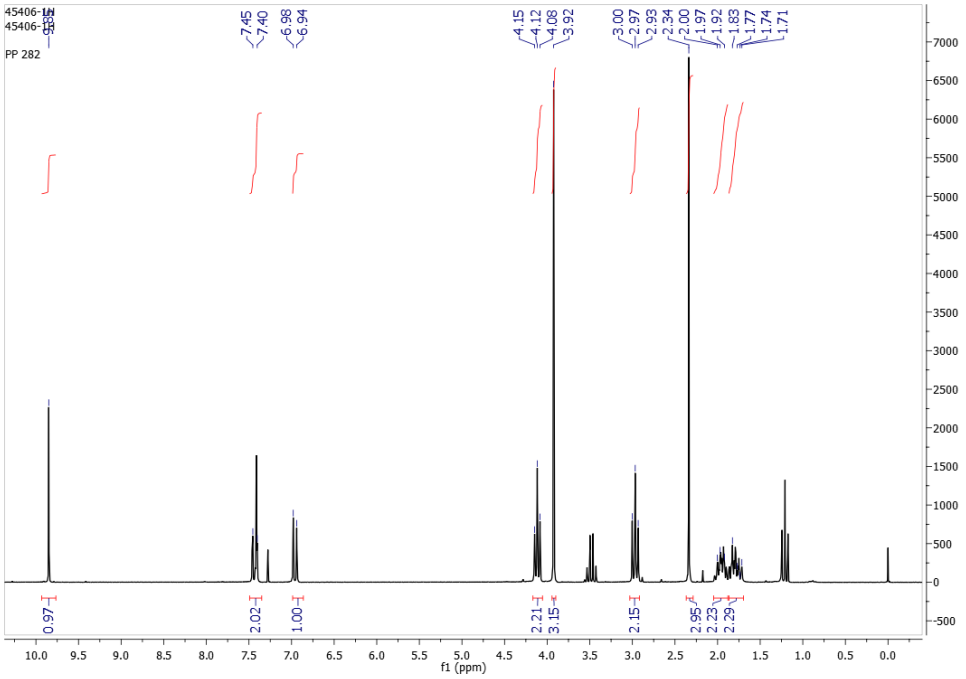


Figure S24. ^{1}H NMR spectrum of 4-(S-acetylthiobutoxy)-3-methoxybenzaldehyde **8**

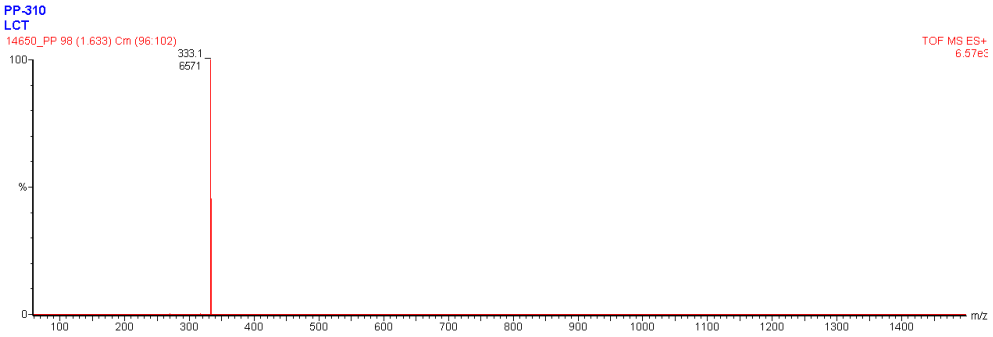


Figure S25. ESI-MS spectrum of 4-(S-acetylthiohexoxy)-3-methoxybenzaldehyde **9**

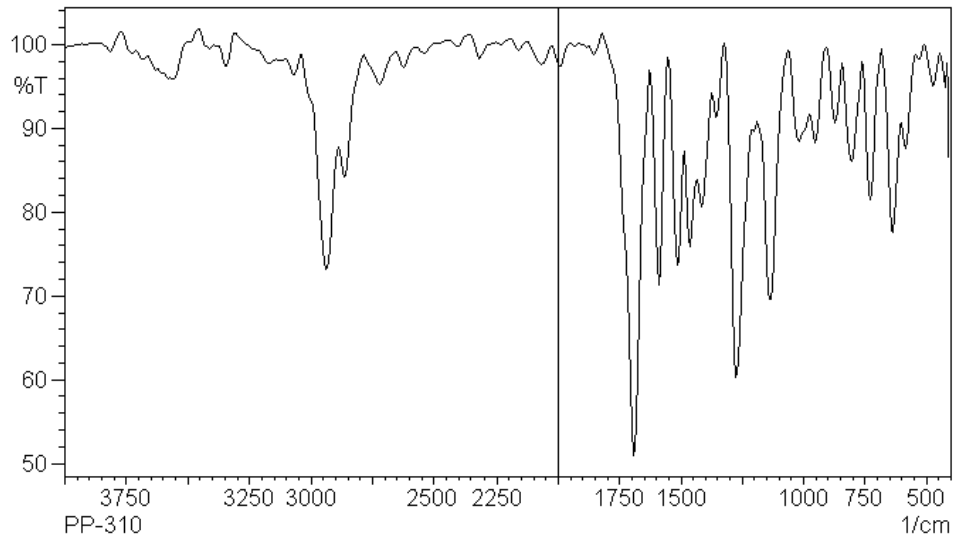


Figure S26. IR spectrum of 4-(S-acetylthiohexoxy)-3-methoxybenzaldehyde **9** (KBr disk)

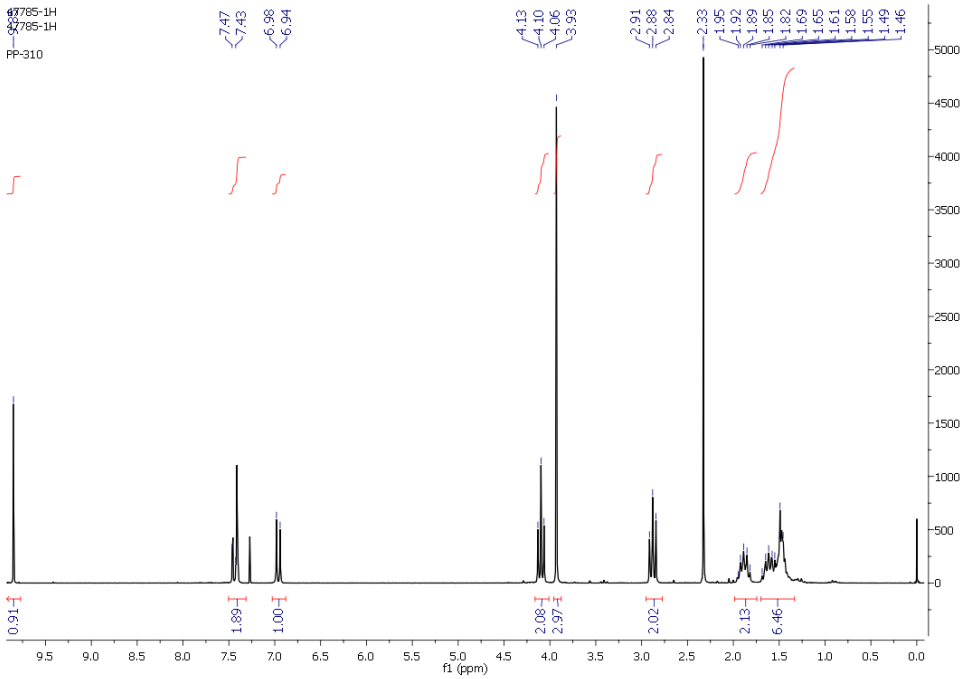


Figure S27. ^{1}H NMR spectrum of 4-(S-acetylthiohexoxy)-3-methoxybenzaldehyde **9**

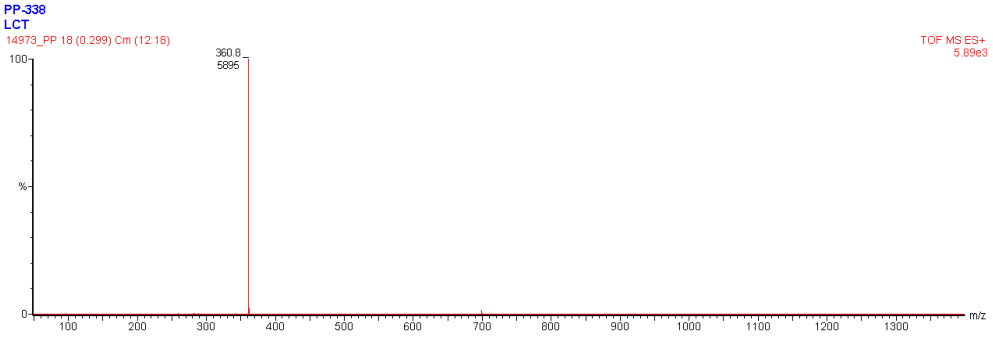


Figure S28. ESI-MS spectrum of 4-(S-acetylthiooctoxy)-3-methoxybenzaldehyde **10**

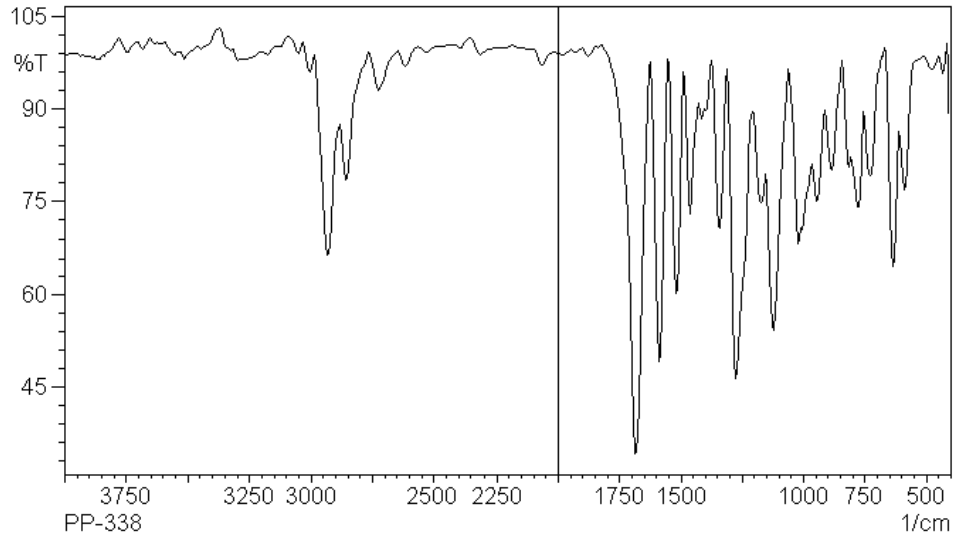


Figure S29. IR spectrum of 4-(S-acetylthiooctoxy)-3-methoxybenzaldehyde **10** (KBr disk)

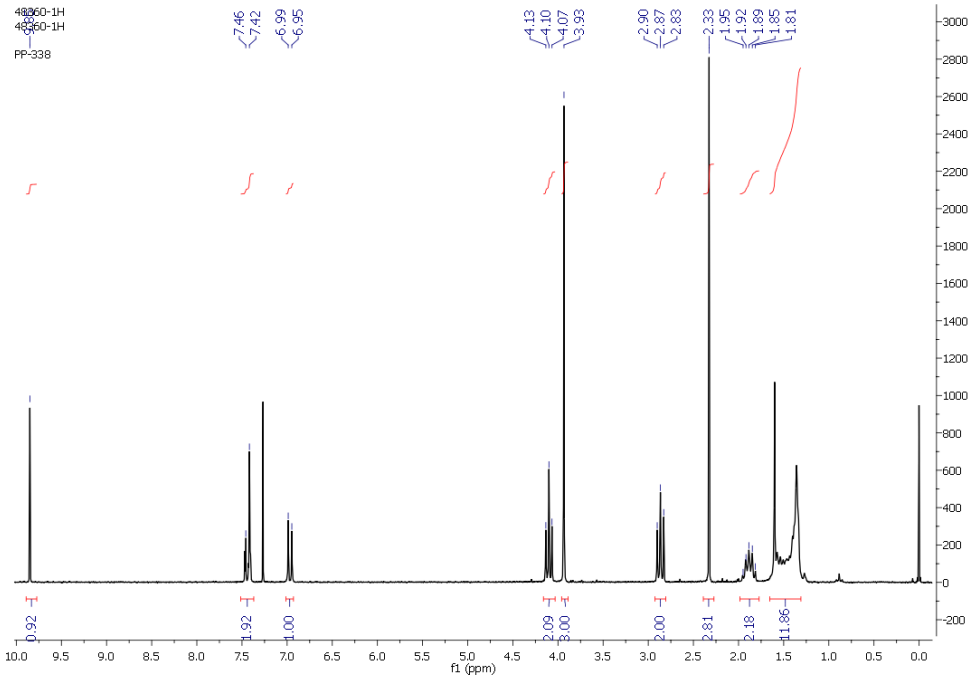


Figure S30. ^{1}H NMR spectrum of 4-(S-acetylthiooctoxy)-3-methoxybenzaldehyde **10**

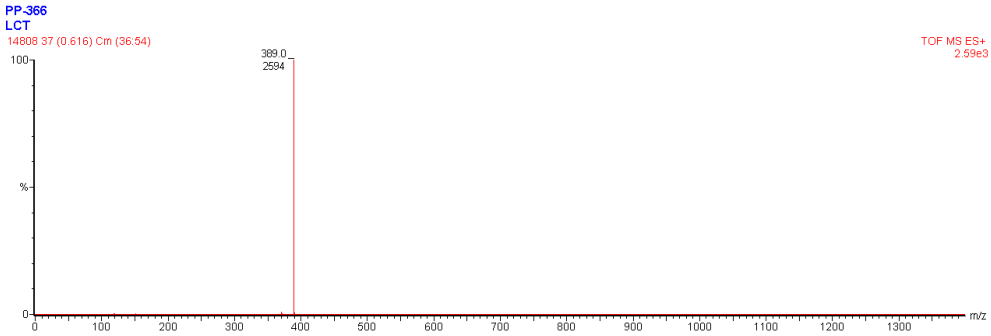


Figure S31. ESI-MS spectrum of 4-(S-acetylthiodecoxy)-3-methoxybenzaldehyde **11**

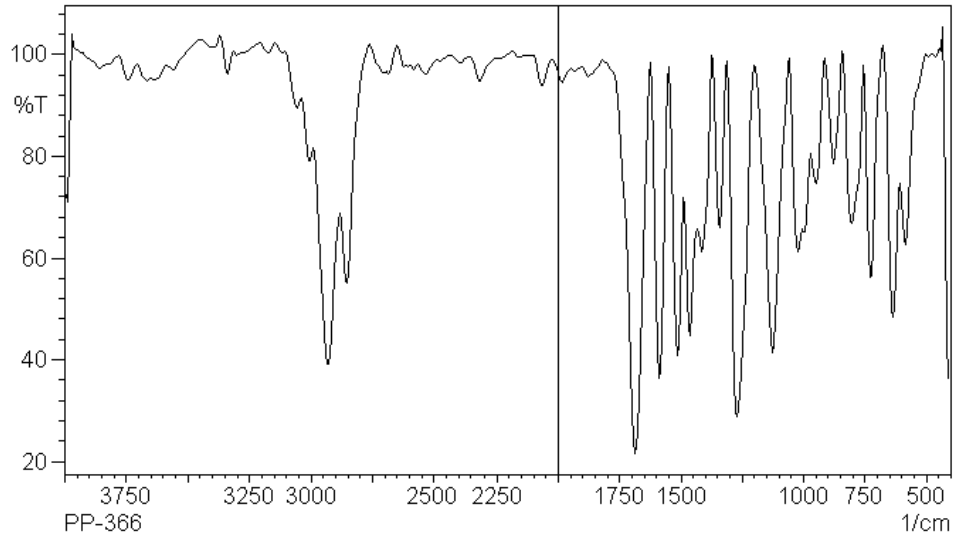


Figure S32. IR spectrum of 4-(S-acetylthiodecoxy)-3-methoxybenzaldehyde **11** (KBr disk)

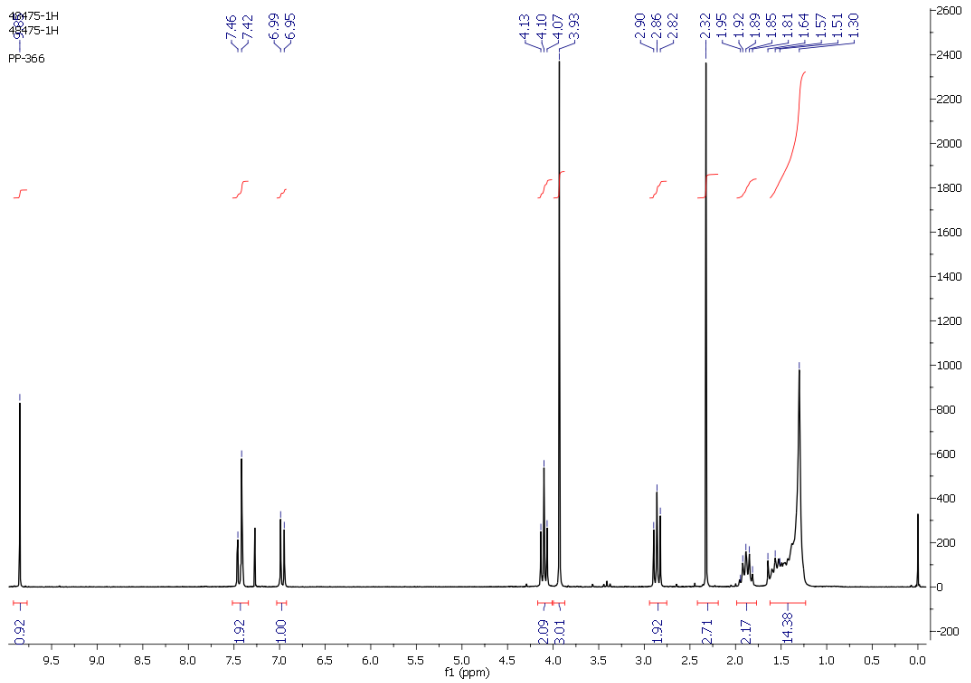


Figure S33. ^{1}H NMR spectrum of 4-(S-acetylthiodecoxy)-3-methoxybenzaldehyde **11**

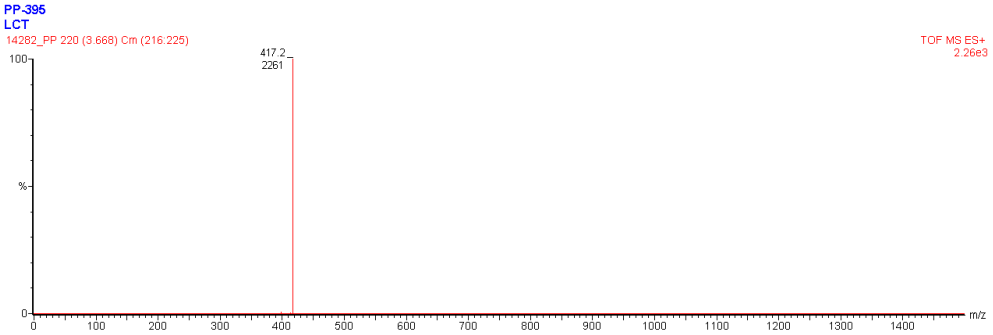


Figure S34. ESI-MS spectrum of 4-(S-acetylthiododecoxy)-3-methoxybenzaldehyde **12**

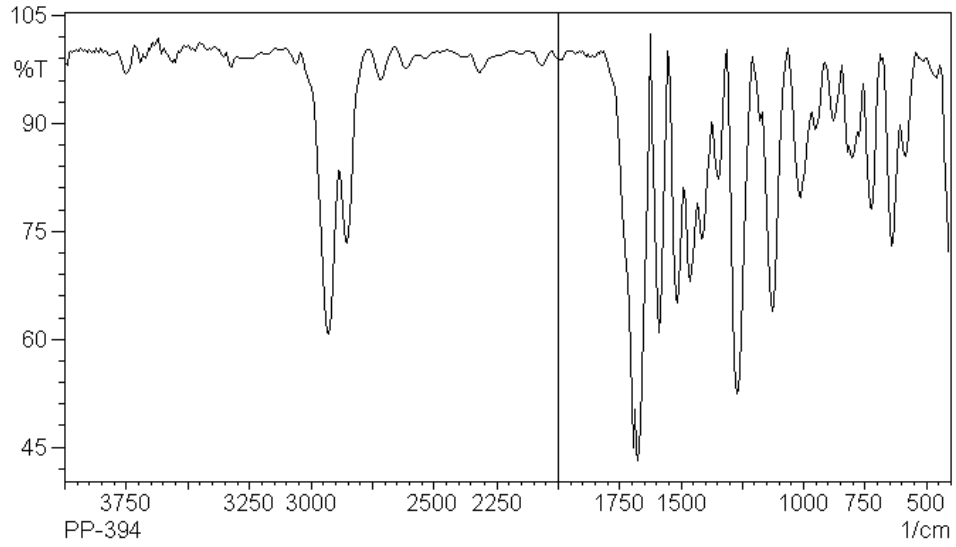


Figure S35. IR spectrum of 4-(S-acetylthiododecoxy)-3-methoxybenzaldehyde **12** (KBr disk)

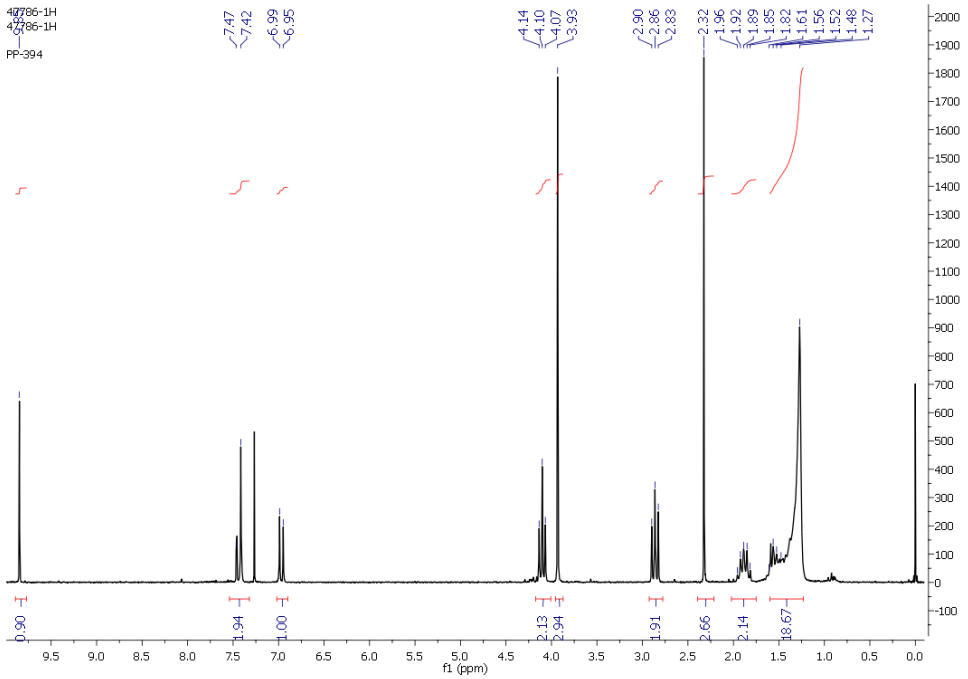


Figure S36. ^{1}H NMR spectrum of 4-(S-acetylthiododecoxy)-3-methoxybenzaldehyde **12**

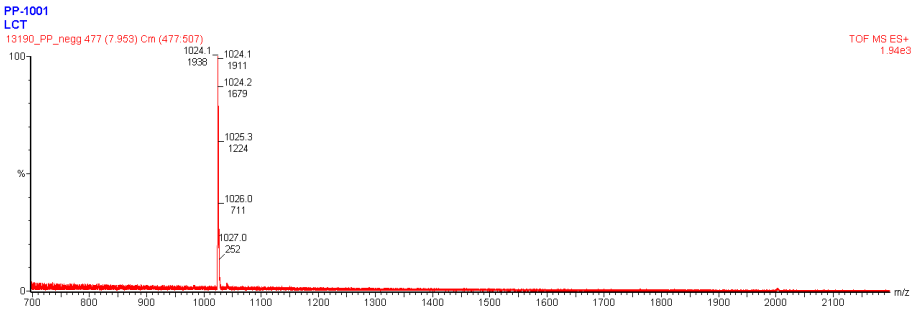


Figure S37. ESI-MS spectrum of fullerene thioacetate **I**

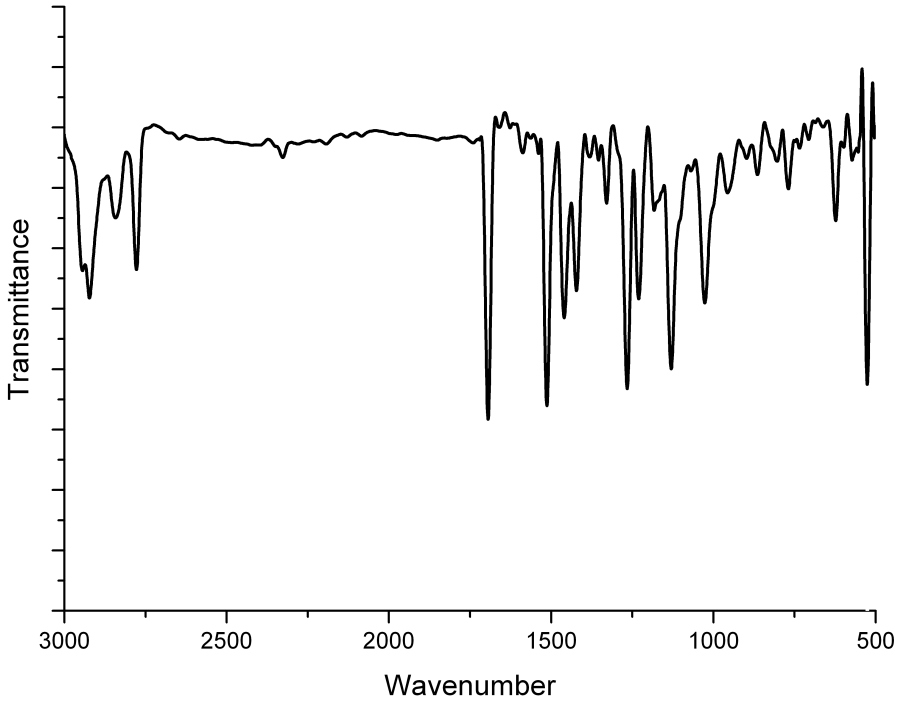


Figure S38. IR spectrum of fullerene thioacetate **I** (KBr disk)

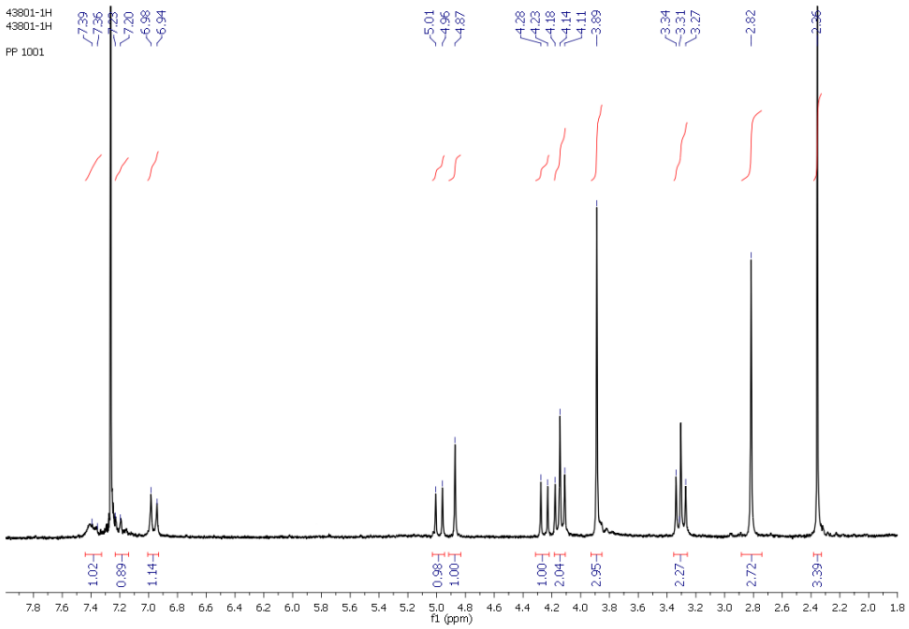


Figure S39. ^{1}H NMR spectrum of fullerene thioacetate **I**

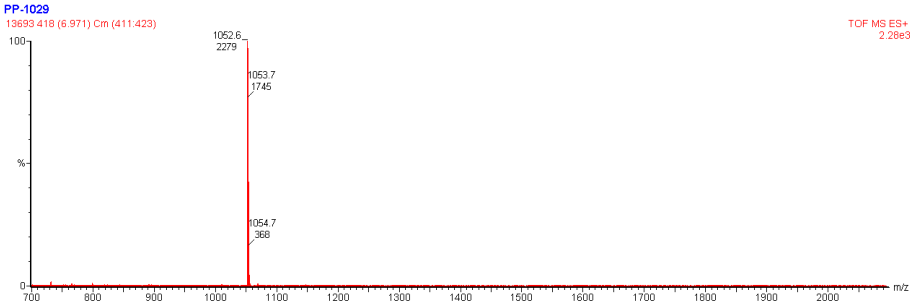


Figure S40. ESI-MS spectrum of fullerene thioacetate **II**

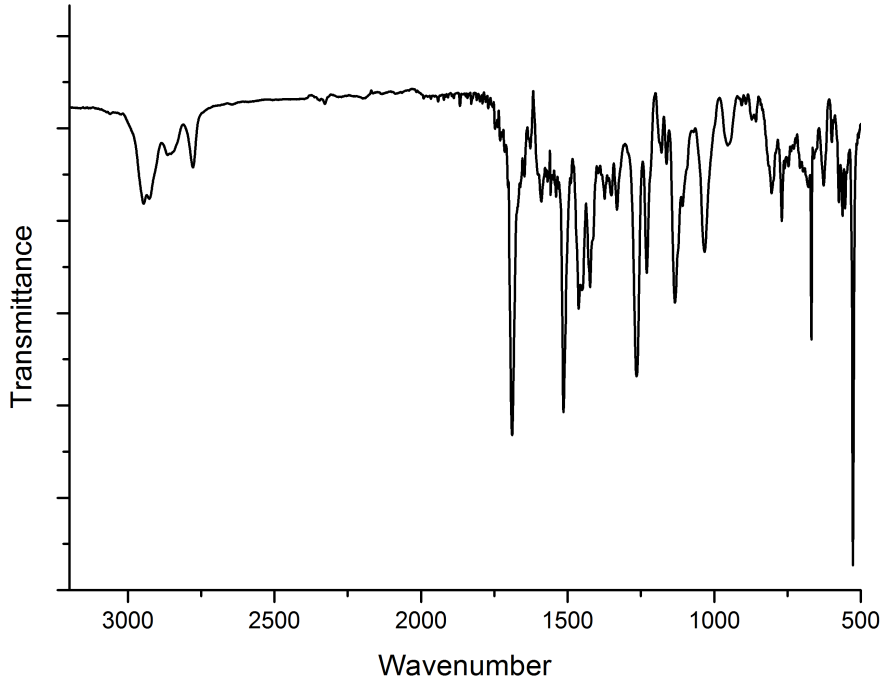


Figure S41. IR spectrum of fullerene thioacetate **II** (KBr disk)

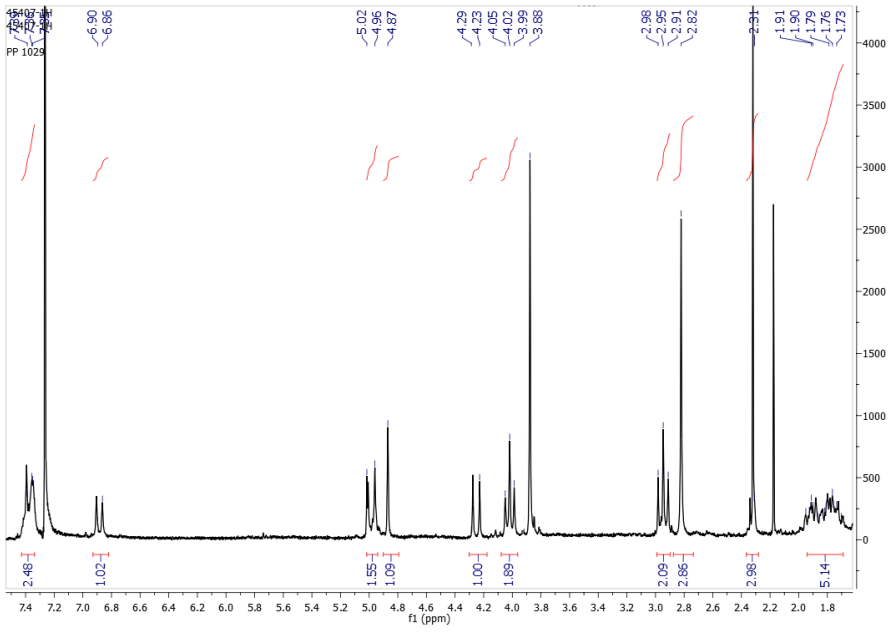


Figure S42. ^{1}H NMR spectrum of fullerene thioacetate **II**

Figure S43. ESI-MS spectrum of fullerene thioacetate **III**

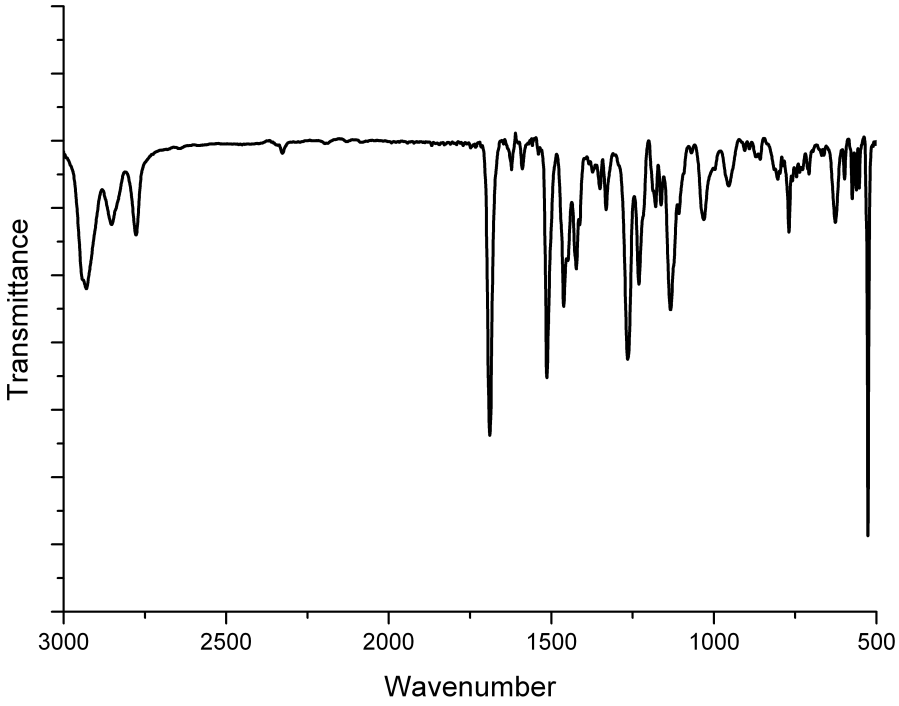


Figure S44. IR spectrum of fullerene thioacetate **III** (KBr disk)

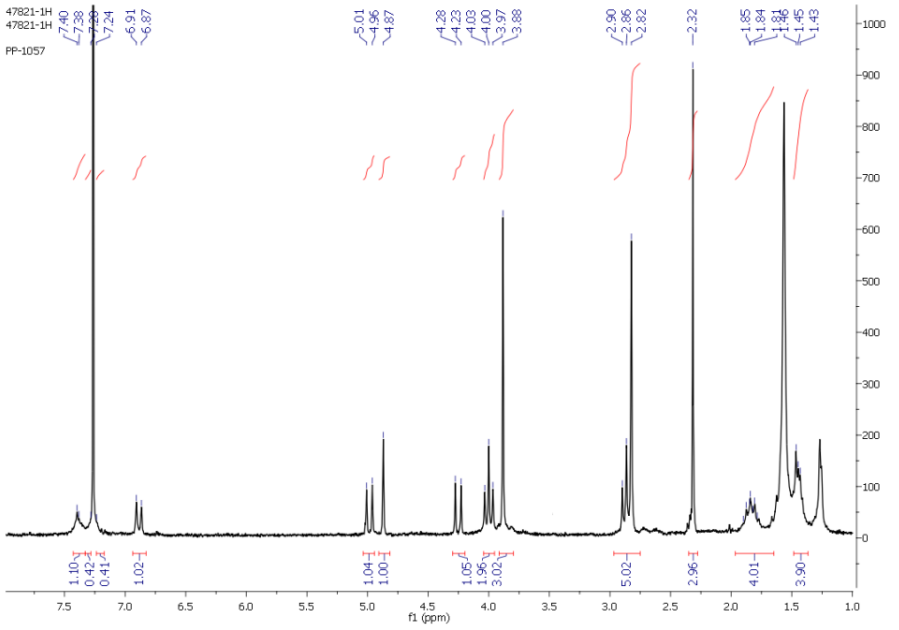


Figure S45. ^{1}H NMR spectrum of fullerene thioacetate **III**

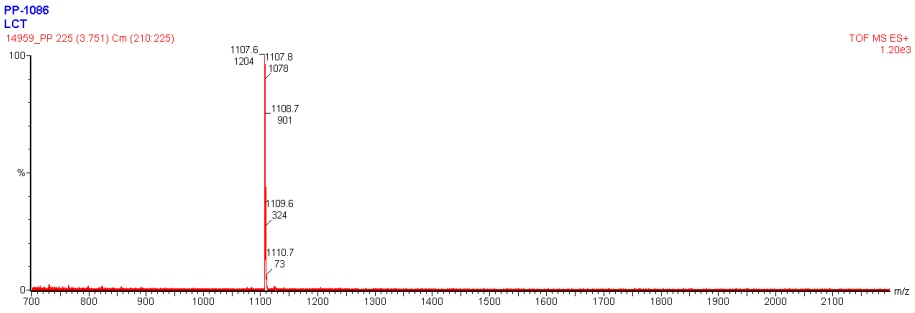


Figure S46. ESI-MS spectrum of fullerene thioacetate **IV**

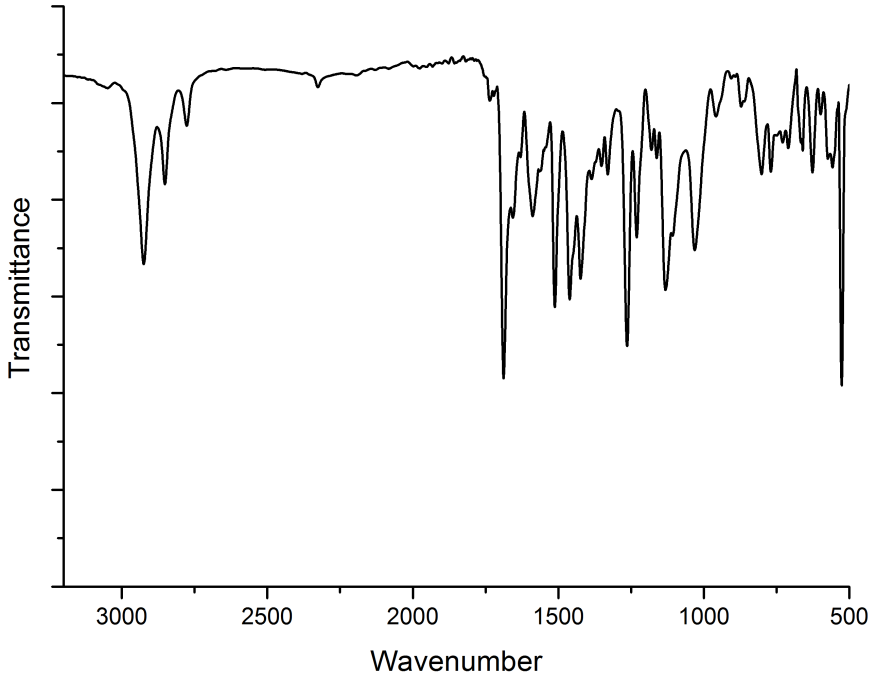


Figure S47. IR spectrum of fullerene thioacetate **IV** (KBr disk)

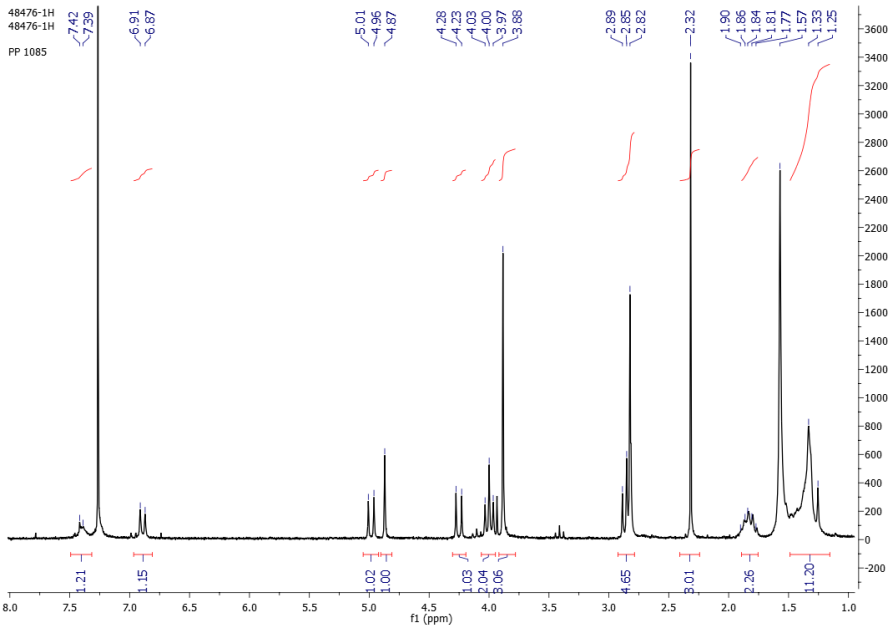


Figure S48. ^{1}H NMR spectrum of fullerene thioacetate **IV**

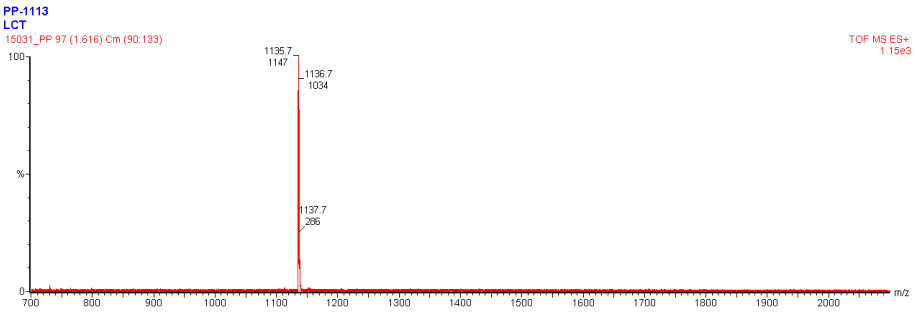


Figure S49. ESI-MS spectrum of fullerene thioacetate **V**

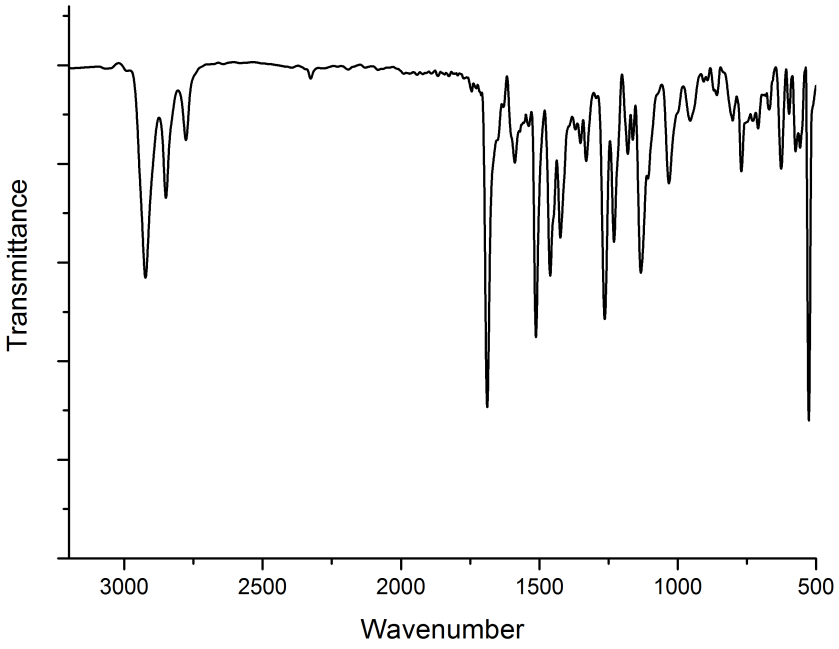


Figure S50. IR spectrum of fullerene thioacetate **V** (KBr disk)

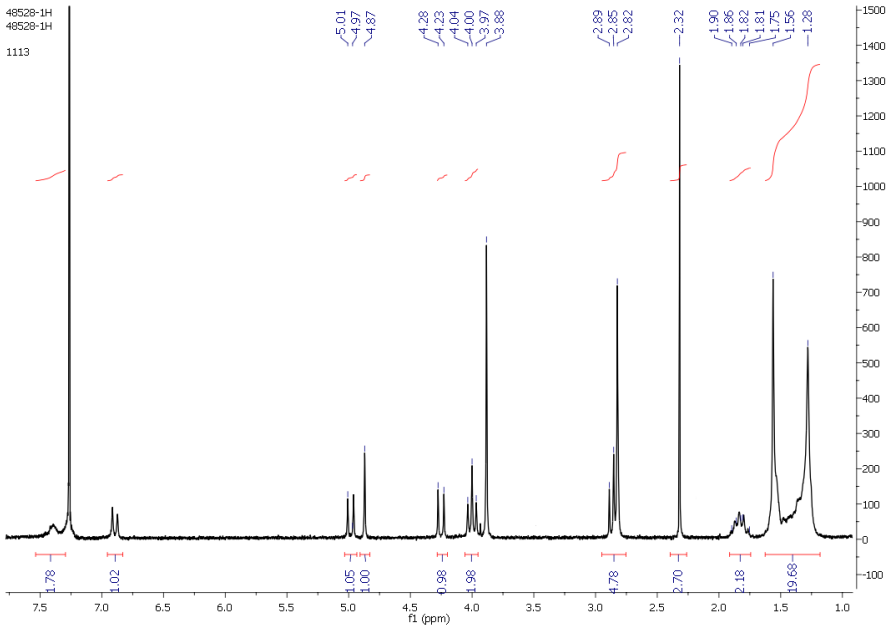


Figure S51 ^{1}H NMR spectrum of fullerene thioacetate **V**

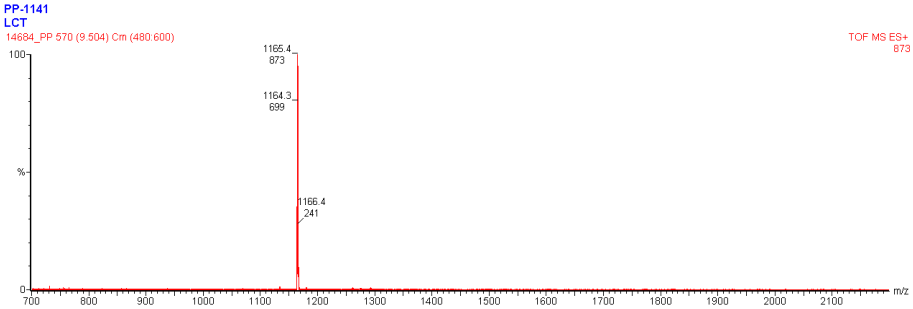


Figure S52. ESI-MS spectrum of fullerene thioacetate **VI**

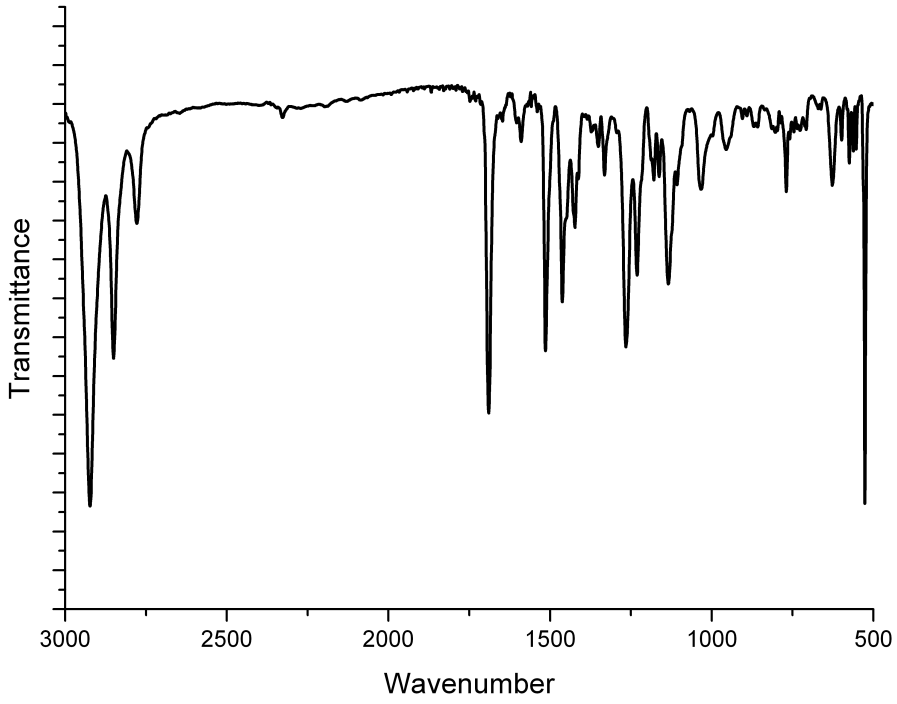


Figure S53 IR spectrum of fullerene thioacetate **VI** (KBr disk)

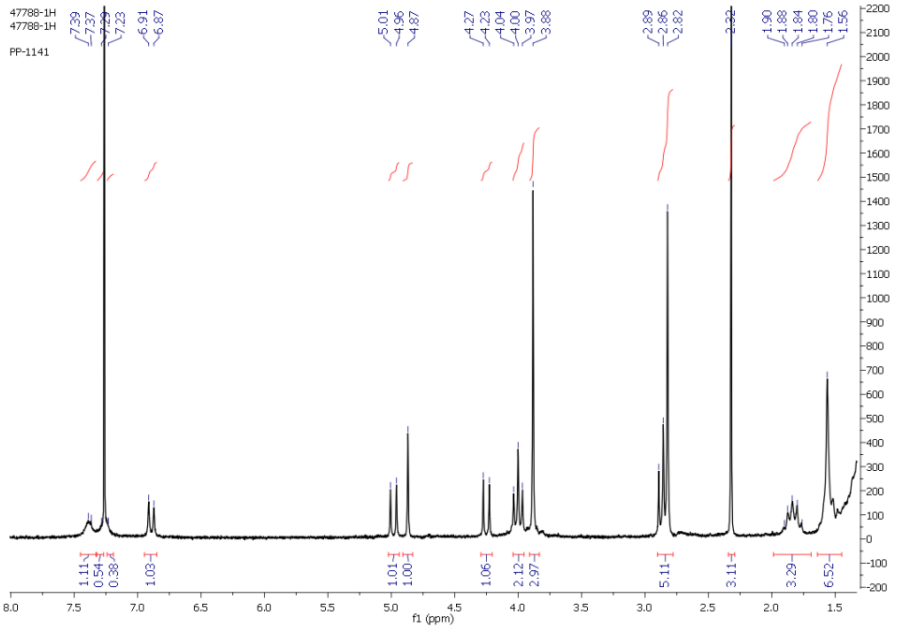


Figure S54. ^{1}H NMR spectrum of fullerene thioacetate **VI**

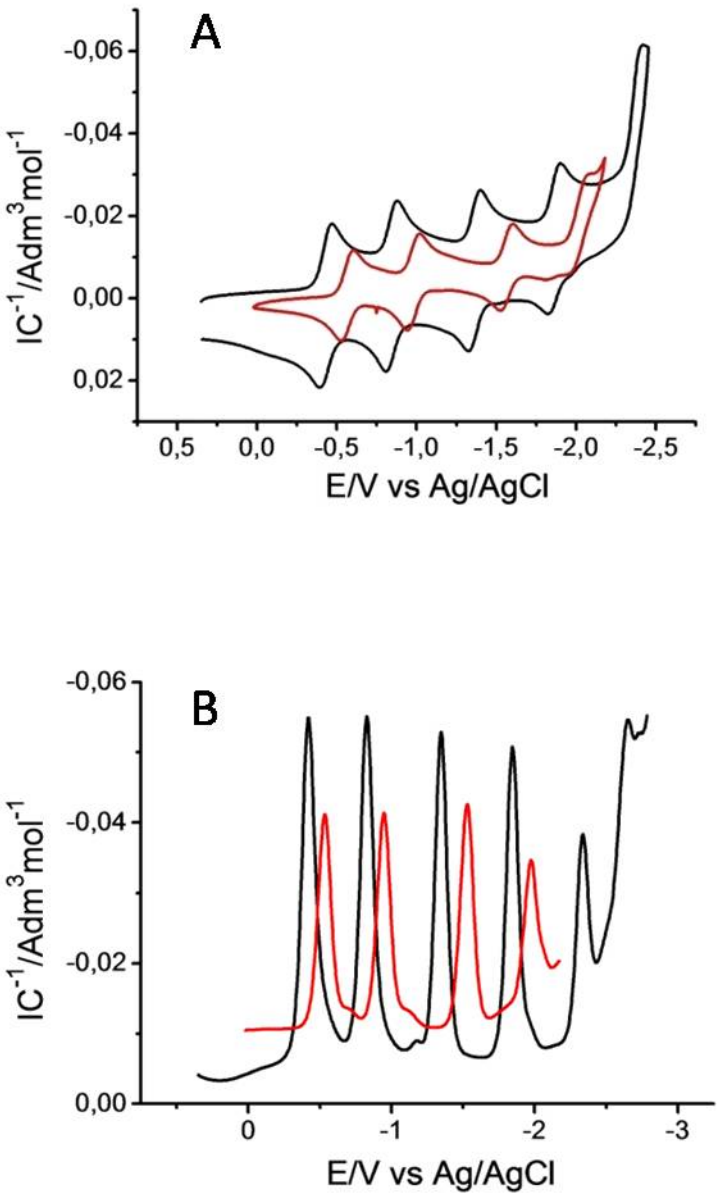


Figure S55. Voltammograms of (black line) C60 and (red line) compound **III** in 0.1 M TBAHFP/ toluene/acetonitrile (4:1), (A) CV, v = 100 mV/s; (B) DPV, tp = 3 ms, ΔE = 50 mV.

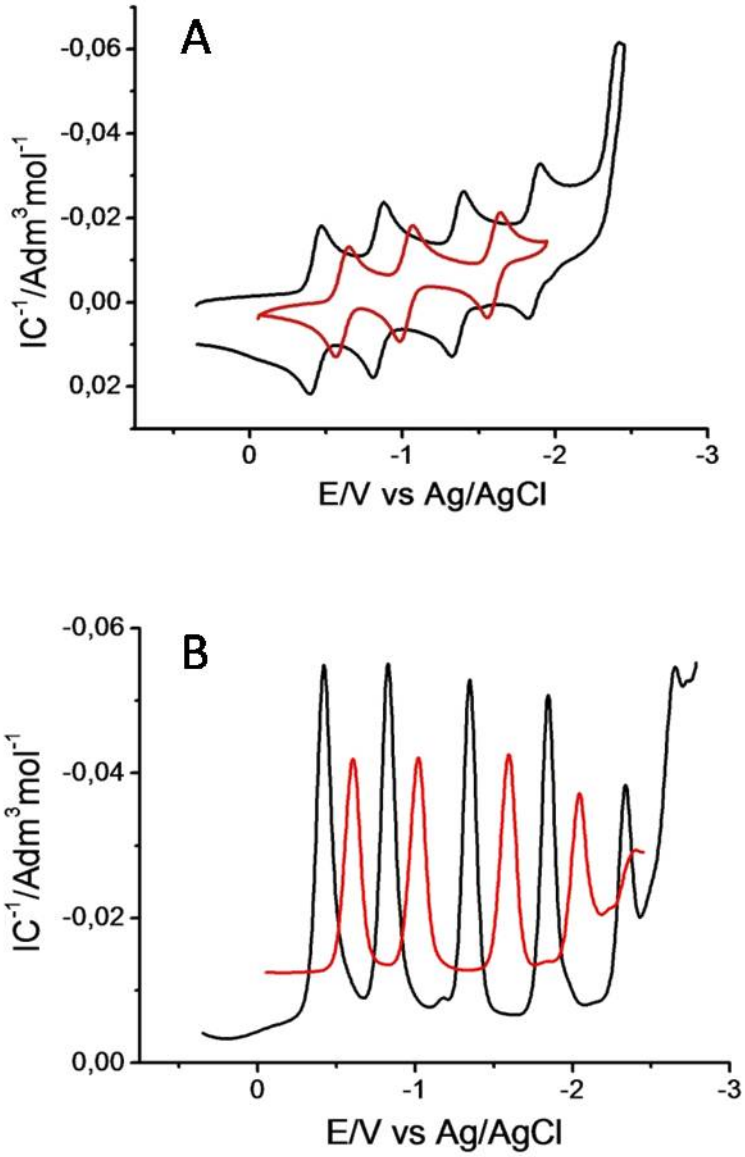


Figure S56. Voltammograms of (black line) C60 and (red line) compound **V** in 0.1 M TBAHFP/ toluene/acetonitrile (4:1), (A) CV, v = 100 mV/s; (B) DPV, tp = 3 ms, ΔE = 50 mV.

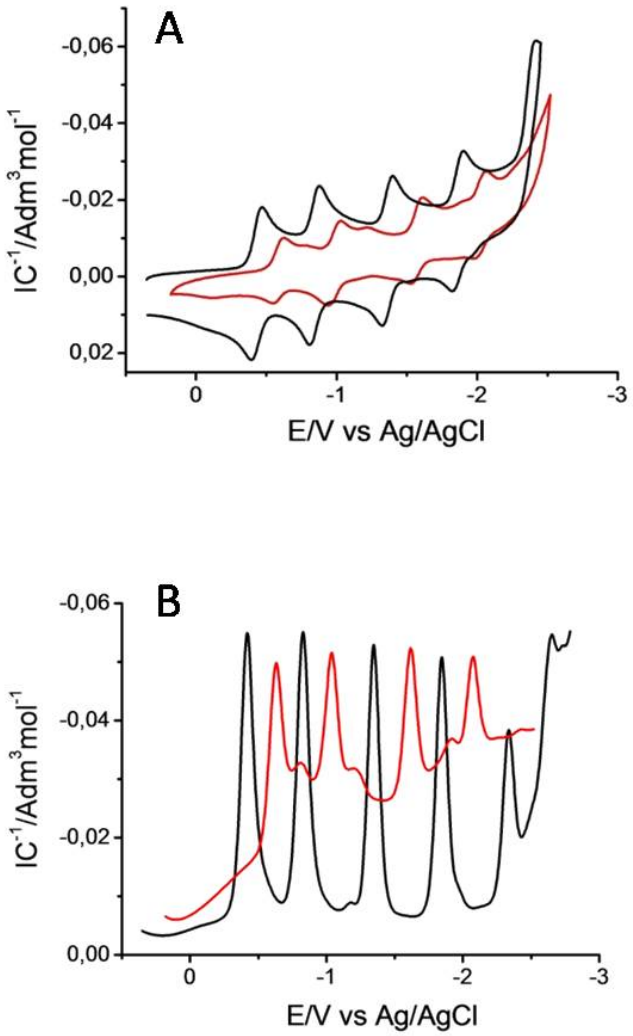


Figure S57. Voltammograms of (black line) C60 and (red line) compound **VI** in 0.1 M TBAHFP/ toluene/acetonitrile (4:1), (A) CV, v = 100 mV/s; (B) DPV, tp = 3 ms, ΔE = 50 mV.

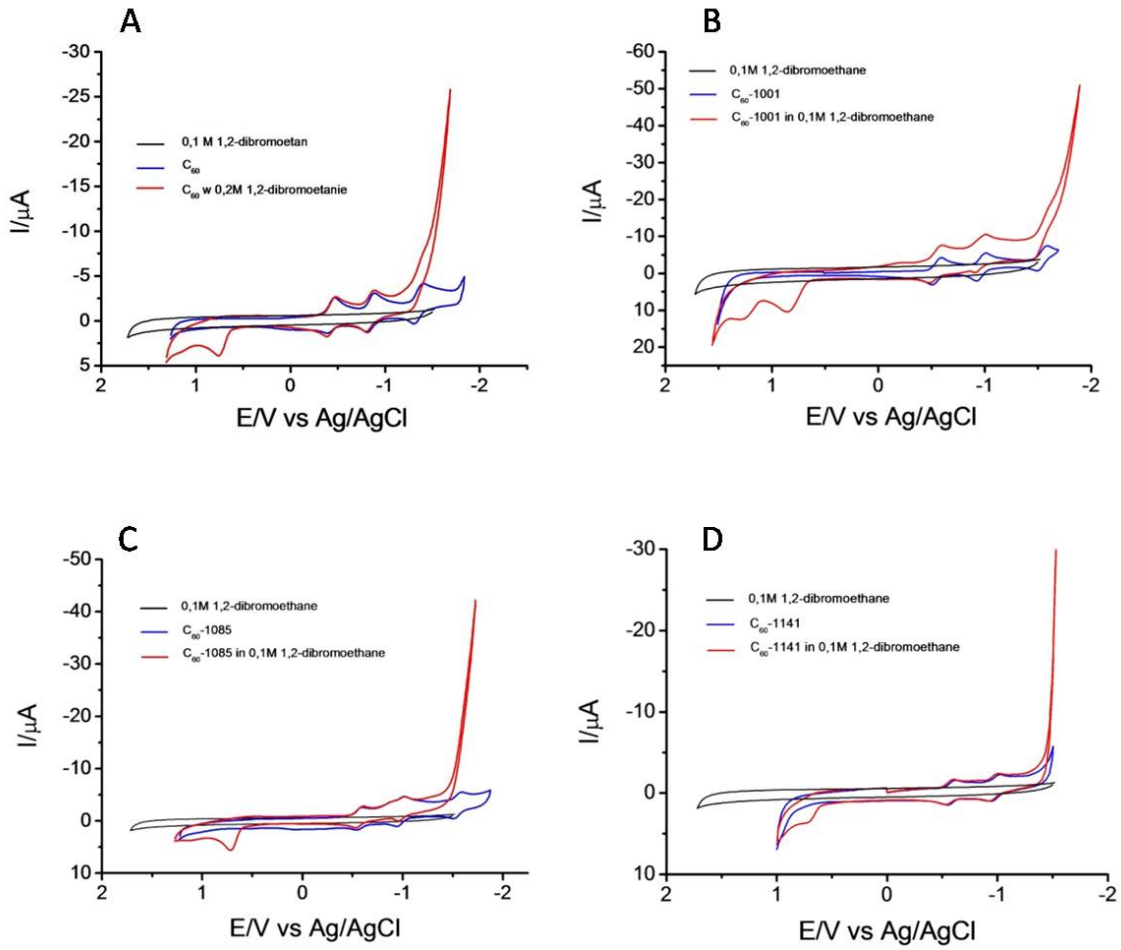


Figure S58. Cyclic voltammograms for $\mathbf{C_{60}}$(A), derivative **I** (B), **IV** (C) and **VI** (D) in absence and presence of 0,1M 1,2-dibromoethane in 0.1 M TBAHFP/ toluene/acetonitrile (4:1), v = 100 mVs^{-1}.

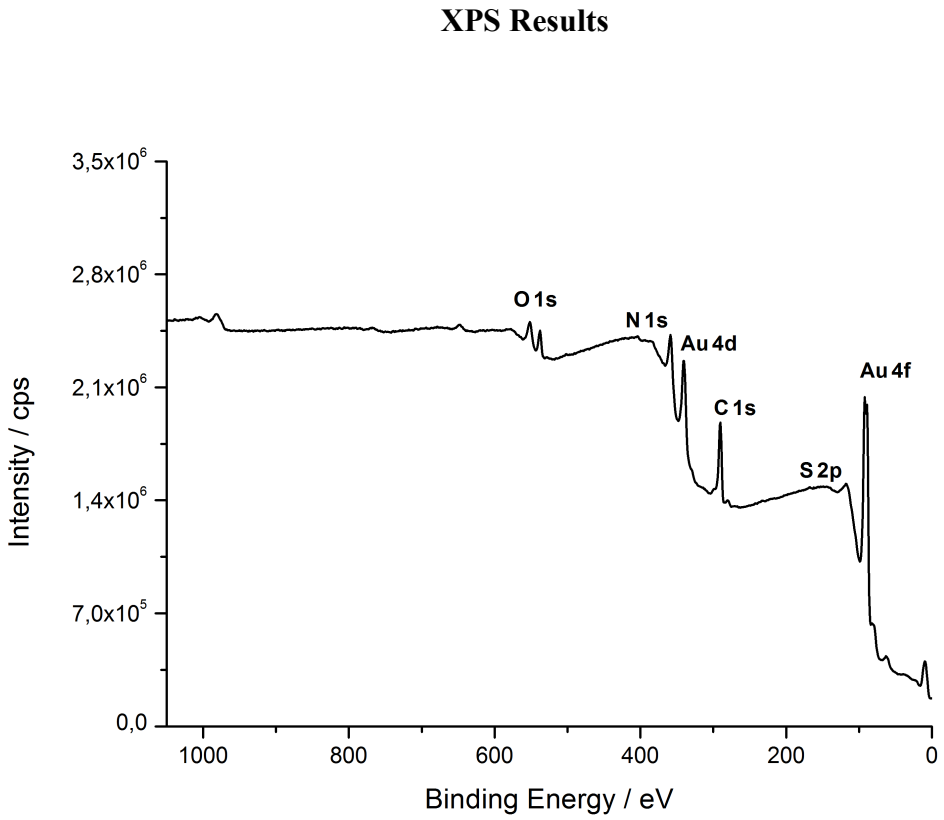


Figure S59. XPS survey spectra of fullerene thioacetate **I** film on gold surface

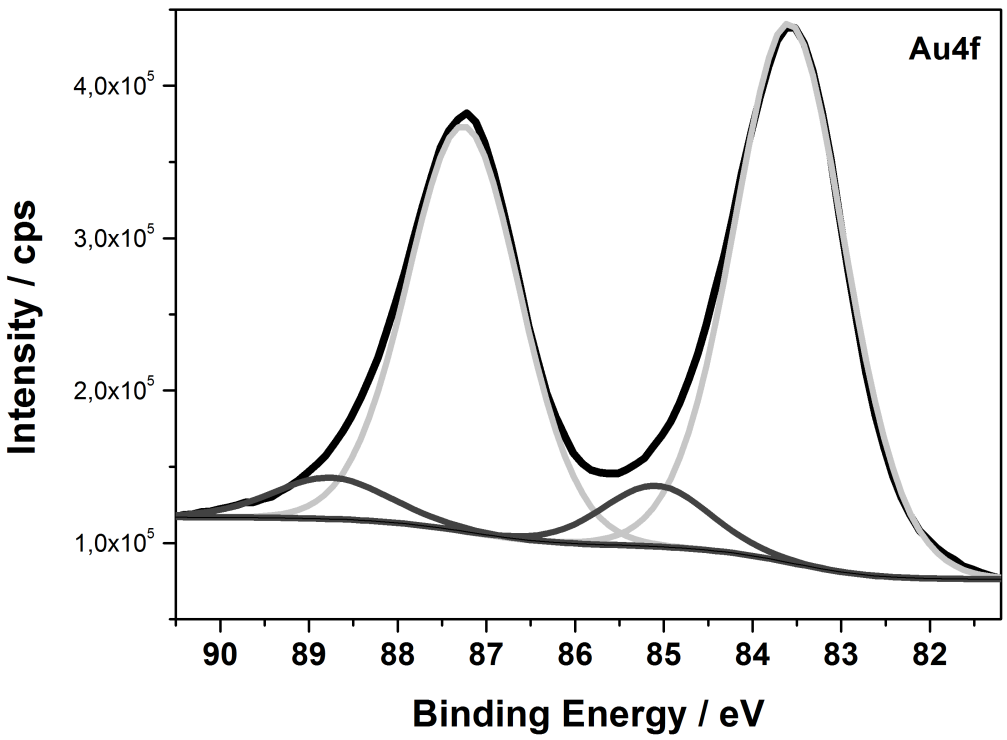


Figure S60. Au4f XPS spectra of fullerene thioacetate **I** film on gold surface

Table S1. Voltammetric characteristics of C_{60} and compound **3**, CV and DPV (bottom)

Compound	C_{60}	I	II	III	IV	V	VI
E_{pc1} [V]	-0.467	-0.582	-0.551	-0.579	-0.606	-0.651	-0.626
E_{pa1} [V]	-0.396	-0.511	-0.475	-0.513	-0.530	-0.564	-0.551
$E_1^{0'}$ [V]	-0.432	-0.547	-0.513	-0.546	-0.568	-0.608	-0.589
E_{pc2} [V]	-0.874	-0.994	-0.965	-0.983	-1.021	-1.069	-1.029
E_{pa2} [V]	-0.807	-0.925	-0.889	-0.921	-0.945	-0.985	-0.943
$E_2^{0'}$ [V]	-0.841	-0.960	-0.927	-0.952	-0.983	-1.027	-0.986
E_{pc3} [V]	-1.40	-1.586	-1.548	-1.574	-1.603	-1.641	-1.614
E_{pa3} [V]	-1.324	-1.51	-1.465	-1.519	-1.526	-1.558	-1.528
$E_3^{0'}$ [V]	-1.362	-1.548	-1.506	-1.547	-1.565	-1.600	-1.571
E_{pc4} [V]	-1.895	-2.07	-1.845	-	-2.074	-	-2.06
E_{pa4} [V]	-1.828	-1.979	-1.763	-	-1.960	-	-1.986
$E_4^{0'}$ [V]	-1.862	-2.025	-1.9804	-	-2.017	-	-2.023
E_{pc5} [V]	-2.417	-	-	-	-	-	-
E_{pa5} [V]	-2.274	-	-	-	-	-	-
$E_5^{0'}$ [V]	-2.346	-	-	-	-	-	-

Compound	C_{60}	I	II	III	IV	V	VI
E_1 [V]	-0.422	-0.540	-0.489	-0.545	-0.536	-0.606	-0.63
$_{b1/2}$ [mV]	103	107	98	59		112	98
E_2 [V]	-0.827	-0.944	-0.904	-0.950	-0.947	-1.022	-1.039
$_{b1/2}$ [mV]	98	98	98	103		112	98
E_3 [V]	-1.342	-1.538	-1.481	-1.551	-1.529	-1.598	-1.618
$_{b1/2}$ [mV]	98	93	103	103		11	98
E_4[V]	-1.845	-2.007	-1.945	-	-1.975	-2.043	-2.074
$_{b1/2}$ [mV]	98	88	83	-		103	88
E_5 [V]	-2.338	-	-	-	-	-	-
$_{b1/2}$ [mV]	88	-	-	-	-	-	-
E_6 [V]	-2.656	-	-	-	-	-	-
$_{b1/2}$ [mV]	44	-	-	-	-	-	-

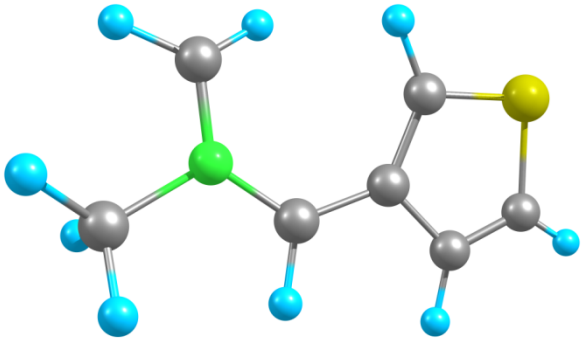
Table S2. Molecular Orbital Energies for Thioacetate Derivatives calculated from CV experiments.

Compound	Energies (eV)		
	HOMO	LUMO	HOMO-LUMO gap
C_{60}	-5.906	-3.921	-1.985
A1	-5.94	-3.805	-2.135
A2	-5.911	-3.865	-2.05
A3	-5.955	-3.921	-2.034
I	-5.952	-3.806	-2.16
II	-5.962	-3.84	-2.112
III	-5.962	-3.807	-2.16
IV	-5.975	-3.785	-2.19
V	-6.028	-3.745	-2.28
VI	-5.97	-3.764	-2.206

Calculations results

Ylide **A1**

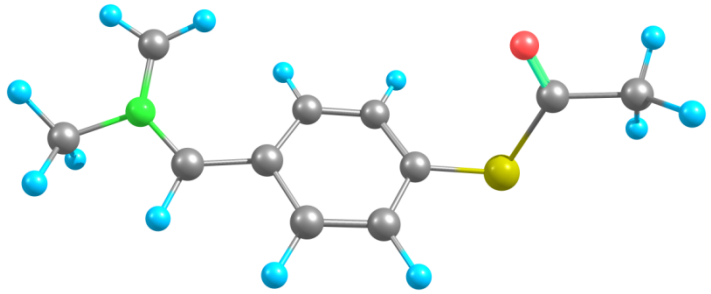
HF=-725.0167322



C	0.024706000	0.034513000	0.014567000
C	0.022687000	0.023675000	2.448823000
C	2.076430000	0.004367000	1.243859000
N	0.597217000	0.037711000	1.238125000
C	-3.149065000	0.045578000	-1.841114000
S	-3.966164000	0.392509000	-0.348212000
C	-2.465962000	0.352239000	0.532354000
C	-1.374648000	0.096548000	-0.287926000
C	-1.808168000	-0.082628000	-1.659552000
H	0.718554000	-0.037657000	-0.810939000
H	-1.030960000	-0.170565000	2.540059000
H	0.670008000	-0.011700000	3.311537000
H	2.455349000	0.436549000	0.317726000
H	2.438816000	0.595584000	2.086061000
H	2.420661000	-1.028322000	1.344936000
H	-3.709750000	-0.054614000	-2.760813000
H	-2.483872000	0.609145000	1.578633000
H	-1.116485000	-0.304557000	-2.466475000

Ylide **A2**

HF=-955.0996732

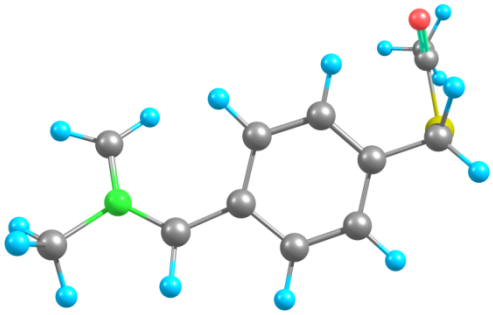


6	0.020382000	-0.004551000	0.003883000
6	0.043481000	0.112332000	1.403099000
16	1.605915000	0.149101000	2.262269000
6	1.560922000	-1.392890000	3.234802000
8	0.606528000	-2.128878000	3.284461000
6	2.864736000	-1.648916000	3.968651000
6	-1.183758000	0.002497000	-0.679037000
6	-2.432090000	0.103329000	-0.006755000
6	-3.608160000	0.134172000	-0.827233000
6	-2.381286000	0.224548000	1.405740000
1	-1.179009000	-0.084268000	-1.763214000
1	0.953056000	-0.103224000	-0.544168000
1	3.459519000	-0.740303000	4.095661000
1	3.453795000	-2.371366000	3.391227000
1	2.643047000	-2.092733000	4.943269000
6	-1.169217000	0.243246000	2.087571000
1	-1.167330000	0.356101000	3.167250000
1	-3.288235000	0.365670000	1.979048000
7	-4.908223000	0.014878000	-0.457267000
1	-3.467865000	0.266046000	-1.891647000
6	-5.877845000	0.379170000	-1.516958000
6	-5.444796000	-0.326508000	0.717348000
1	-5.493401000	0.049010000	-2.482628000
1	-6.016337000	1.462985000	-1.529875000

1	-6.828268000	-0.118542000	-1.322659000
1	-4.817444000	-0.681513000	1.515617000
1	-6.519715000	-0.338038000	0.804326000

Ylide **A3**

HF=-994.4175207



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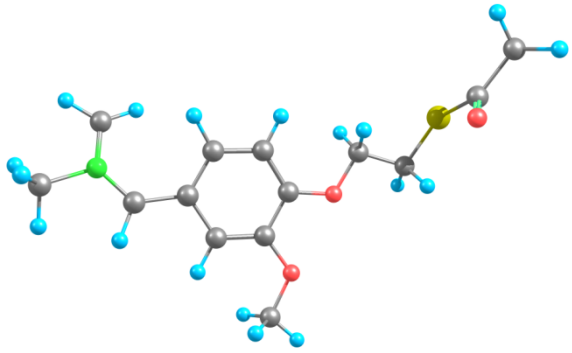
1	1.237530000	0.327592000	8.153230000
1	1.204218000	-1.368581000	8.680166000
1	1.013467000	-2.798725000	5.462287000
1	0.872636000	-3.026721000	7.319838000
7	0.819010000	-1.068317000	6.628449000
6	0.783919000	-0.058938000	5.724469000
6	0.620699000	-0.130895000	4.299270000
6	0.873568000	1.057323000	3.563096000
6	0.172679000	-1.249265000	3.551626000
6	0.001789000	-1.175894000	2.172460000
6	0.709906000	1.116987000	2.189196000
6	0.275519000	-0.001905000	1.459675000
6	0.724384000	-0.627782000	8.039562000
6	0.867831000	-2.392716000	6.447379000
1	-0.350159000	-2.051296000	1.632547000
1	-0.102206000	-2.169175000	4.051524000
1	1.205619000	1.943778000	4.099245000
1	0.921398000	2.048933000	1.668070000
1	0.901749000	0.923769000	6.160996000
16	1.594812000	-0.506120000	-0.999143000
1	1.738555000	-3.649107000	-2.784419000
1	2.733130000	-3.644633000	-1.318331000

1	2.953242000	-2.357076000	-2.525035000
8	0.092863000	-2.714914000	-0.954442000
6	1.142500000	-2.220992000	-1.309076000
6	2.216026000	-3.003279000	-2.041794000
1	-0.703186000	-0.589420000	-0.375232000
1	-0.078607000	1.076977000	-0.377034000

Ylide **I**

HF=-1223.4549502



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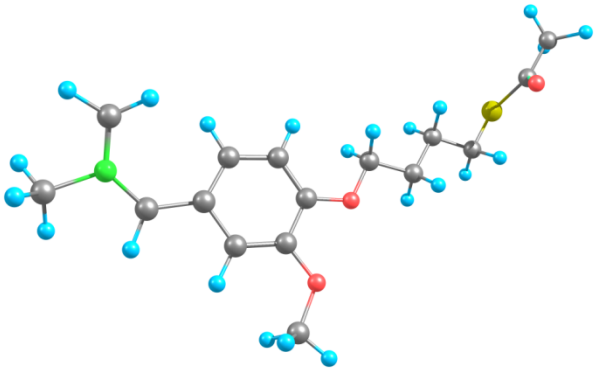
6	2.163158000	1.043486000	-0.205961000
6	1.790868000	2.127126000	0.580778000
6	3.493130000	0.985342000	-0.698856000
1	0.775952000	2.201942000	0.955521000
6	2.701701000	3.139170000	0.907609000
6	4.389109000	1.992551000	-0.379821000
8	3.782255000	-0.105428000	-1.468727000
1	-0.520068000	0.906788000	-0.464857000
6	-0.647033000	-1.242410000	-0.660524000
16	-2.375138000	-1.439441000	-0.091016000
6	-3.222807000	-0.417796000	-1.320338000
1	-0.105911000	-2.134376000	-0.334634000
1	-0.657179000	-1.208908000	-1.752267000
6	4.027137000	3.102831000	0.435610000
1	2.338685000	3.984339000	1.476752000
1	5.405552000	1.942889000	-0.754961000
6	5.089094000	-0.214663000	-2.000766000
6	5.041965000	4.103147000	0.644878000
1	5.099894000	-1.140640000	-2.579344000
1	5.330236000	0.628653000	-2.662497000

1	5.847289000	-0.274177000	-1.207628000
7	5.060860000	5.105434000	1.553087000
1	5.913992000	4.070089000	0.005813000
8	-2.640784000	0.149915000	-2.216673000
6	-4.719876000	-0.325894000	-1.101826000
1	-5.220781000	-0.351888000	-2.073679000
1	-4.945644000	0.638189000	-0.630844000
1	-5.101331000	-1.124952000	-0.460957000
6	6.124384000	6.111962000	1.337344000
6	4.230862000	5.369981000	2.572879000
1	6.986700000	5.634977000	0.871033000
1	6.423848000	6.527369000	2.300897000
1	5.750986000	6.909132000	0.689450000
1	3.480877000	4.652734000	2.855000000
1	4.448113000	6.225794000	3.192498000

Ylide **II**

HF=-1302.0835368



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6	0.227349000	0.060441000	-2.391400000
1	0.205744000	1.087010000	-2.767030000
1	-0.776512000	-0.363815000	-2.398266000
1	0.873508000	-0.547254000	-3.026768000
6	2.104839000	0.081931000	-0.934712000
1	2.582069000	0.298383000	0.004884000
1	2.658671000	0.111418000	-1.860461000
6	-1.105907000	0.301375000	2.197186000
6	-1.071423000	0.228243000	3.579900000
1	-2.017531000	0.615691000	1.700655000
6	0.120156000	-0.180796000	4.235648000
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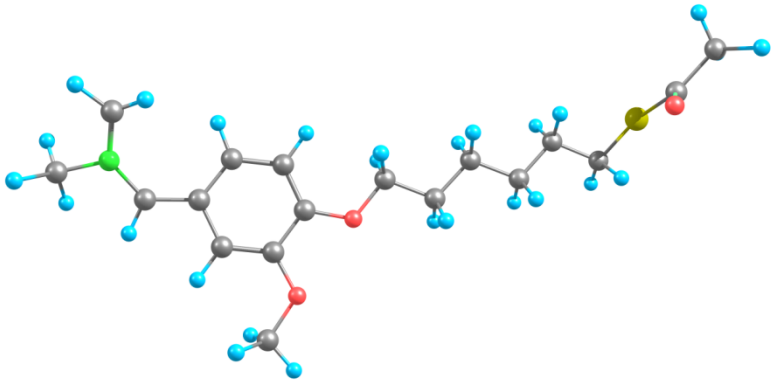
6	1.190513000	-0.425689000	2.061992000
6	1.225965000	-0.509650000	3.459510000
1	2.064000000	-0.748867000	1.512260000
1	2.143554000	-0.837132000	3.935556000
1	-1.185009000	0.141637000	-0.397608000
8	0.066959000	-0.214704000	5.600740000
6	-3.331179000	0.949748000	3.812498000
6	1.218543000	-0.655531000	6.307344000

1	-3.754806000	0.174619000	3.158824000
1	-4.018880000	1.138187000	4.639497000
1	-3.200886000	1.873517000	3.231907000
1	1.489418000	-1.674855000	5.991530000
1	2.074372000	0.000859000	6.087531000
6	0.884815000	-0.623931000	7.793907000
1	0.000197000	-1.251019000	7.964588000
1	0.604484000	0.400545000	8.068530000
6	2.055553000	-1.104717000	8.662419000
1	2.932828000	-0.469082000	8.493508000
1	2.339482000	-2.126428000	8.378404000
6	1.705999000	-1.068870000	10.151992000
1	0.848571000	-1.710948000	10.377645000
1	1.470879000	-0.049805000	10.471677000
16	3.059511000	-1.659790000	11.243967000
6	4.029485000	-0.143102000	11.372959000
6	5.300581000	-0.300825000	12.184439000
8	3.701124000	0.896097000	10.843858000
1	6.149110000	-0.375222000	11.493994000
1	5.287392000	-1.191160000	12.818309000
1	5.442382000	0.594260000	12.796849000

Ylide **III**

HF=-1380.7112605

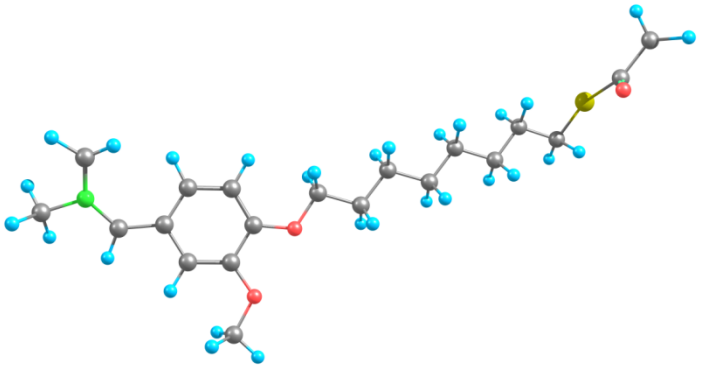


6	-0.370486000	0.099008000	-0.153524000
6	-0.066855000	0.012143000	1.251833000
7	0.485856000	0.122046000	-1.198722000
6	-0.157235000	0.155689000	-2.531766000
1	-0.213462000	1.188079000	-2.887367000
1	-1.156288000	-0.275166000	-2.468100000
1	0.441130000	-0.437198000	-3.225292000
6	1.827516000	0.166414000	-1.224680000
1	2.374473000	0.371664000	-0.321245000
1	2.307591000	0.216125000	-2.189923000
6	-1.130068000	0.314163000	2.150311000
6	-0.987461000	0.218290000	3.524665000
1	-2.078889000	0.632157000	1.731893000
6	0.252979000	-0.196054000	4.078901000
8	-1.967192000	0.500477000	4.434446000
6	1.151503000	-0.398643000	1.824156000
6	1.296080000	-0.505984000	3.213043000
1	1.980677000	-0.707899000	1.202430000
1	2.249075000	-0.836832000	3.610712000
1	-1.411083000	0.194109000	-0.433131000
8	0.306531000	-0.253824000	5.442579000
6	-3.225645000	0.922107000	3.944007000
6	1.508399000	-0.711375000	6.049691000

1	-3.694656000	0.154185000	3.313220000
1	-3.847917000	1.093548000	4.824794000
1	-3.145942000	1.855341000	3.369367000
1	1.751579000	-1.723081000	5.689777000
1	2.346046000	-0.050880000	5.777214000
6	1.292784000	-0.714456000	7.557694000
6	2.519803000	-1.218793000	8.327154000
1	0.421137000	-1.342483000	7.782479000
1	1.036767000	0.303642000	7.877659000
6	2.310207000	-1.234417000	9.847334000
1	3.389744000	-0.589237000	8.089818000
1	2.774848000	-2.233479000	7.987544000
1	1.436518000	-1.858818000	10.085666000
1	2.065123000	-0.219414000	10.190867000
6	3.535075000	-1.750822000	10.615600000
1	4.402531000	-1.116864000	10.396644000
1	3.786162000	-2.764394000	10.276523000
6	3.303657000	-1.760507000	12.128297000
1	2.463122000	-2.406634000	12.401782000
1	3.100465000	-0.751412000	12.498068000
16	4.735266000	-2.388892000	13.093438000
6	5.715632000	-0.878104000	13.202610000
6	7.046605000	-1.065776000	13.904590000
8	5.349747000	0.180859000	12.741299000
1	7.838098000	-1.109380000	13.147037000
1	7.082990000	-1.981490000	14.500263000
1	7.236930000	-0.196346000	14.540421000

Ylide **IV**

HF=-1459.338769



6	7.828571000	-0.665774000	-0.115992000
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6	4.743795000	1.411822000	0.186960000
1	6.859773000	1.716104000	0.266375000
6	3.694924000	0.466118000	0.034741000
8	4.340936000	2.704720000	0.369801000
7	8.446194000	-1.864649000	-0.029706000
6	9.915108000	-1.824360000	-0.209296000
1	10.404497000	-1.791670000	0.767881000
1	10.189081000	-0.948192000	-0.796726000
1	10.228148000	-2.722206000	-0.744481000
6	7.949750000	-3.082869000	0.239296000
1	6.942568000	-3.182439000	0.604182000
1	8.646112000	-3.905458000	0.294705000
1	8.504171000	0.172397000	-0.221256000
6	4.029286000	-0.869480000	-0.161078000
8	2.426340000	0.968398000	0.095382000
6	5.339910000	3.693777000	0.530273000
6	5.363652000	-1.293868000	-0.190254000
1	5.559981000	-2.336068000	-0.402369000
1	3.247244000	-1.609027000	-0.292579000
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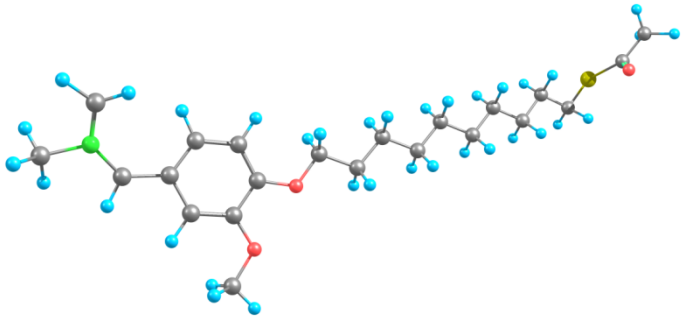

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Ylide **VI**

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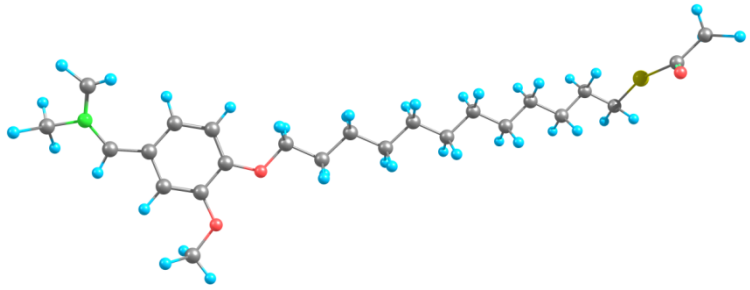

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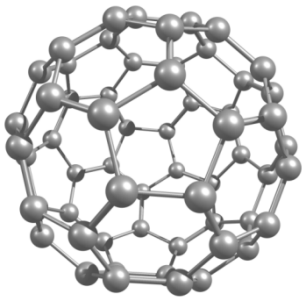

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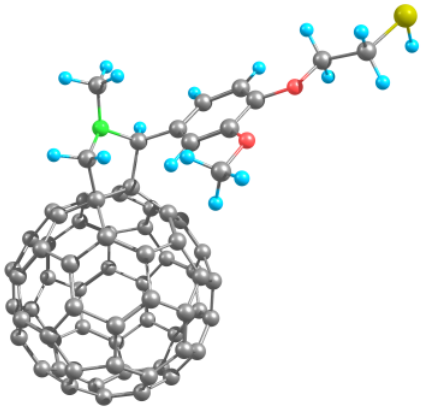

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Deprotected **II**

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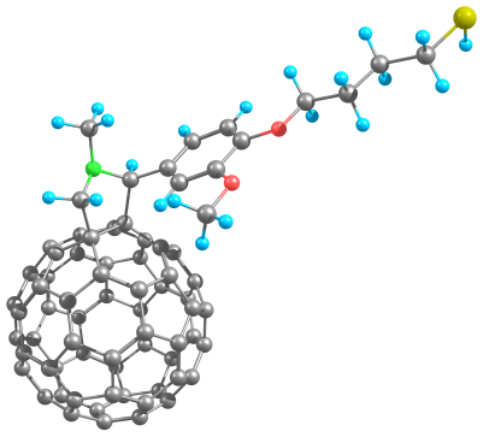

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6	0.449786000	-1.725075000	1.156600000
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6	0.856011000	-0.361321000	0.902705000
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6	0.263899000	0.486344000	1.963509000
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6	-1.089257000	-0.559874000	-3.243806000
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1	3.445436000	0.469771000	3.246226000

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Deprotected **III**

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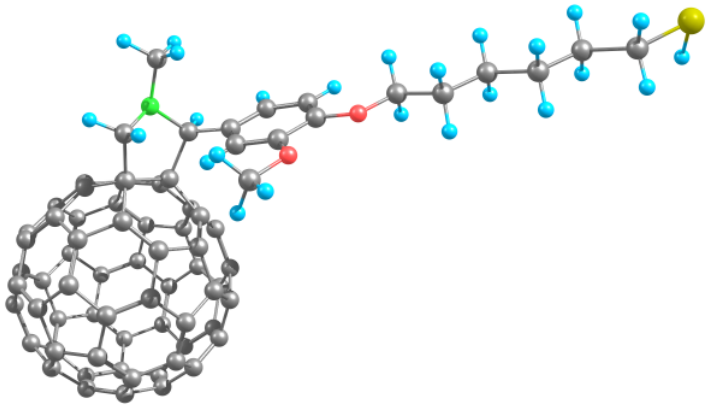

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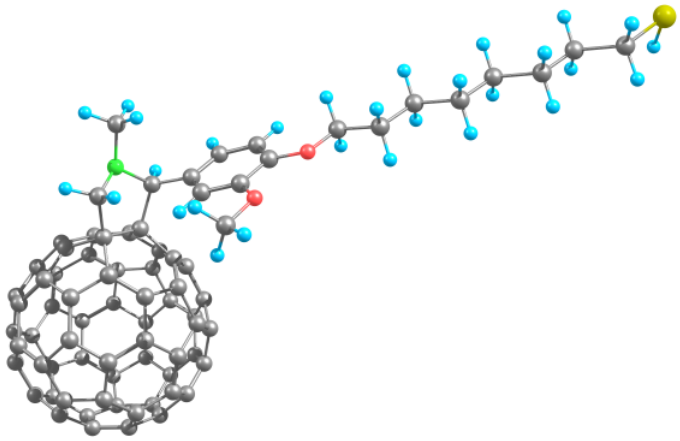
Deprotected **IV**

HF=-3592.9232137



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1	1.627987000	5.047933000	-2.181210000
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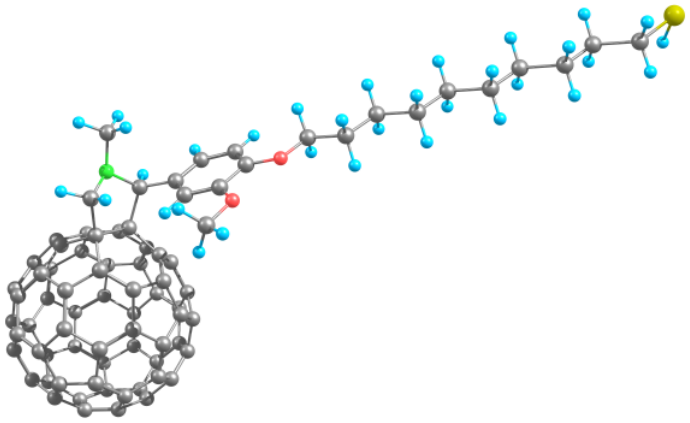
Deprotected **V**

HF=-3671.5507809



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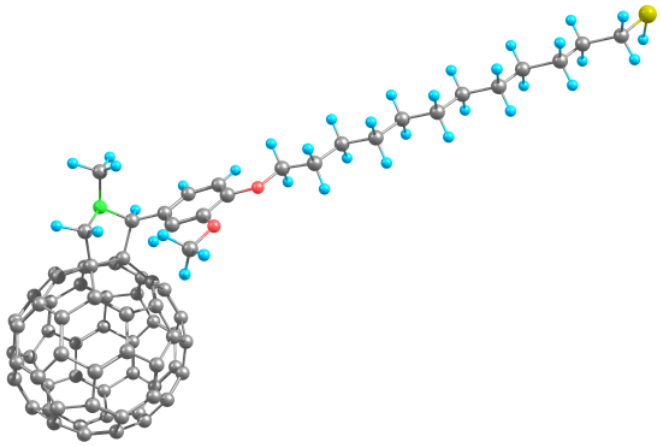
Deprotected **VI**

HF=-3750.1782389



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