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Chiral Gold Amides as Anticancer Drugs: Synthesis and Activity Studies

Sonya Newcombe[≠1], Mariusz Bobin[≠1,2], Amruta Shrikhande[≠1], Chris Gallop[2], Yannick Pace[1,2], Helen Yong[1], Rebecca Gates[1], Shuvashri Chaudhuri[1,2], M. Roe[2], Eddy M. E. Viseux[2], Eva Hoffmann[1]**

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Acknowledgements

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I. Experimental Procedures

All reagents and solvents were used without further purification from commercially available sources unless otherwise stated. Triflic amide was prepared using the procedure reported by Burdon *et. al.*[1] Dry diethyl ether and tetrahydrofuran were distilled from sodium/benzophenone under an atmosphere of nitrogen. Dichloromethane, toluene, triethylamine, and diisopropylamine were distilled from calcium hydride under atmosphere of nitrogen. Under anhydrous conditions, all apparatus was flame-dried before either cooling under reduced pressure (0.3 mmHg) or under a continuous flow of nitrogen or argon. Evaporation under reduced pressure was performed on a Büchi rotary evaporator, using a diaphragm pump. Reduced pressure was achieved by using a Leybold static oil pump (0.05 mmHg) unless otherwise stated. The IR spectra were recorded on spectrometer Perkin Elmer FT-IR Spectrum One equipped with a diamond top plate. Mass spectra were obtained using VG Autospec Magnetic Sector MS and Bruker Daltonic FT-ICR-MS Ape III instruments, using electron impact (EI) or fast atom bombardment (FAB). The ^{1}H nuclear magnetic resonance spectra were recorded on a Varian 400 (400 MHz) or Varian 500 (500 MHz). Chemical shifts are reported in parts per million (ppm) relative to residual $CHCl_3$ (δ 7.26 ppm), H_2O (δ 4.80 ppm), DMSO (δ 2.50 ppm), CH_3OH (δ 4.87 ppm). The following abbreviations are used to describe the multiplicity of given signals: s = singlet, d = doublet, t = triplet, q = quartet, quin = quintet, sex = sextet, sept = septet, m = multiplet and br = broad. Coupling constants, *J*, are given wherever appropriate in Hertz. The ^{13}C nuclear magnetic resonance spectra were recorded on a Varian 500 (126 MHz). Chemical shifts are reported in parts per million (ppm) relative to $CDCl_3$ (central line of triplet δ 77.00 ppm), DMSO (central line of septet δ 39.51 ppm), CD_3OD (central line of septet δ 49.15 ppm). The following abbreviations are used to describe the given signals: C = quaternary, CH = methane, CH_2 = methylene, CH_3 =methyl. The ^{31}P nuclear magnetic resonance spectra were recorded on a Varian 400 (162 MHz) and are referenced to 85% phosphoric acid in water (δ 0 ppm). The ^{19}F nuclear magnetic resonance spectra were recorded on a Varian 400 (376 MHz). The units for the reported $[\alpha]_D$ values are: $[\alpha] = deg cm^3 g^{-1} dm^{-1}$, $c = g cm^{-3}$. All reactions were monitored, where appropriate, by T.L.C. using Macherey-Nagel plates with a 0.2 mm layer of 60 F_{254} silica gel containing a fluorescent indicator. Visualization was achieved with U.V. light (254 mm) followed by an ethanolic solution of phosphomolibdic acid or aqueous solution of potassium permanganate. Flash column chromatography was carried out using Apollo Zeoprep 60 Hyd 35-70 micron silica gel. Petroleum ether (PET) usually refers to the fraction distilled narrow alkene hydrocarbons distillate fraction from crude oil in the 40 to 60 °C range, unless otherwise stated, and was distilled prior to use.

The ICP-MS (Agilent 7500ce) was operated in standard (i.e.no collision/reaction cell gas) mode. The conditions used are as follow: RF Power 1500W, Carrier Gas 0.8L/min, Spray Chamber temp. 2 °C. The instrument for Au was calibrated using an external calibration procedure: calibration solutions were prepared, typically containing 0 ng/ml Au, 50 ng/ml Au and 100 ng/ml Au, all diluted from a 1000ug/ml Au stock solution – dilutions were performed using ultra-pure water.

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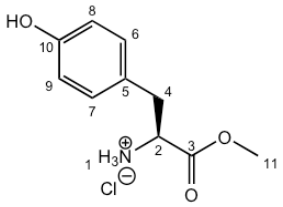
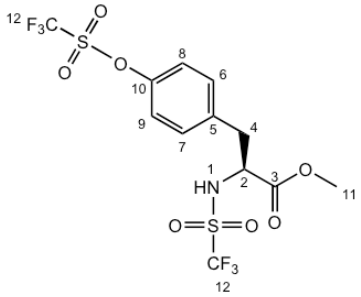


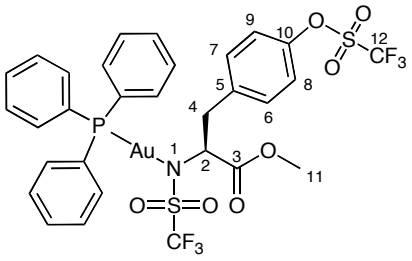
(2*S*)-3-(4-hydroxyphenyl)-1-methoxy-1-oxopropan-2-aminium chloride

Thionyl chloride (0.48 mL, 6.62 mmol) was added dropwise to a solution of *L*-tyrosine (0.60 g, 3.31 mmol) in methanol (22 mL). The reaction was heated to reflux with vigorous stirring for 24 h. After cooling, the reaction mixture was concentrated under reduced pressure and the residual methanol removed by azeotropic distillation with dichloromethane (10 mL) under reduced pressure to give the title compound as a white solid (0.65 g, 84%). **$[\alpha]_D^{23.0}$** = −4.7 (*c* = 1.00, water); **^{1}H NMR (500 MHz, D_2O)** δ = 7.08 (2H, d, *J*=7.7, 6, 7-H), 6.83 (2H, d, *J*=7.7, 8, 9-H), 4.31 (1H, t, *J*=5.9, 2-H), 3.76 (3H, s, 11-H), 3.24 – 3.02 (2H, m, 4-H); **^{13}C NMR (126 MHz, D_2O)** δ = 170.1 (3-C), 155.2 (10-C), 130.8 (6, 7-CH), 125.4 (5-C), 116.0 (8, 9-CH), 54.2 (2-CH), 53.5 (11-CH_3), 34.8 (4-CH_2); **IR (diamond, ν_{MAX}, cm^{-1})** 3335 (NH st), 2877 (N^+-H st), 1983 (Ar comb), 1741 (C=O st), 1225 (CO-O st as), 1199 (C-O st as); **Acc. Mass (FAB)** $C_{10}H_{14}NO_3$ *Found: 196.0962 m/z, Calculated: 196.0968 m/z.*



(*S*)-methyl 3-(4-(((trifluoromethyl)sulfonyl)oxy)phenyl)-2-(trifluoromethylsulfonamido)propanoate

Triflic anhydride (0.56 mL, 3.31 mmol) in dichloromethane (3.3 mL) was added dropwise to a solution of (2*S*)-3-(4-hydroxyphenyl)-1-methoxy-1-oxopropan-2-aminium chloride (0.767 g, 3.31 mmol) and triethylamine (1.38 mL, 9.93 mmol) in dichloromethane (12.8 mL) at −78 °C. The mixture was stirred for 24 h. at room temperature. Water (5 mL) was added and the pH adjusted to pH=5 using 32% hydrochloric acid. The aqueous layer was extracted with diethyl ether. The organics extracts were combined, dried over anhydrous magnesium sulfate, filtered and concentrated under reduced pressure. Purification by column chromatography (diethyl ether) afforded the title compound as yellow solid (0.704 g, 49%). **X-Ray**: see appendix (The compound was recrystallised by slow evaporation of diethyl ether at room temperature). **$[\alpha]_D^{25.5}$** = 17.1 (*c* = 1.00, dichloromethane); **^{1}H NMR (500 MHz, $CDCl_3$)** δ = 7.29 – 7.22 (4H, m, 6, 7, 8, 9-H), 4.49 (1H, t, *J*=6.0, 1H, 2-H), 3.78 (3H, s, 11-H), 3.23 – 3.13 (2H, m, 4-H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ = 170.4 (3-C), 149.2 (10-C), 134.8 (5-C), 131.3 (6, 7-CH), 123.1 (12-CF), 121.8 (8, 9-CH), 120.6 (12-CF), 120.0 (12-CF), 118.0 (12-CF), 117.4 (12-CF), 115.8 (12-CF), 57.7 (2-CH), 53.2 (11-CH_3), 38.9 (4-CH_2); **IR (diamond, ν_{MAX}, cm^{-1})** 3349 (O-H st), 3221 (NH st), 2176 (Ar comb), 1724 (C=O st), 1238 (CO-O st), 1199 (S-O st as), 1141 (S-O st sy); **Acc. Mass (FAB)** $C_{14}H_{10}F_6NO_7S_2$ *Found: 481.9778 m/z, Calculated: 481.9797 m/z.*



Triphenylphosphine gold (*S*)-methyl 3-(4-(((trifluoromethyl)sulfonyl)oxy)phenyl)-2-(trifluoromethylsulfonamido)propanoate

Silver carbonate (42.1 mg, 0.153 mmol) was added to a solution of (*S*)-methyl 3-(4-(((trifluoromethyl)sulfonyl)oxy)phenyl)-2-(trifluoromethylsulfonamido)propanoate (50 mg, 0.153 mmol) in dichloromethane (3.82 mL) and stirred for 5 min. under an atmosphere of nitrogen. Triphenylphosphine gold chloride (75.6 mg, 0.153 mmol) was added and stirred for 1.5 h. The reaction mixture was filtered through Celite and the filtrate concentrated under reduced pressure to give the corresponding compound as white solid (1.548 g, 90% from **^{1}H NMR** based on CH_3 peak). **X-Ray**: see appendix (The complex (30 mg, 0.033 mmol) was recrystallised from dichloromethane (0.1 mL) into pentane (0.4 mL) at -25 °C (a few crystals)). (The pure complex for these experiments were obtained by extracting trilenylphosphine gold chloride from acetone and then recrystallization of the desired complex in diethyl ether at -25 °C (see NMR)). **$[\alpha]_D^{23.9}$** = 2.0 (*c* = 1.00, dichloromethane); **^{1}H NMR (500 MHz, $CDCl_3$)** δ = 7.52 – 7.44 (15H, m, Ar), 7.27 (2H, d, *J*=9.6, 6, 7-H), 7.00 (2H, d, *J*=8.6, 2H, 8, 9-H), 4.91 (1H, m, 2-H), 3.67 (3H, s, 11-H), 3.26 – 3.16 (2H, m, 4-H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ = 170.8 (3-C), 148.4 (10-Ar), 137.0 (5-Ar), 134.2 (Ar), 134.1 (Ar), 132.01 (Ar), 132.01 (Ar), 131.6 (6, 7-Ar), 129.4 (Ar), 129.3 (Ar), 128.9 (Ar), 128.4 (Ar), 121.1 (8, 9-Ar), 61.5 (2-CH), 52.1 (11-CH_3), 41.7 (4-CH_2); **^{31}P NMR (162 MHz, $CDCl_3$)** δ = 31.30 (s); **IR (diamond, ν_{MAX}, cm^{-1})** 2956 (O-H st), 2073 (Ar comb), 1738 (C=O st), 1249 (CO-O st), 1176 (S-O st as), 1137 (S-O st sy); **Acc. Mass (FAB)** $C_{30}H_{25}AuF_6NO_7PS_2$ *Found: 940.0383 m/z, Calculated: 940.0272 m/z.*

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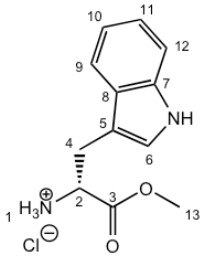
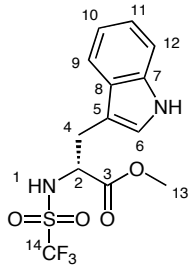


(2*R*)-3-(1*H*-indol-3-yl)-1-methoxy-1-oxopropan-2-aminium chloride

Thionyl chloride (0.72 mL, 9.87 mmol) was added dropwise to a solution of *D*-tryptophan (1.000 g, 4.89 mmol) in methanol (33 mL). The reaction was heated to reflux with vigorous stirring for 24 h. After cooling, the reaction mixture was concentrated under reduced pressure and residual methanol traces removed by azeotropic distillation with dichloromethane (10 mL) under reduced pressure to give the title compound as a white solid (1.070 g, 86%). **$[\alpha]_D^{22.8}$** = −15.2 (*c* = 1.00, water); **^{1}H NMR (500 MHz, D_2O)** δ = 7.52 (1H, d, *J*=7.9, 9-H), 7.46 (1H, d, *J*=8.1, 12-H), 7.26 – 7.10 (3H, m, 4, 5, 9-H), 4.37 (1H, t, *J*=6.0, 2-H), 3.73 (3H, s, 13-H), 3.44 – 3.31 (2H, m, 4-H); **^{13}C NMR (126 MHz, D_2O)** δ = 170.4 (2-C), 136.3 (7-C), 126.4 (8-C), 125.4 (6-C), 122.3 (11-CH), 119.6 (10-CH), 118.1 (9-CH), 112.1 (12-CH), 106.0 (5-C), 53.6 (13-CH_3), 53.3 (2-CH), 25.7 (4-CH_2); **IR (diamond, ν_{MAX}, cm^{-1})** 3261 (NH st), 2870 (N^+-H st), 2023 (Ar comb), 1748 (C=O st), 1229, 1211 (CO-O st as), 1181 (C-O st as); **Acc. Mass (FAB)** $C_{12}H_{15}N_2O_2$ *Found: 219.1120 m/z, Calculated: 219.1128 m/z.*



Methyl *N*-[(trifluoromethyl)sulfonyl]-*D*-tryptophanate

Triflic anhydride (0.83 mL, 4.89 mmol) in dichloromethane (4.9 mL) was added dropwise to a solution of (2*R*)-3-(1H-indol-3-yl)-1-methoxy-1-oxopropan-2-aminium chloride (1.073 g, 4.89 mmol) and triethylamine (2.05 mL, 14.69 mmol) in dichloromethane (18.9 mL) at −78 °C. The mixture was stirred for 24 h. at room temperature. Water (5 mL) was added and the pH was adjusted to pH=5 using 32% hydrochloric acid. The aqueous layer was extracted with diethyl ether. The organic extracts were combined, dried over anhydrous magnesium sulfate, filtered and concentrated under reduced pressure. Purification by column chromatography (diethyl ether) afforded the title compound as brown-yellow solid (1.548 g, 90%). **$[\alpha]_D^{25.5}$** = −31.8 (*c* = 1.00, dichloromethane); **^{1}H NMR (500 MHz, $CDCl_3$)** δ = 8.17 (1H, s,1-NH), 7.52 (1H, d, *J*=7.9, 9-H), 7.37 (1H, d, *J*=8.1, 12-H), 7.24 – 7.19 (1H, m, 10-H), 7.17 – 7.12 (1H, m, 11-H), 7.04 (1H, d, *J*=2.3, 1H, 6-H), 8.17 (1H, s, NH) 4.57 (1H, t, *J*=5.0, 1H, 2-H), 3.71 (3H, s, 13-H), 3.38 (2H, m, 4-H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ = 170.7 (3-C), 136.2 (7-C), 127.1 (8-C), 125.1 (14-CF), 124.6 (14-CF), 123.5 (6-CH), 123.3 (14-CF), 122.5 (11-CH), 120.7 (14-CF), 120.0 (10-CH), 118.3 (9-CH), 118.2 (14-CF), 111.4 (12-CH), 108.0 (5-C), 57.4 (2-CH), 53.0 (13-CH_3), 29.3 (4-CH_2); **IR (diamond, ν_{MAX}, cm^{-1})** 3402.9 (ar NH st), 3261.5 (NH st), 2197.0, 2157.2, 1031.4 (Ar comb), 1712.6 (C=O st), 1230.6 (CO-O st),1185.0 (S-O st as), 1145.5 (S-O st sy); **Acc. Mass (FAB)** $C_{13}H_{13}F_3N_2O_4SNa$ *Found: 373.0446 m/z, Calculated: 373.0440 m/z.*

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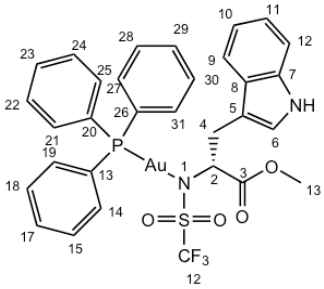
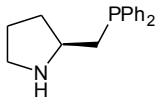


Triphenylphosphine gold methyl *N*-[(trifluoromethyl)sulfonyl]-*D*-tryptophanate

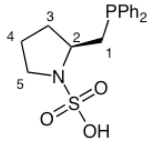
Silver carbonate (38.6 mg, 0.143 mmol) was added to a solution of Methyl *N*-[(trifluoromethyl)sulfonyl]-*D*-tryptophanate (50 mg, 0.143 mmol) in dichloromethane (3.6 mL) and stirred for 5 min. under an atmosphere of nitrogen. Triphenylphosphine gold chloride (70.6 mg, 0.143 mmol) was added and stirred for 1.5 h. The reaction was filtered through Celite and the solvent evaporated under reduced pressure to give the corresponding compound as pale yellow solid (0.115 g, 90% from **^{1}H NMR** based on CH_3 peak). **X-Ray**: see appendix (The complex (30 mg, 0.038 mmol) was recrystallised by slow diffusion of chloroform (0.1 mL) into benzene (0.4 mL) at +5 °C to get pure compound for experiments (see NMR)). **$[\alpha]_D^{23.7}$** = −42.5 (*c* = 1.00, dichloromethane); **^{1}H NMR (500 MHz, $CDCl_3$)** δ = 7.58 – 6.97 (20H m, Ar), 5.06 (1H, q, *J*=6.1, 2-H), 3.65 (3H, s, 13-H), 3.39 (2H, ddd, *J*=5.7, 14.7, 21.2, 4-H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ = 174.1 (3-C), 135.9 (7-C), 134.2 (Ar), 134.10 (Ar), 131.7 (Ar), 129.1 (Ar), 129.0 (Ar), 128.6 (Ar), 127.8 (8-CH), 123.7 (6-CH), 122.0 (11-CH), 119.4 (10-CH), 119.0 (9-CH), 111.1 (12-CH), 110.5 (5-C), 60.8 (2-CH), 52.0 (13-CH_3), 31.7 (4-CH); **^{31}P NMR (162 MHz, $CDCl_3$)** δ = 31.01 (s); **IR (diamond, ν_{MAX}, cm^{-1})** 3398 (ar NH st), 2180 (Ar comb),

1738 (C=O st), 1212 (CO-O st), 1176 (S-O st as), 1101 (S-O st sy); **Acc. Mass (FAB)** $C_{31}H_{27}AuF_3N_2O_4PSNa$ *Found: 831.0944 m/z, Calculated: 831.0939 m/z.*



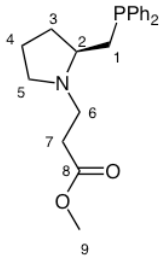
(*L*)-(-).2-[(Diphenylphosphino)methyl]pyrrolidine

Deoxygenated 32% HCl (2 mL) was added to a round bottomed flask containing (*S*)-2-((diphenylphosphino)methyl)pyrrolidine-1-sulfonic acid (100 mg, 0.30 mmol) under an atmosphere of nitrogen and stirred for 16 h. at 85 °C. After cooling, the pH was adjusted to pH=12 using potassium hydroxide and extracted with dichloromethane (3x7 mL). The reaction was concentrated under reduced pressure to give the title compound as yellow oil (53 mg, 65%). All data is identical to that reported: Tomioka *Tetrahedron .Lett*. **1999**. *55*. 3843



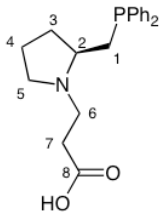
(*S*)-2-((diphenylphosphino)methyl)pyrrolidine-1-sulfonic acid

(*S*)-hexahydropyrrolo[1,2-*b*]isothiazole 1,1-dioxide (0.850 g, 5.21 mmol) was added to a solution of diphenylphosphinelithium (5.21 mmol) in dry tetrahydrofuran (12.4 mL). The reaction was stirred for 3 h. and then quenched with 8 mL of water. The crude residue was extracted with dichloromethane (3x10 mL). The organic layers were combined and concentrated under reduced pressure. Purification by column chromatography (methanol : dichloromethane, [10:90]) afforded the title compound as white solid (1.648 g, 91%). **^{1}H NMR (500 MHz, $CDCl_3$)** δ = 7.94 – 6.95 (10H, m, Ar), 3.76 (1H, s, 2-H), 3.32 – 2.80 (3H, m, 1, 5-H), 2.03 (1H, s, 1-H), 1.77 (1H, s, 3-H), 1.52 (3H, s, 3, 4-H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ = 139.1 (s, Ar), 139.0 (s, Ar), 132.8 (s, Ar), 132.6 (s, Ar), 128.5 (s, Ar), 128.4 (s, Ar), 128.4 (s, Ar), 128.3 (s, Ar), 128.3 (s, Ar), 58.8 (d, *J*=21.0, 2-CH), 50.2 (s, 5-CH_2), 35.6 (s, 1-CH_2), 32.0 (s, 3-CH_2), 24.3 (s, 4-CH_2); **^{31}P NMR (243 MHz, $CDCl_3$)** δ = −21.26 (s); **IR (diamond, ν_{MAX}, cm^{-1})** 1433 (H-C-H st as), 1174 (-SO_3^- st as), 1041 (-SO_3^- st sy); **Acc. Mass (FAB):** $C_{17}H_{20}NaNO_3PS$ *Found: 372.0803 m/z Calculated: 372.0794 m/z.*



Methyl 3-{(2*S*)-2-[(diphenylphosphino)methyl]pyrrolidin-1-yl} propanoate

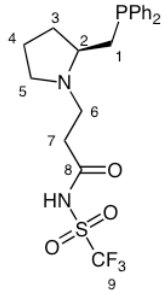
Methyl-3-bromopropionate (1.0 mL, 9.28 mmol) in dichloromethane (8.0 mL) was added dropwise to a solution of triethylamine (2.61 mL, 18.57 mmol) and (2*S*)-2-[(diphenylphosphino)methyl]pyrrolidine (2.50 g, 9.28 mmol) in dichloromethane (27 mL). The resultant solution was stirred at 30 °C for 18 h. The reaction mixture was poured into water/dichloromethane (1:1, 200 mL). The aqeous phase was extracted with dichloromethane (100 mL) and the combined organic phases washed with water (100 mL) and brine (100 mL); dried over anhydrous sodium sulfate, filtered and concentrated under reduced pressure. Purification by column chromatography (methanol : dichloromethane, [5:95]) afforded the title compound as a yellow cloudy viscous oil (1.57 g, 47%). **$[\alpha]_D^{25.5}$** = −78.2 (*c* = 1.00, dichloromethane); **^{1}H NMR (500 MHz, $CDCl_3$)** δ = 7.50 – 7.39 (4H, m, Ar), 7.37 – 7.28 (6H, m, Ar), 3.66 (3H, s, 9-H), 3.19 – 3.03 (2H, m, 5, 6-H), 2.54 (1H, dt, *J*=3.3, 13.3, 4-H), 2.49 – 2.29 (4H, m, 6, 7-H), 2.15 – 2.06 (1H, m, 5-H), 2.06 – 1.91 (2H, m, 1, 3-H), 1.83 – 1.53 (3H, m, 3, 4-H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ = 172.7 (s, 8-C), 139.3 (d, *J*=12.1, Ar), 138.5 (d, *J*=13.3, Ar), 133.0 (d, *J*=19.3, Ar), 132.6 (d, *J*=18.7, Ar), 128.7 (s, Ar), 128.5 (s, Ar), 128.4 (s, Ar), 128.4 (s, Ar), 128.3 (s, Ar), 128.3 (s, Ar), 62.1 (d, *J*=19.3, 2-CH), 53.4 (d, *J*=0.8, 5-CH_2), 51.5 (s, 9-CH_3), 49.1 (s, 6-CH_2), 33.6 (d, *J*=13.3, 1-CH_2), 33.5 (s, 7-CH_2), 31.7 (d, *J*=7.8, 3-CH_2), 22.1 (d, *J*=0.6, 4-CH_2); **^{31}P NMR (162 MHz, $CDCl_3$)** δ = −21.19 (s); **IR (diamond, ν_{MAX}, cm^{-1})** 2961, 2802 (CH_3O st), 1735 (C=O st), 1433 (H-C-H st as), 1175 (C-O st as); **Acc. Mass (FAB)** $C_{21}H_{27}NO_2P$ *Found: 356.1778, Calculated: 356.1774.*



3-{(2*S*)-2-[(diphenylphosphino)methyl]pyrrolidin-1-yl}propanoic acid

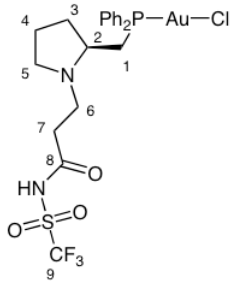
1N sodium hydroxide (34.3 mL) was added to methyl 3-{(2*S*)-2-[(diphenylphosphino)methyl]pyrrolidin-1-yl}propanoate (0.50 g, 1.41 mmol) in

methanol (22.9 mL). After stirring for 20 h. at room temperature the reaction mixture was neutralized with 32% hydrochloric acid (3.5 mL). The resulting solution was lyophilized. The crude product was dissolved in methanol and the insoluble salts were removed by filtration. The resultant solution was dried over anhydrous magnesium sulfate, filtered and concentrated under reduced pressure to give the corresponding compound as a yellow and cloudy viscous oil (0.57 g, 100%). **$[\alpha]_D^{25.8}$** = −40.0 (*c* = 1.00, dichloromethane); **^{1}H NMR (500 MHz, $CDCl_3$)** δ = 7.40 (10H, m, Ar), 3.70-3-80 (1H, m, 5-H), 3.61 – 3.49 (1H, m, 7-H), 3.06 – 2.72 (6H, m, 1, 6, 7, 5-H), 2.64 (1H, t, *J*=12.1, 1-H), 2.24 – 1.82 (m, 4H, 3, 4-H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ = 173.2 (s, 8-C), 136.8 (d, *J*=11.3, Ar), 136.1 (d, *J*=12.7, Ar), 133.0 (d, *J*=20.2, Ar), 132.5 (d, *J*=19.2, Ar), 129.6 (s, Ar), 129.1 (s, Ar), 128.9 (d, *J*=7.3, Ar), 128.7 (d, *J*=6.9, Ar), 66.9 (d, *J*=23.2, 2-CH), 52.8 (s, 5-CH_2), 49.4 (s, 7-CH_2), 31.1 (s, 6-CH_2), 30.5 (d, *J*=7.4, 3-CH_2), 29.6 (d, *J*=16.2, 1-CH_2), 21.7 (s, 4-CH_2); **^{31}P NMR (162 MHz, $CDCl_3$)** δ = −20.61 (s), 30.40 (s, P=O, 5%); **IR (diamond, ν_{MAX}, cm^{-1})** 2956, 2547 (HO st), 1720 (C=O st), 1432 (H-C-H st as); **Acc. Mass (FAB)** $C_{20}H_{25}NO_2P$ *Found: 342.1608 m/z, Calculated: 342.1617 m/z.*



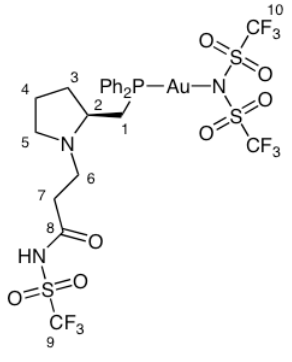
3-{(2*S*)-2-[(diphenylphosphino)methyl]pyrrolidin-1-yl}-*N*-[(trifluoromethyl)sulfonyl]propanamide

3-{(2*S*)-2-[(diphenylphosphino)methyl]pyrrolidin-1-yl}propanoic acid (0.50 g, 1.46 mmol), triflic amide (0.218 g, 1.46 mmol) and HOBt∗H_2O (0.224 g, 1.46 mmol) were dissolved in dichloromethane (3.85 mL) and cooled to 0 °C under an atmosphere of nitrogen. EDC (0.233 g, 1.50 mmol) was added and the mixture stirred for 15 min at 0 °C and then at room temperature for 18 h. The precipitate was removed by filtration and the filtrate concentrated under reduced pressure. The residue was dissolved in dichloromethane (20 mL) and washed with 1M citric acid (20 mL), saturated sodium bicarbonate (20 mL), brine (20 mL) and dried over anhydrous magnesium sulfate, filtered and concentrated under reduced pressure. Purification by column chromatography (methanol:dichloromethane, [5:95]) afforded the title compound as white solid (0.34 g, 49%). **X-Ray:** see appendix (The complex (30 mg, 0.062 mmol) was recrystallised from chloroform or benzene at room temperature). **$[\alpha]_D^{25.7}$** = −27.7 (*c* = 1.00, dichloromethane); **^{1}H NMR (500 MHz, $(CD_3)_2SO$)** δ = 7.55 – 7.32 (10H, m, Ar), 3.75 – 3.45 (2H, m, 5, 6-H), 3.22 (1H, s, 2-H,), 3.11 – 2.89 (3H, m, 1 ,5 ,6-H), 2.55 – 2.45 (2H, m, 7-H), 2.28 (1H, t, *J*=12.1, 1-H), 2.07 (1H, m, 3-H), 1.94 – 1.77 (2H, m, 4-H), 1.67 (1H, m, 3-H); **^{13}C NMR (126 MHz, $(CD_3)_2SO$)** δ = 174.3 (s, 8-C), 137.3 (d, *J*=12.2, Ar), 136.2 (d, *J*=13.2, Ar), 132.7 (d, *J*=19.9, Ar), 132.4 (d, *J*=19.6, Ar), 129.2 (d, *J*=33.7, Ar), 128.8 (d, *J*=7.1, Ar), 128.6 (d, *J*=7.0, Ar), 124.1 (s, 9-CF), 121.5 (s, 9-CF), 118.9 (s, 9-CF), 116.4 (s, 9-CF), 66.1 (d, *J*=23.5, 2-CH), 52.8 (s, 5-CH_2), 49.6 (s, 6-CH_2), 34.3 (s, 7-CH_2), 30.1 (s, 3-CH_2), 28.9 (d, *J*=13.0, 1-CH_2), 21.4 (s, 4-CH_2); **^{31}P NMR (162 MHz, DMSO)** δ = −21.76 (s); **^{19}F NMR (376 MHz, $(CD_3)_2SO$)** δ = −77.71 (s); **IR (diamond, ν_{MAX}, cm^{-1})** 3052, 2967 (NH st), 2192 (Ar comb), 1598 (C=O st amide), 1431 (H-C-H st as), 1176 (S-O st as), 1123 (S-O st sy); **Acc. Mass (FAB)** $C_{21}H_{24}F_3N_2NaO_3PS$ *Found: 495.1117 m/z, Calculated: 495.1090 m/z;*



3-{(2*S*)-2-[(diphenylphosphino)methyl]pyrrolidin-1-yl}-*N*-[(trifluoromethyl)sulfonyl]propanamide gold chloride

3-{(2*S*)-2-[(diphenylphosphino)methyl]pyrrolidin-1-yl}-*N*-[(trifluoromethyl) sulfonyl]propanamide (50 mg, 0.106 mmol) was dissolved in dry dichloromethane (1 mL) under an atmosphere of nitrogen. Dimethyl sulfide gold chloride (31 mg, 0.106 mmol) was added in one portion and the resultant mixture stirred for 3 h. Concentration of the reaction mixture under reduced pressure afforded the title compound as a white solid (70 mg, 94%). **$[\alpha]_D^{26.1}$** = −12.3 (*c* = 1.00, dichloromethane); **^{1}H NMR (500 MHz, $CDCl_3$)** δ = 7.92 (2H, dd, *J*=7.1, 13.6, Ar), 7.80 (2H, dd, *J*=7.1, 13.4, Ar), 7.59 – 7.42 (6H, m, Ar), 4.26 (1H, m, 5-H), 3.86 – 3.58 (2H, m, 6-H), 3.53 – 3.37 (2H, m, 1-H), 3.02 – 2.90 (2H, m, 5,6-H), 2.83 – 2.55 (2H, m, 7-H), 2.19 – 1.91 (3H, m, 3,4-H), 1.80 – 1.67 (1H, m, 3-H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ = 175.6 (s, 8-C), 134.1 (d, *J*=14.3, Ar), 133.1 (d, *J*=13.6, Ar), 132.6 (dd, *J*=2.1, 52.4, Ar), 129.5 (dd, *J*=6.8, 12.1, Ar), 128.6 (d, *J*=63.1, Ar), 127.9 (d, *J*=61.7, Ar), 124.12(s, 9-CF), 121.5 (s, 9-CF), 119.0 (s, 9-CF), 116.4 (s, 9-CF), 67.7 (s, 2-CH), 54.6 (s, 5-CH_2), 52.3 (s, 6-CH_2), 34.5 (s, 7-CH_2), 30.4 (s, 3-CH_2), 29.1 (d, *J*=38.9, 1-CH_2), 21.9 (s, 4-CH_2); **^{31}P NMR (162 MHz, $CDCl_3$)** δ = 26.38 (s); **^{19}F NMR (376 MHz, $CDCl_3$)** δ = −78.34 (s); **IR (diamond, ν_{MAX}, cm^{-1})** 3055 (NH st), 2191 (Ar comb), 1610 (C=O st amide), 1437 (H-C-H st as), 1173 (S-O st as), 1124 (S-O st sy); **Acc. Mass (FAB)** $C_{21}H_{24}AuClF_3N_2NaO_3PS$ *Found: 727.0440 m/z, Calculated: 727.0444 m/z.*



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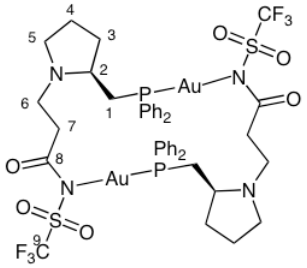
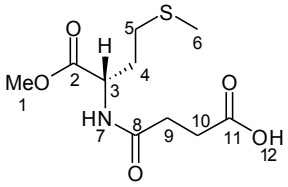
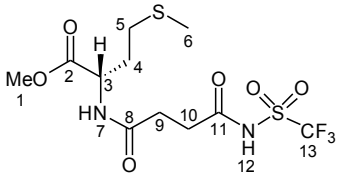
3-{(2*S*)-2-[(diphenylphosphino)methyl]pyrrolidin-1-yl}-*N*-[(trifluoromethyl)sulfonyl]propanamide gold bis(trifluoromethanesulfonate)
Bistriflic amide (26 mg, 0.092 mmol) and silver carbonate (25.5 mg, 0.092 mmol) in dry dichloromethane (2 mL) was stirred for 5 min. under an atmosphere of nitrogen. Triphenylphosphine gold chloride (65.2 mg, 0.092 mmol) in dichloromethane (0.31 mL) was added and stirred for 2 h. excluding light. The mixture was filtered through Celite and concentrated under reduced pressure to give the title compound as an off white solid with (70.5 mg, 80%). **$[\alpha]_D^{26.1}$** = −23.6 (*c* = 1.00, dichloromethane); **^{1}H NMR (500 MHz, CDCl$_3$)** δ = 8.17 – 6.96 (10H, m, Ar), 4.33 -2.89 (9H, m, 1,5,6,7-H), 2.22 – 1.75 (3H, m, 3,4-H), 1.47 – 1.21 (1H, m, 3-H); **^{13}C NMR (126 MHz, CDCl$_3$)** δ = 174.8 (s, C-8), 134.9 (d, *J*=14.0, Ar), 133.8 (s, Ar), 132.2 (s, Ar), 131.7 (d, *J*=12.2, Ar), 130.0 (s, Ar), 129.6 (s, Ar), 129.4 (d, *J*=11.7, Ar), 123.4 (s, CF), 120.9 (s, CF), 118.3 (s, CF), 115.7 (s, CF), 64.4 (s, 2-CH), 52.8 (s, 5-CH_2), 44.9 (s, 6-CH_2), 29.5, 29.1 (s, 1, 3, 7-CH_2), 20.8 (s, 4-CH_2); **^{31}P NMR (162 MHz, CDCl$_3$)** δ = 26.78 (s); **^{19}F NMR (376 MHz, CDCl$_3$)** δ = −76.56 (s), −78.68 (s). **IR (diamond, ν_{MAX}, cm^{-1})** 2178 (Ar comb), 1669 (C=O st amide), 1439 (H-C-H st as), 1178 (S-O st as), 1128 (S-O st sy).



bis(3-{(2*S*)-2-[(diphenylphosphino)methyl]pyrrolidin-1-yl}-*N*-[(trifluoromethyl)sulfonyl]propanamide) di-gold
3-{(2*S*)-2-[(diphenylphosphino)methyl]pyrrolidin-1-yl}-*N*-[(trifluoromethyl)sulfonyl] propanamide (100 mg, 0.212 mmol) was dissolved in dry dichloromethane (2.1 mL) in a flame dried flask, under an atmosphere of nitrogen. Dimethyl sulfide gold chloride (62 mg, 0.212 mmol) was added in one portion and the mixture stirred for 15 min. Silver carbonate (58 mg, 0.212 mmol) was added in one portion and the resultant mixture stirred for 18 h. The reaction mixture was filtered through Celite and concentrated under reduced pressure to give the title compound as a yellow solid (139 mg, 98%). **X-Ray:** see appendix (The complex (30 mg, 0.023 mmol) was recrystallised by slow diffusion of dichloromethane (0.2 mL) into benzene (0.3 mL) at +5 °C with slow evaporation). **$[\alpha]_D^{23.5}$** = −21.2 (*c* = 1.00, dichlorometahne); **^{1}H NMR (500 MHz, CDCl$_3$)** δ = 7.91 – 7.37 (10H m, Ar), 3.36 – 1.23 (13H m, 1-7-H); **^{13}C NMR (126 MHz, CDCl$_3$)** δ = 176.6 (s, 8-C), 133.6 (s, Ar), 133.0 (s, Ar), 132.2 (s, Ar), 129.9 (s, Ar), 129.4 (s, Ar), 129.3 (s, Ar), 125.4 (s, 9-CF), 122.1 (s, 9-CF), 118.7 (s, 9-CF), 115.5 (s, 9-CF), 61.8 (s, 2-CH), 53.4 (s, 5-CH_2), 50.04 (s, 6-CH_2), 37.4 (s, 7-CH_2), 33.2 (s, 3-CH_2), 31.9 (s, 1-CH_2), 22.8 (s, 4-CH_2); **^{31}P NMR (162 MHz, CDCl$_3$)** δ = 21.92 (s), 20.81 (s); **IR (diamond, ν_{MAX}, cm^{-1})** 2962 (NH st), 2168 (Ar comb), 1683 (C=O st amide), 1437 (H-C-H st as), 1177 (S-O st as), 1121 (S-O st sy); **Acc. Mass (FAB)** $C_{42}H_{47}Au_2F_6N_4O_6P_2S_2$ *Found: 1337.1704 m/z, Calculated: 1337.1704 m/z.*



***(S)*-4-((1-methoxy-4-(methylthio)-1-oxobutan-2-yl)amino)-4-oxobutanoic acid**
L-methionine methyl ester hydrochloride (250 mg, 1.25 mmol) was suspended in dichloromethane (12.5 mL) under an atmosphere of nitrogen. Triethylamine (0.26 mL, 1.88 mmol) was added and the suspension stirred for 10 min. 4-dimethylaminopyridine (15 mg, 0.12 mmol) and succinic anhydride (125 mg, 1.25 mmol) were added and the reaction stirred for 16 h. The reaction mixture was shaken with 3 x 20 mL portions of hydrochloric acid (2 M) and the aqueous washings extracted with diethyl ether (3x20 mL). The combined organic phases were dried over anhydrous magnesium sulfate, filtered and concentrated under reduced pressure to yield the title compound as a white solid (0.199 g, 60%). **$[\alpha]_D^{25.4}$** = 29.3 (*c* = 1.05, dichloromethane); **^{1}H NMR (500 MHz, CDCl$_3$)** δ = 10.6 (1H, s, 12-H), 6.44 (1H, d, *J*=7.8, 7-NH), 4.73 (1H, td, *J*=7.3, 5.4, 3-H), 3.77 (3H, s, 1-H), 2.66 − 2.81 (2H, m, 9-H), 2.57 (2H, t, *J*=6.8, 10-H), 2.49 − 2.54 (2H, m, 5-H), 2.13 − 2.22 (1H, m, 4-H), 2.10 (3H, s, 6-H), 1.94 − 2.06 (1H, m, 4-H); **^{13}C NMR (126 MHz, CDCl3)** δ = 176.9(11-C=O), 172.5(2-C=O), 171.9 (8-C=O), 52.8 (1-CH_3), 51.6 (3-CH), 31.5 (4-CH_2), 30.5 (10-CH_2), 29.9 (5-CH_2), 29.3 (9-CH_2), 15.4 (6-CH_3); **IR (diamond, ν_{MAX}, cm^{-1})** 3309, 3104 (O-H st), 2923, 1746 (C=O st), 1715 (C=O st), 1651 (C=O st), 1533, 1410.1, 1227 (CO-O st) 1204, 1159 (C-OC); **Acc. Mass (FAB)** $C_{10}H_{17}NNaO_5S$, *Found: 286.0726 m/z*, *Calculated: 286.0720 m/z.*



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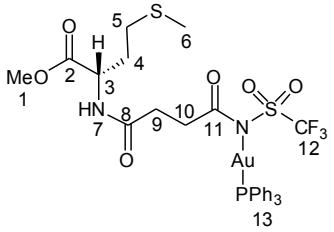
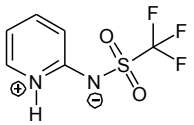
(*S*)-methyl 4-(methylthio)-2-(4-oxo-4 (trifluoromethylsulfonamido)butanamido)butanoate

(*S*)-4-((1-methoxy-4-(methylthio)-1-oxobutan-2-yl)amino)-4-oxobutanoic acid (0.53 g, 2.01 mmol) and triflic amide (0.3 g, 2.01 mmol) were dissolved in dichloromethane (7.5 mL) and cooled to 0 °C under an atmosphere of nitrogen. EDC (0.36ml, 2.06 mmol) was added and the reaction mixture stirred at 0 °C for 15 min., and then at room temperature for 48 h. The reaction mixture was concentrated under reduced pressure and the residue dissolved in ethyl acetate (10 mL). The solution was washed with citric acid (sat.), sodium hydrogen carbonate (sat.) and brine. The combined aqueous washings were then extracted with diethyl ether using continuous extraction equipment for 24 h. The organic phase was separated and dried over anhydrous magnesium sulfate, filtered and concentrated under reduced pressure to yield a yellow oil. The crude oil was purified by column chromatography using a gradient solvent system (0-5% methanol in diethyl ether) to yield the title compound as a pale yellow oil (0.18 g, 23%). **$[\alpha]_D^{26.0}$** = 22.1 (*c* = 1.085, dichloromethane); **^{1}H NMR (500 MHz, $CDCl_3$)** δ = 6.83 (1H, d, *J*=8.3, 7-NH), 4.70 − 4.77 (1H, m, 3-H), 3.77 (3H, s, 1-H), 2.87 – 2.79 (2H, m, 10-H), 2.66 − 2.75 (2H, m, 9-H), 2.45 − 2.55 (2H, m, 5-H), 2.16 (1H, m, 4-H), 2.09 (3H, s, 6-H), 1.95 − 2.05 (1H, m, 4-H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ = 172.4 (2-C=O), 171.9 (8-C=O), 169.4 (11-C=O), 52.8 (1-CH_3), 52.0 (3-CH), 32.2 (10-CH_2), 31.0(4-CH_2), 29.8(5-CH_2), 29.7 (9-CH_2), 15.4 (6-CH_3); **IR (diamond, ν_{MAX}, cm^{-1})** 3371, 2919.4, 1734.5 (C=O), 1649.6, 1537.7, 1441.2, 1387.2, 1201.6 + 1134.8 + 1096.8 (C-O); **Acc. Mass (FAB)** $C_{11}H_{18}F_3N_2O_6S_2$ *Found: 395.0544 m/z, Calculated: 395.0553.*



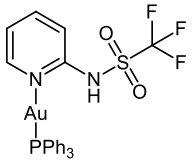
Triphenylphosphine gold (*S*)-methyl 4-(methylthio)-2-(4-oxo-4 (trifluoromethylsulfonamido)butanamido)butanoate

(*S*)-methyl 4-(methylthio)-2-(4-oxo-4 (trifluoromethylsulfonamido)butanamido)butanoate (48.9 mg, 0.12 mmol) was dissolved in dichloromethane (2.5 mL). Ag_2CO_3 (0.034g, 0.12 mmol) was added and the mixture stirred for 5 min. excluding light, under an atmosphere of nitrogen. Triphenylphosphine gold chloride (0.061g, 0.12 mmol) was added in one portion and the reaction stirred for 1.5 h. The reaction mixture was diluted with dichloromethane (10ml), filtered through Celite and concentrated under reduced pressure to afford the title compound as an off white solid (90.3 mg, 85%). **$[\alpha]_D^{26.2}$** = 6.4 (*c* = 1.025, dichloromethane); **^{1}H NMR (500 MHz, $CDCl_3$)** δ = 7.57 − 7.45 (15H, m, Ar), 6.49 (1H, d, *J*=8.3, 7-NH), 4.7 (1H, m, 3-H), 3.72 (3H, s, 1-H), 3.17 – 3.02 (2H, m, 10-H), 2.59 – 2.53 (4H, m, 9,5-H), 2.20 – 2.13 (1H, m, 4-H), 2.08 (3H, s, 6-CH_3), 1.98 (1H, m, 4-CH_2); **^{13}C NMR (126 MHz, $CDCl_3$)** δ = 177.35(11-C=O), 172.2(2-C=O), 171.7(8-C=O), 134.2(Ar), 134.1(Ar), 132.1(Ar), 132.1(Ar), 129.4(Ar), 129.3(Ar), 52.4(1-CH_3), 51.5(3-CH), 33.9(10-CH_2), 31.8(4-CH_2), 31.3(9-CH_2), 30.2(5-CH_2), 15.8 (6-CH_3); **^{31}P NMR(162Mhz, $CDCl_3$)** δ = 30.5 (s); **IR (diamond, ν_{MAX}, cm^{-1})** 2933, 1737, 1671, 1436, 1354, 1174, 1138, 1101; **Acc. Mass (FAB)** *$C_{29}H_{31}AuF_3N_2NaO_6PS_2$ Found: 875.0871 m/z, Calculated: 875.0819 m/z.*



Pyridinium-2-yl(trifluoromethylsulfonyl)amide

2-aminopyridine (0.5 g, 5.3 mmol) and pyridine (0.43 mL, 5.3 mol) were dissolved in dichloromethane (9.75 mL) under an atmosphere of nitrogen. The reaction mixture was cooled to −78 °C and a solution of triflic anhydride (0.89 mL, 5.3 mmol) in dichloromethane (1.8 mL) was added dropwise via cannula over 20 min. with vigorous stirring, after which the mixture was stirred at −78 °C for 2 h. and then at room temperature for 19 h. The reaction was quenched with water (30 mL). The aqueous layer was extracted with chloroform (4x50 mL) and the combined organic layers washed with water (50 mL), 10% NaOH (50 mL) and brine (50 mL), dried over anhydrous magnesium sulfate. The pH of the aqueous layer was brought down to 8 by adding dilute hydrochloric acid dropwise and further extracted with diethyl ether (3x50 mL). The organic layer was dried over anhydrous magnesium sulphate and filtered. The chloroform and ether solutions were combined and concentrated under reduced pressure to leave a pale brown solid. The solid was recrystallised from methanol to yield the title compound as an off white solid (0.19 g, 16%). **^{1}H NMR (400MHz, CD_3OD)** δ = 8.05 (1H, ddd, *J*=9.0, 7.1, 1.5), 7.98 (1H, d, *J*=6.4), 7.72 (1H, d, *J*=9.3), 7.11 (1H, t, *J*=6.6); **^{13}C NMR (126 MHz, CD_3OD)** δ = 115.0, 118.0, 136.8, 144.4; **IR (diamond, ν_{MAX}, cm^{-1})** 777.29, 1128.94, 1155.04, 1323.58, 1357.99, 1540.07, 1614.62, 1632.61; **Acc. Mass (FAB)** $C_6H_5F_3N_2NaO_2S$ *Found: 248.9918 m/z, Calculated: 248.9916 m/z.*



Triphenylphosphine gold pyridinium-2-yl(trifluoromethylsulfonyl)amide

2-(*N*-triflyl)pyridine (50mg, 0.2 mmol) was dissolved in of dry dichloromethane (2.2 mL) under an atmosphere of nitrogen. Silver carbonate (66 mg, 0.2 mmol) and subsequently triphenylphosphine gold chloride (0.108 g, 0.2 mmol) were added and the reaction mixture stirred for 19 h. The reaction mixture was filtered through Celite and concentrated under reduced pressure to yield the title compound as a white crystalline solid. 0.133 g (87%). **^{1}H NMR (400 MHz, $(CD_3)_2SO$)** δ = 8.26 (1H, d, *J*=4.4), 7.87 (1H, t, *J*=7.8), 7.48 – 7.80 (16H, m), 7.08 (1H, t, *J*=5.9). **^{13}C NMR (126 MHz, $(CD_3)_2SO$)** δ = 141.1, 134.1, 133.9, 132.31, 132.29, 129.6, 129.5, 128.3, 127.8, 116.6, 116.3; **^{31}P NMR (162 MHz, $(CD_3)_2SO$)** δ = 29.6 (s); **Acc. Mass (FAB):** $C_{24}H_{20}AuF_3N_2O_2PS$, *Found: 685.0658 m/z, Calculated: 685.0595 m/z.*

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References
[1] Burdon, J.; Farazmand, I.; Stacey, M.; Tatlow, J. C.; *J. Chem. Soc.* **1957**, 2574.

2. Determination of Lipophilicity

The octanol-water partition coefficients (log *P*) of $Ph3PAuNTf_2$ and complexes **3** and **6** were determined using a shake-flask method. A biphasic mixture of water (50 mL, milli-Q purification) and *n*-octanol (50 mL, vacuum distilled) was shaken using a laboratory shaker for 48 h to allow saturation of both phases. Stock solutions of the three compounds (50 μM) were prepared in the organic phase and aliquots (3 mL) of each of these stock solutions were then added to an equal volume of the water phase. The resultant biphasic solutions were mixed for 60 minutes before being centrifuged (2000 g for 5 min) to separate the phases. The concentrations of the gold element in the aqueous phases was then determined using ICP-MS. Log *P* was defined as the logarithm of the ratio of the concentrations in the organic and aqueous phases (Log *P* = Log {[Au(org)]/[Au(aq)]}. The values reported are the means of three separate determinations.

Complex	Log P
Ph3PAuNTf2	4.07
Complex **3**	3.05
Complex **6**	3.33

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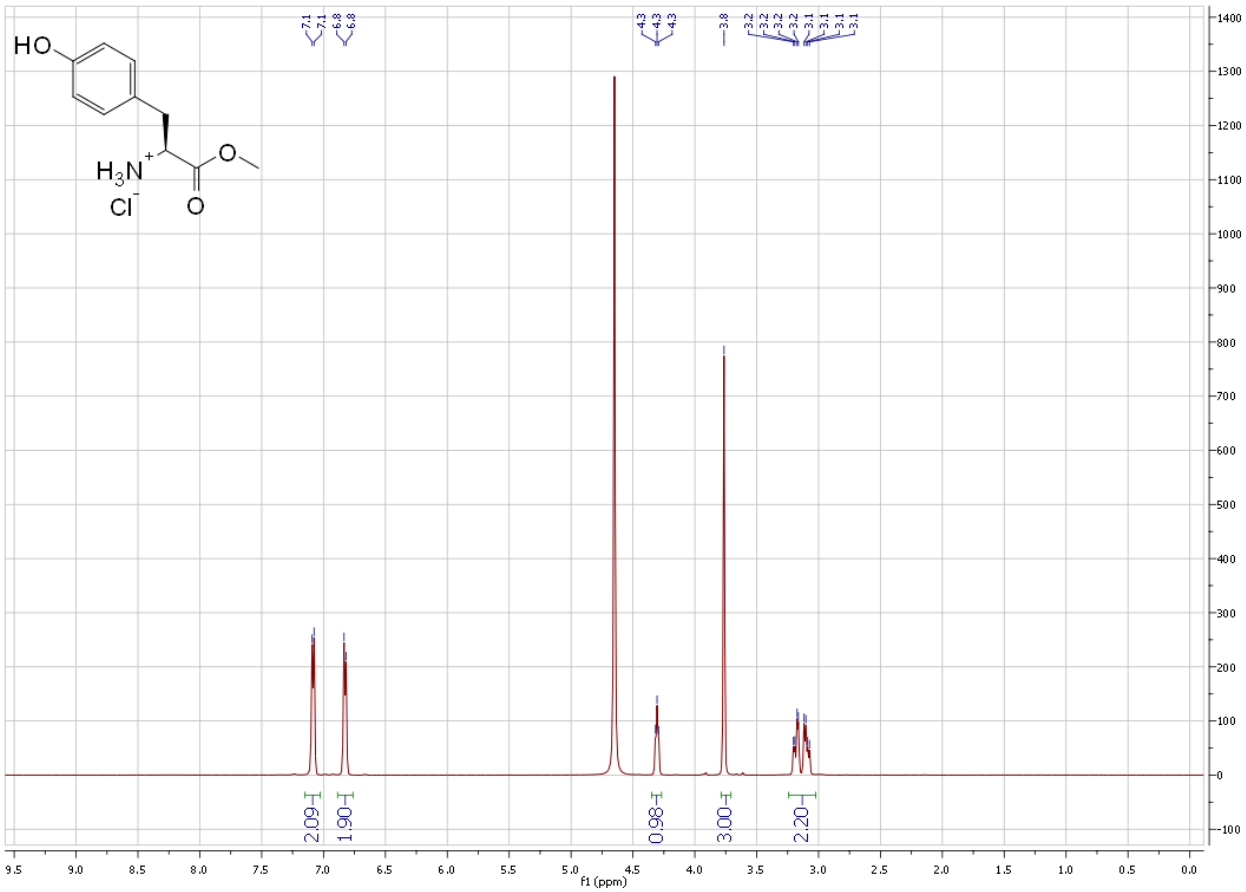
3. Spectral Data

(2*S*)-3-(4-hydroxyphenyl)-1-methoxy-1-oxopropan-2-aminium chloride



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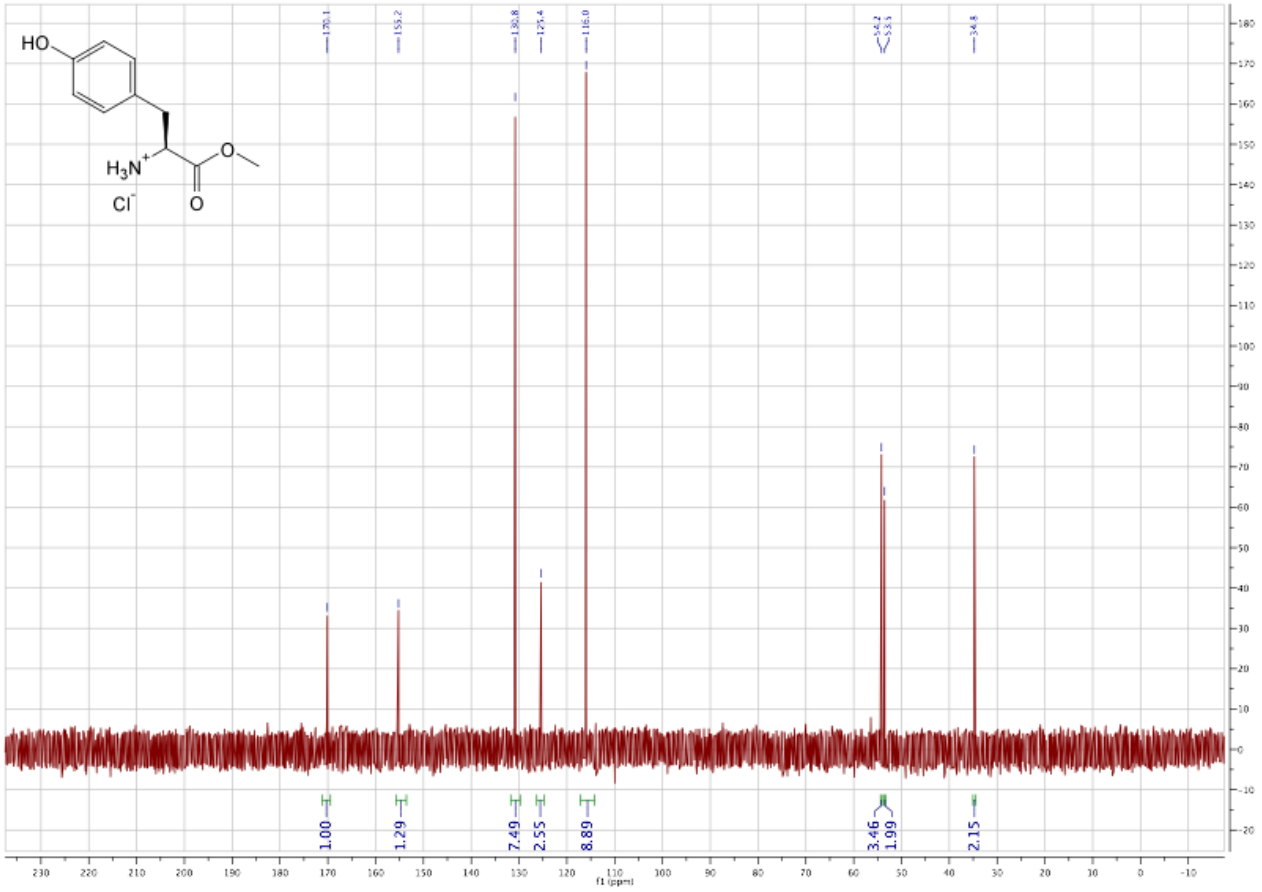
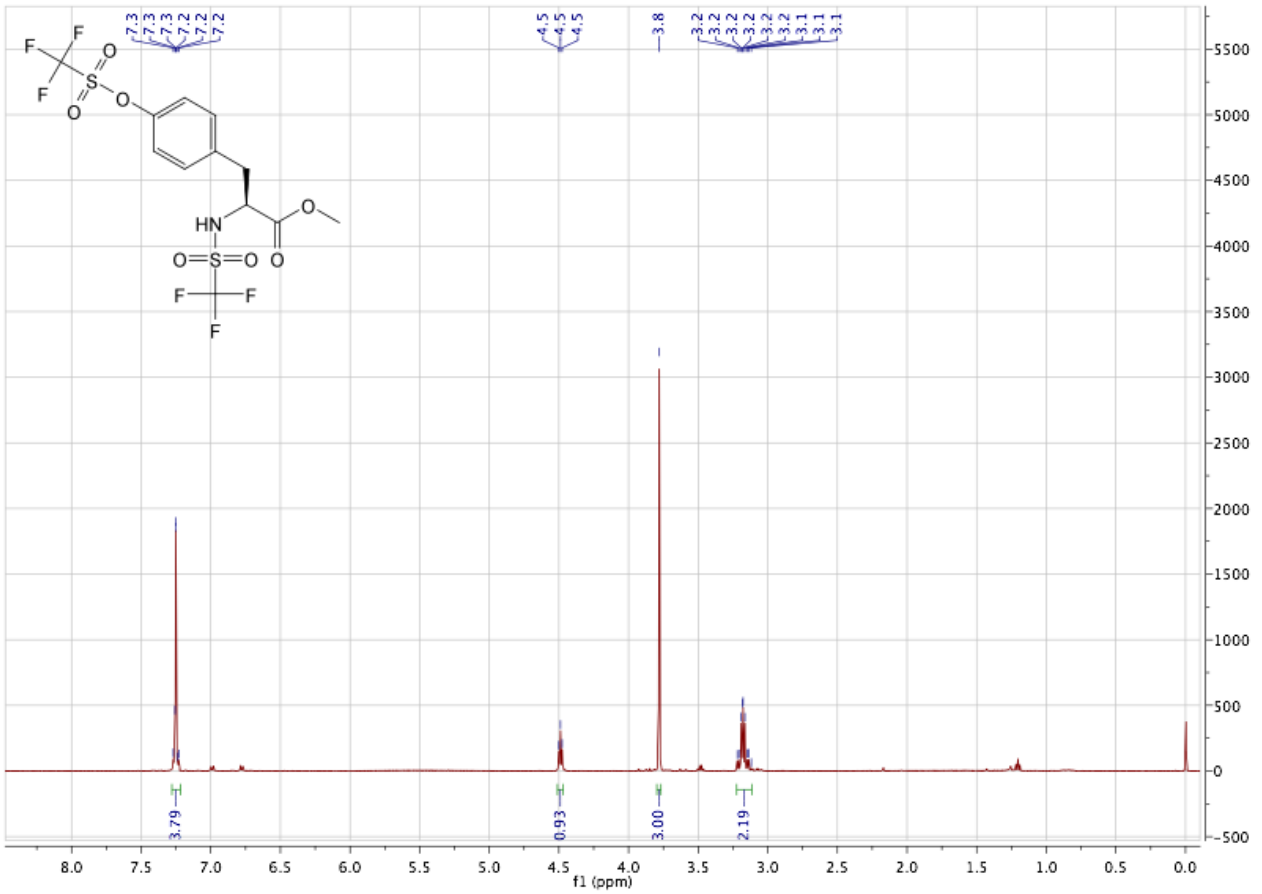


(*S*)-methyl 3-(4-(((trifluoromethyl)sulfonyl)oxy)phenyl)-2-(trifluoromethylsulfonamido)propanoate



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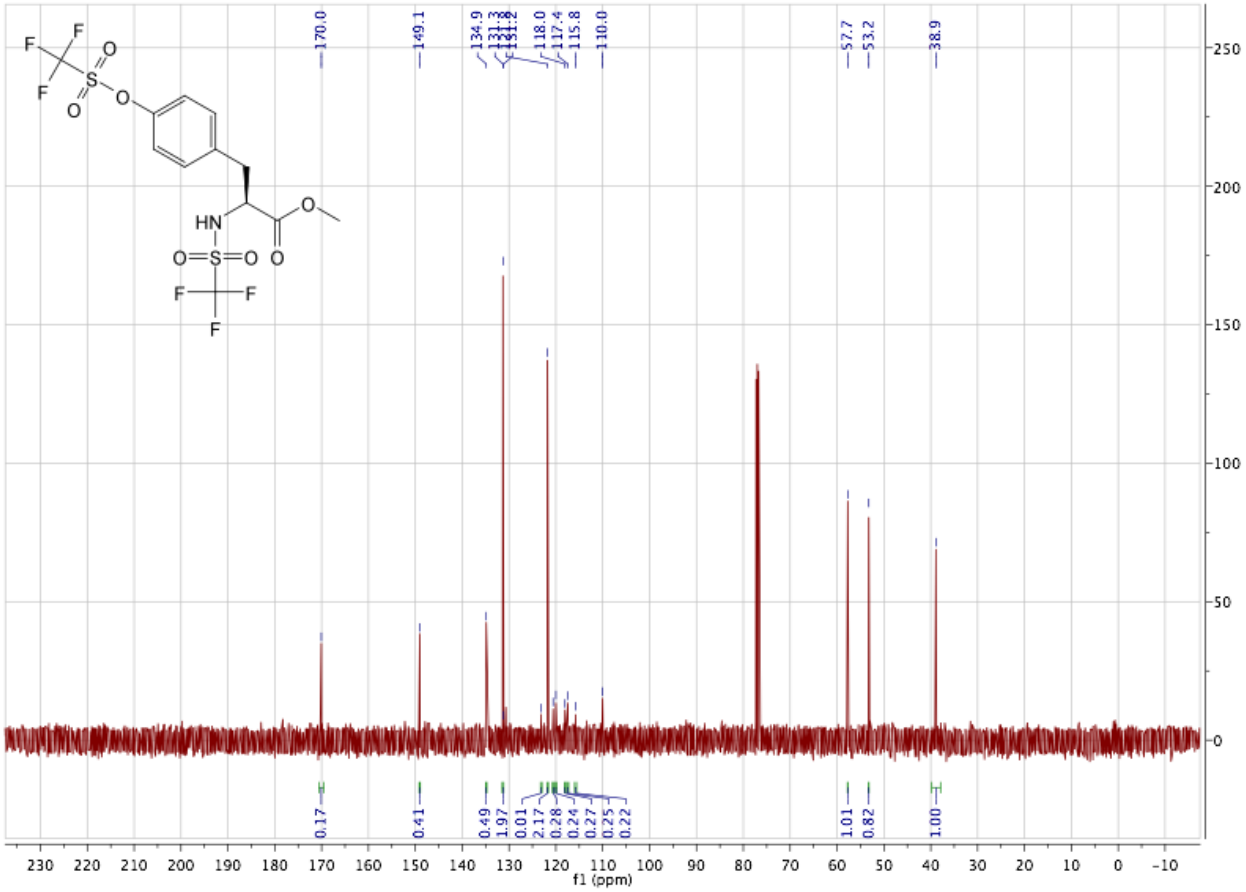
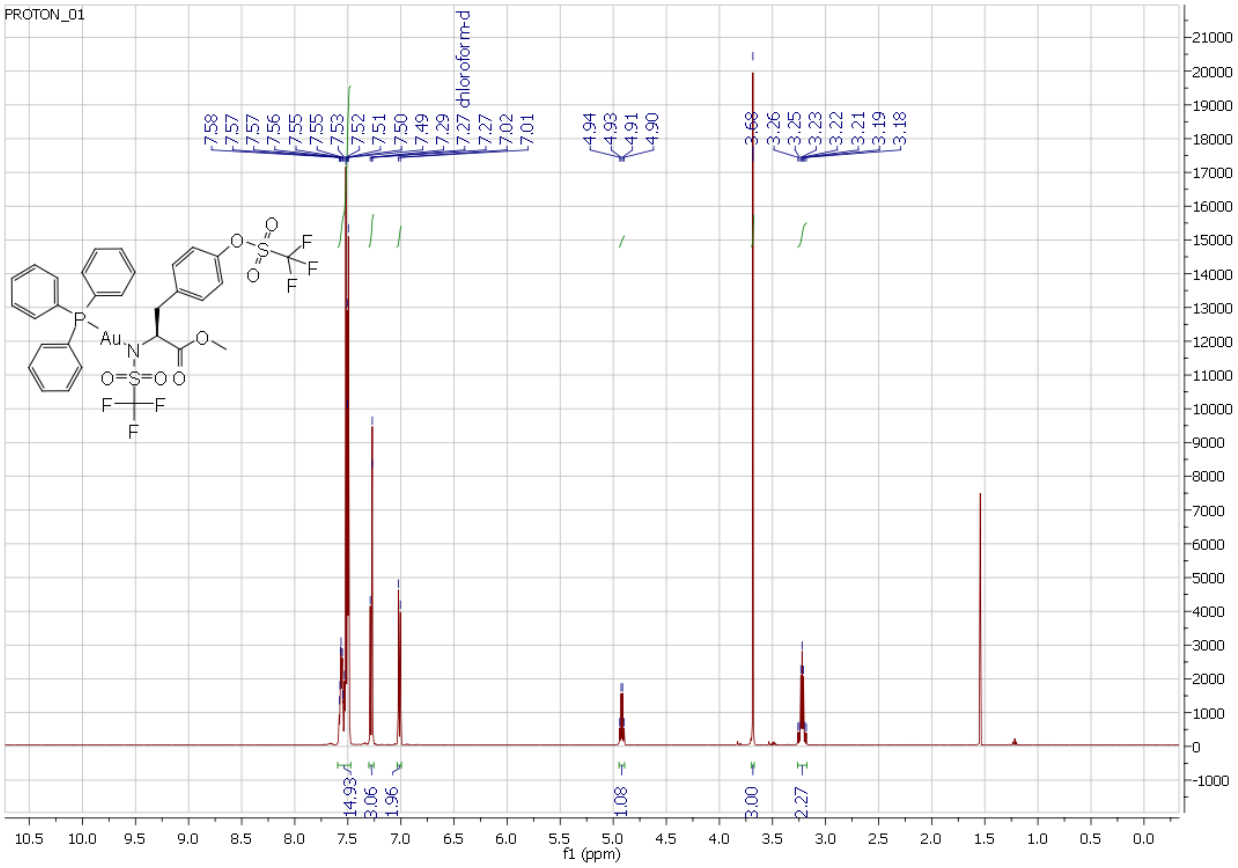


Triphenylphosphine gold (*S*)-methyl 3-(4-(((trifluoromethyl)sulfonyl)oxy)phenyl)-2-(trifluoromethylsulfonamido)propanoate



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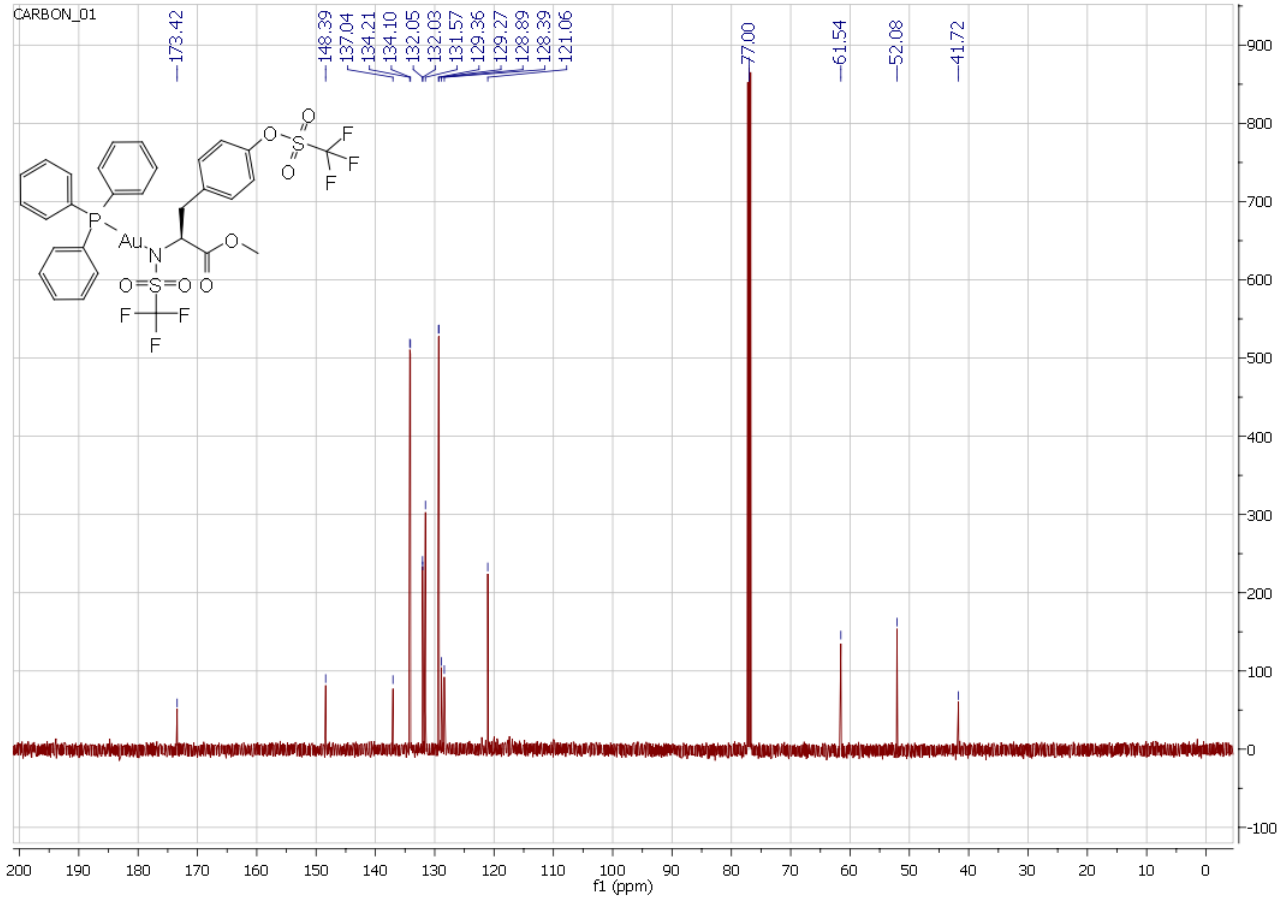

(2*R*)-3-(1*H*-indol-3-yl)-1-methoxy-1-oxopropan-2-aminium chloride

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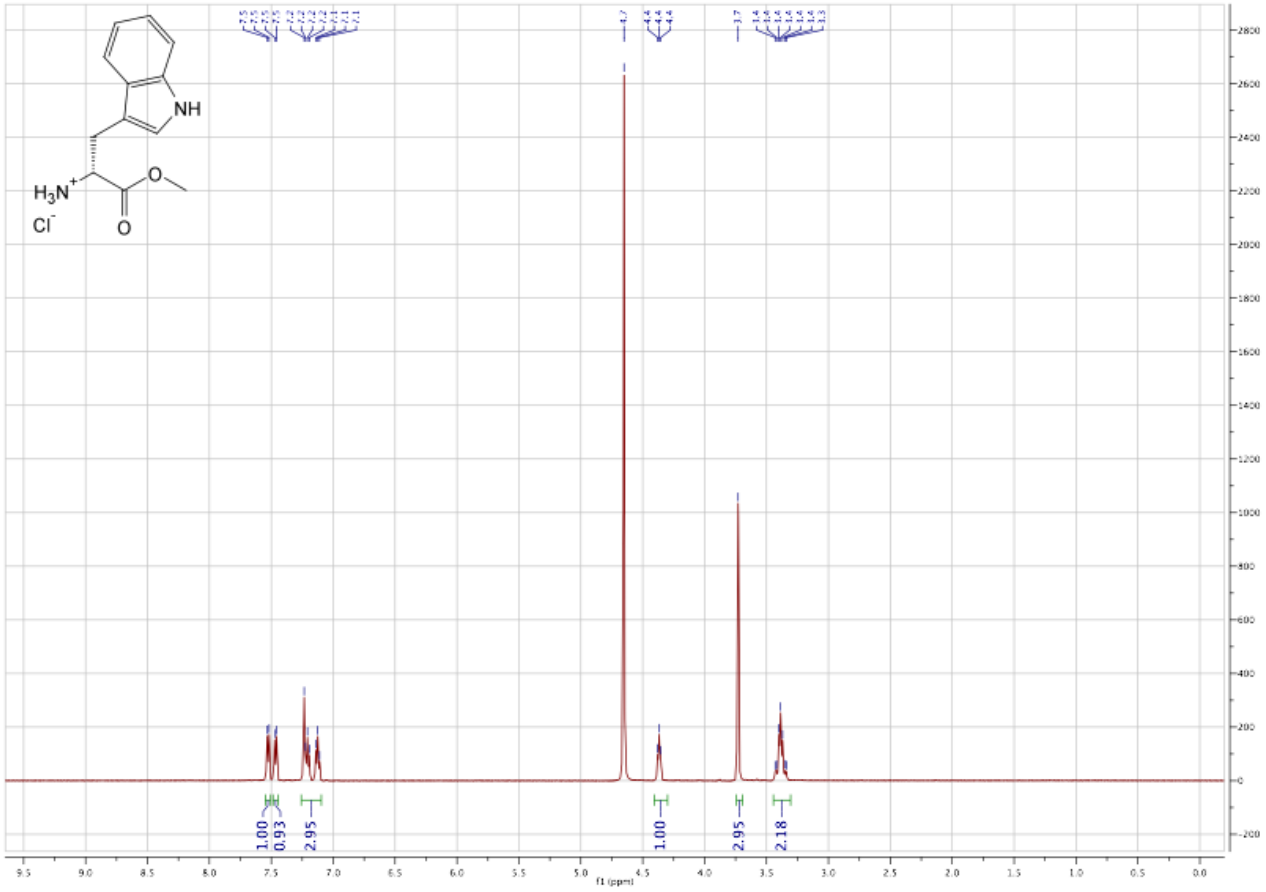

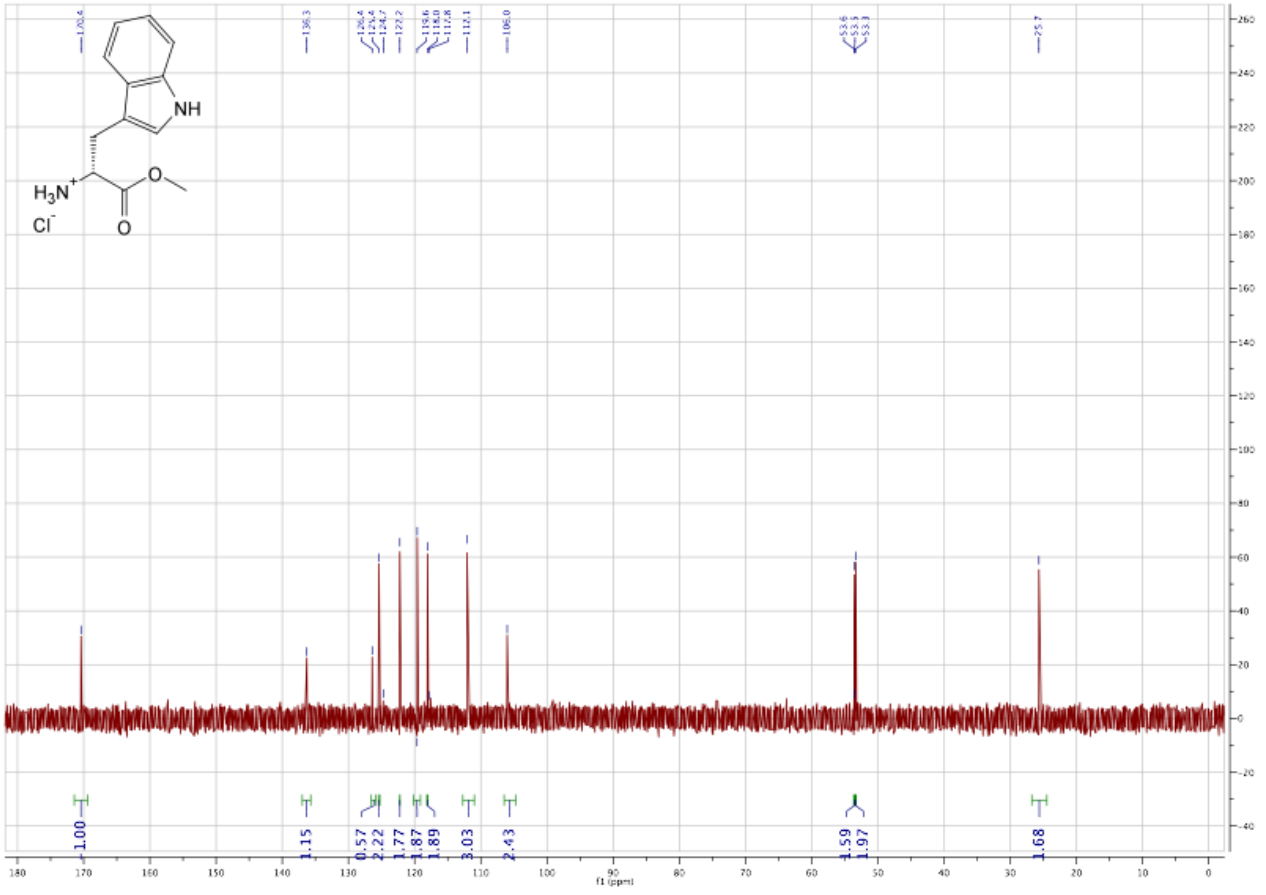

Methyl *N*-[(trifluoromethyl)sulfonyl]-*D*-tryptophanate

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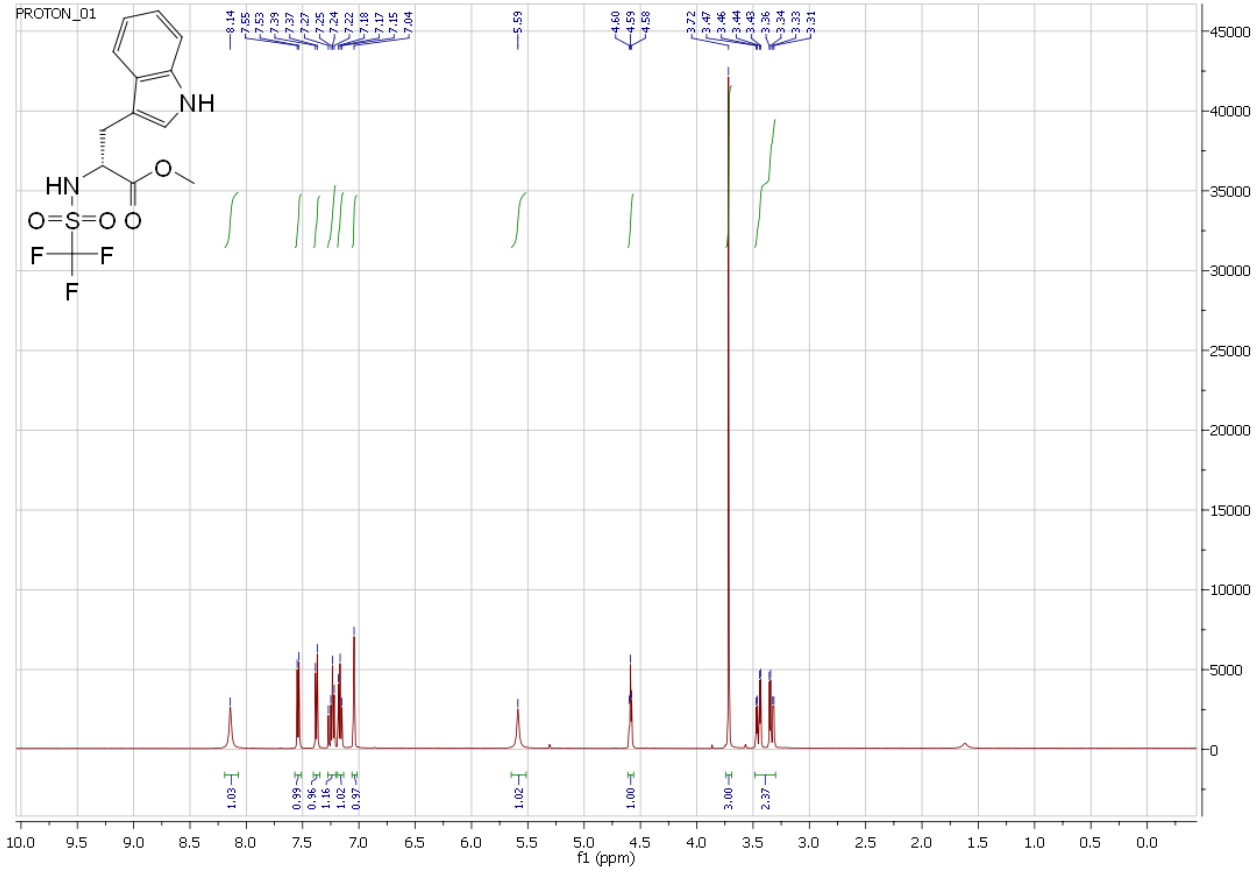

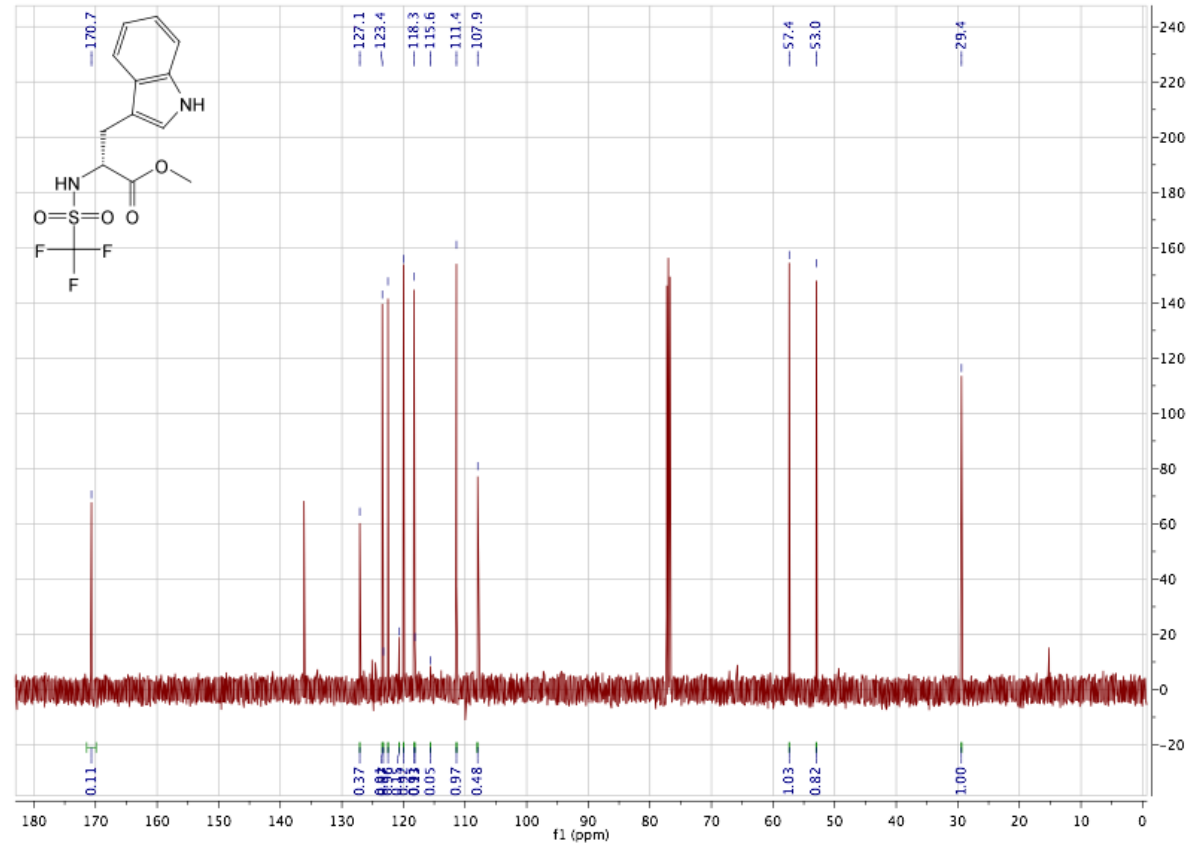

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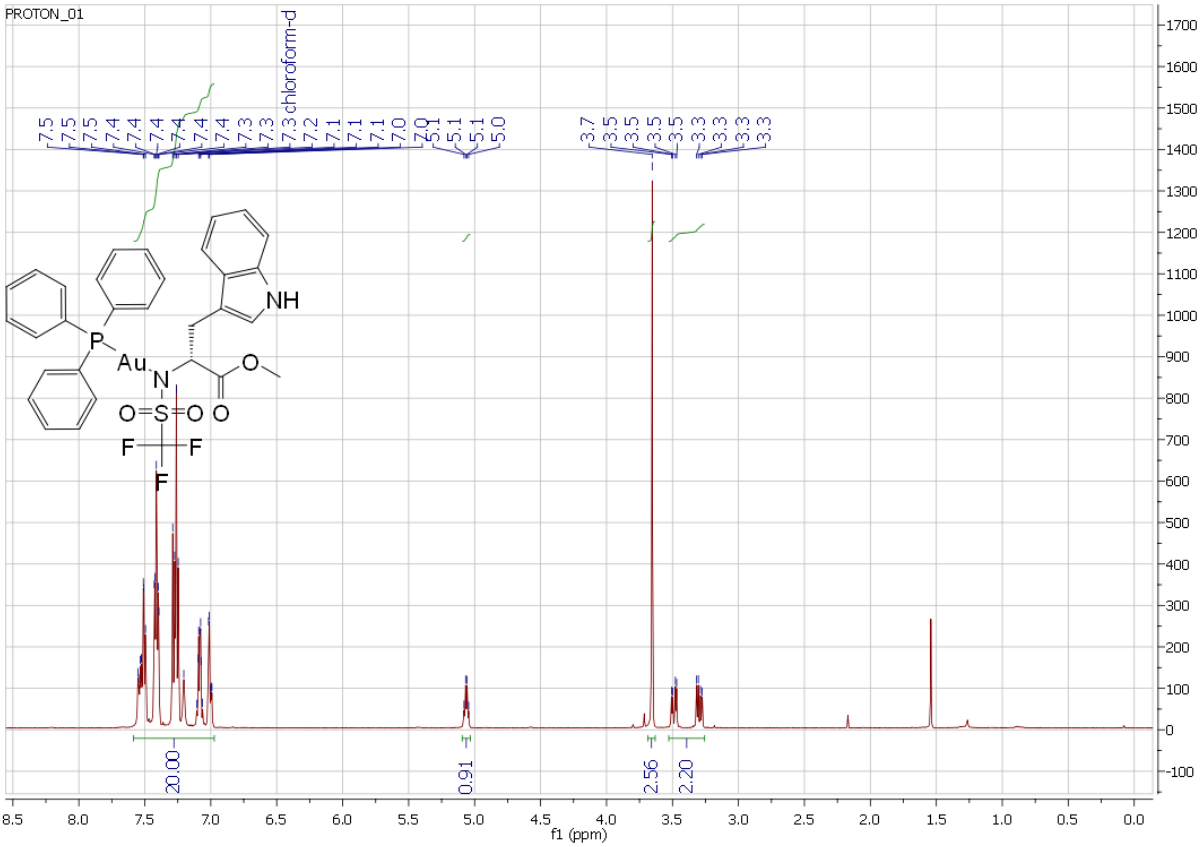
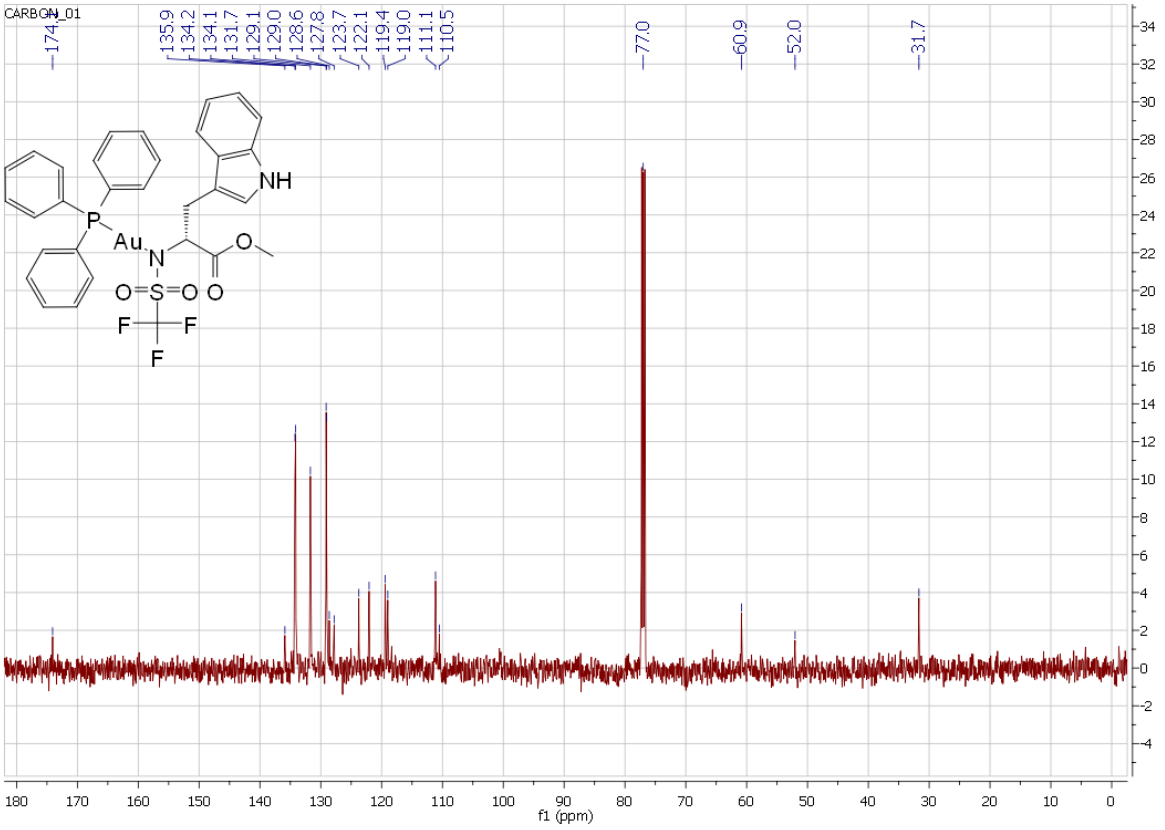
Triphenylphosphine gold methyl *N*-[(trifluoromethyl)sulfonyl]-*D*-tryptophanate





(*S*)-2-((diphenylphosphino)methyl)pyrrolidine-1-sulfonic acid

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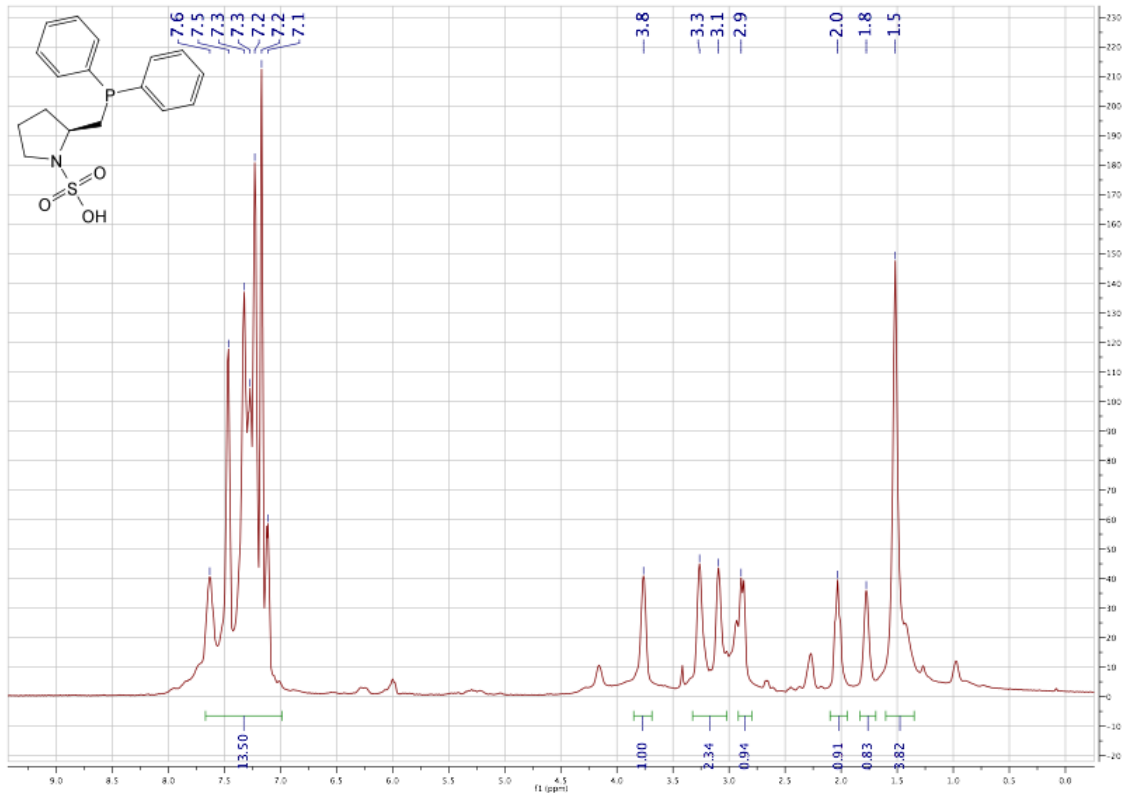

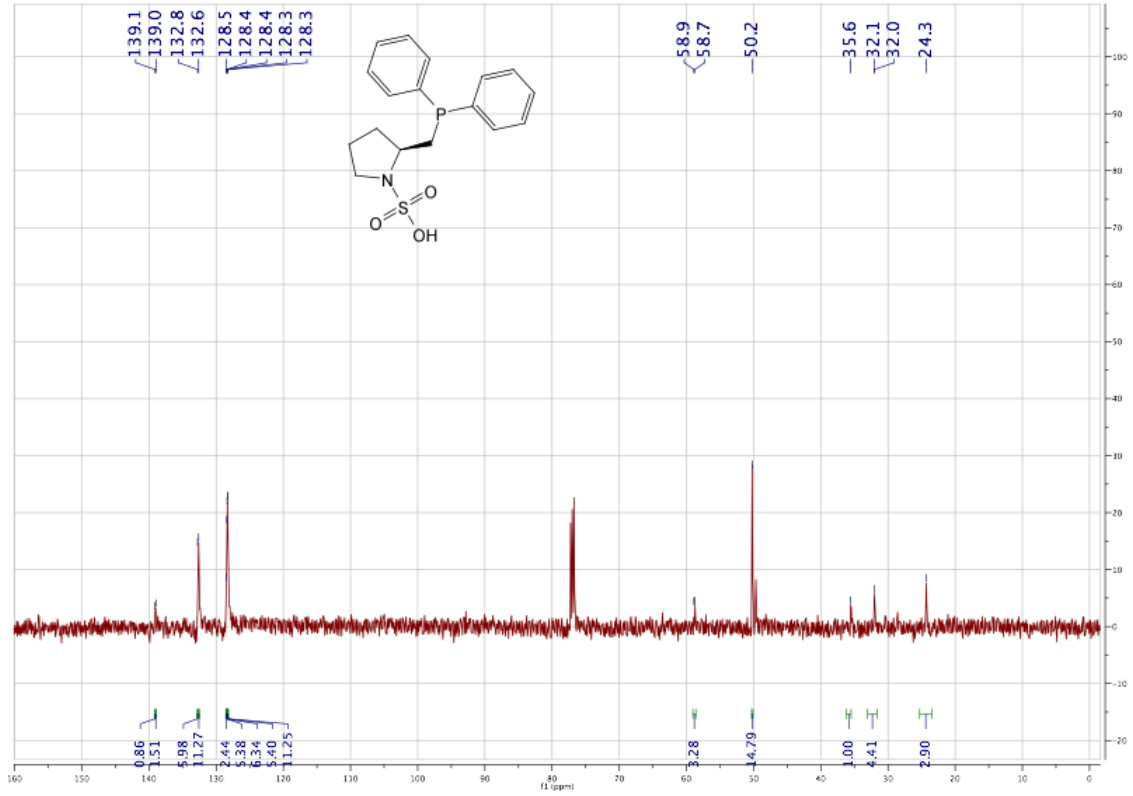

Methyl 3-{(2*S*)-2-[(diphenylphosphino)methyl]pyrrolidin-1-yl} propanoate

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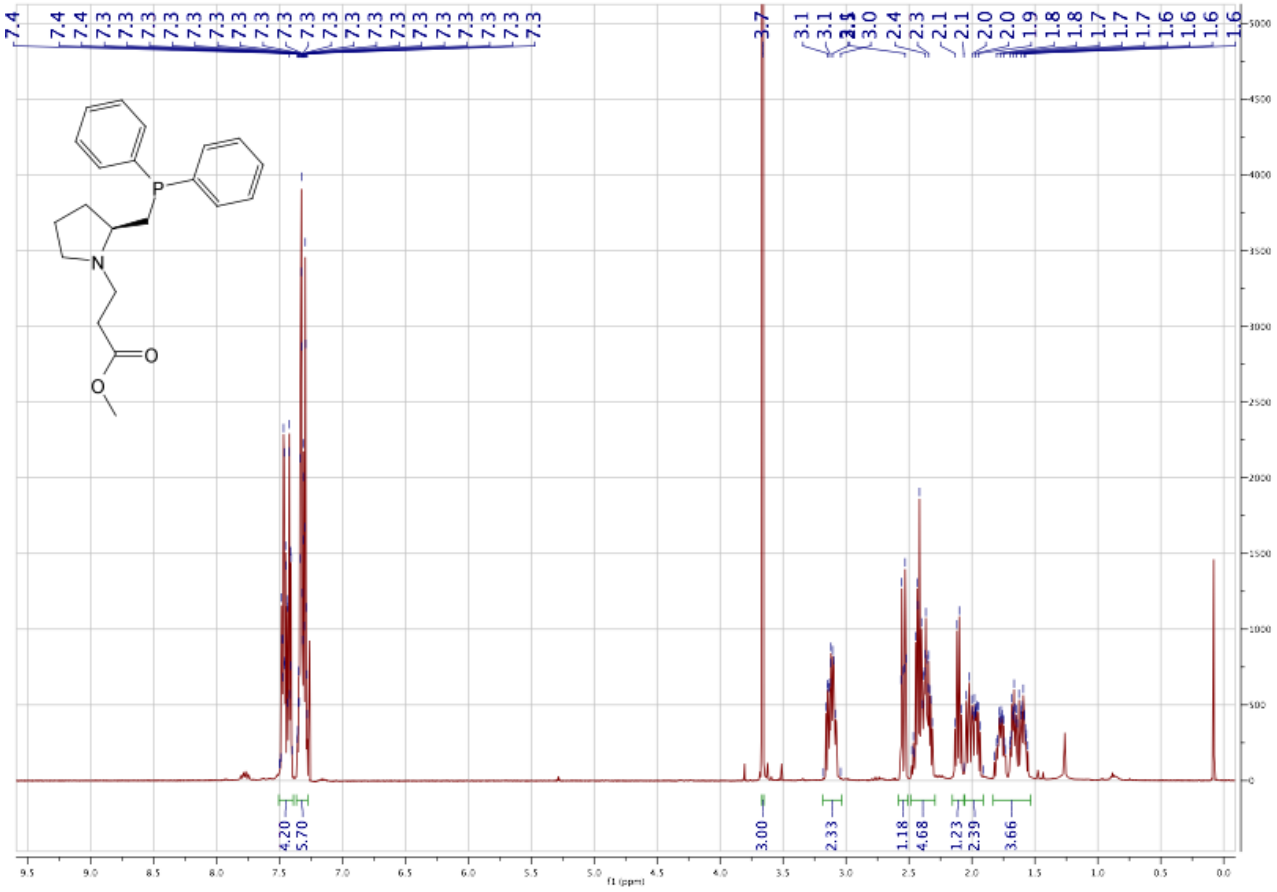

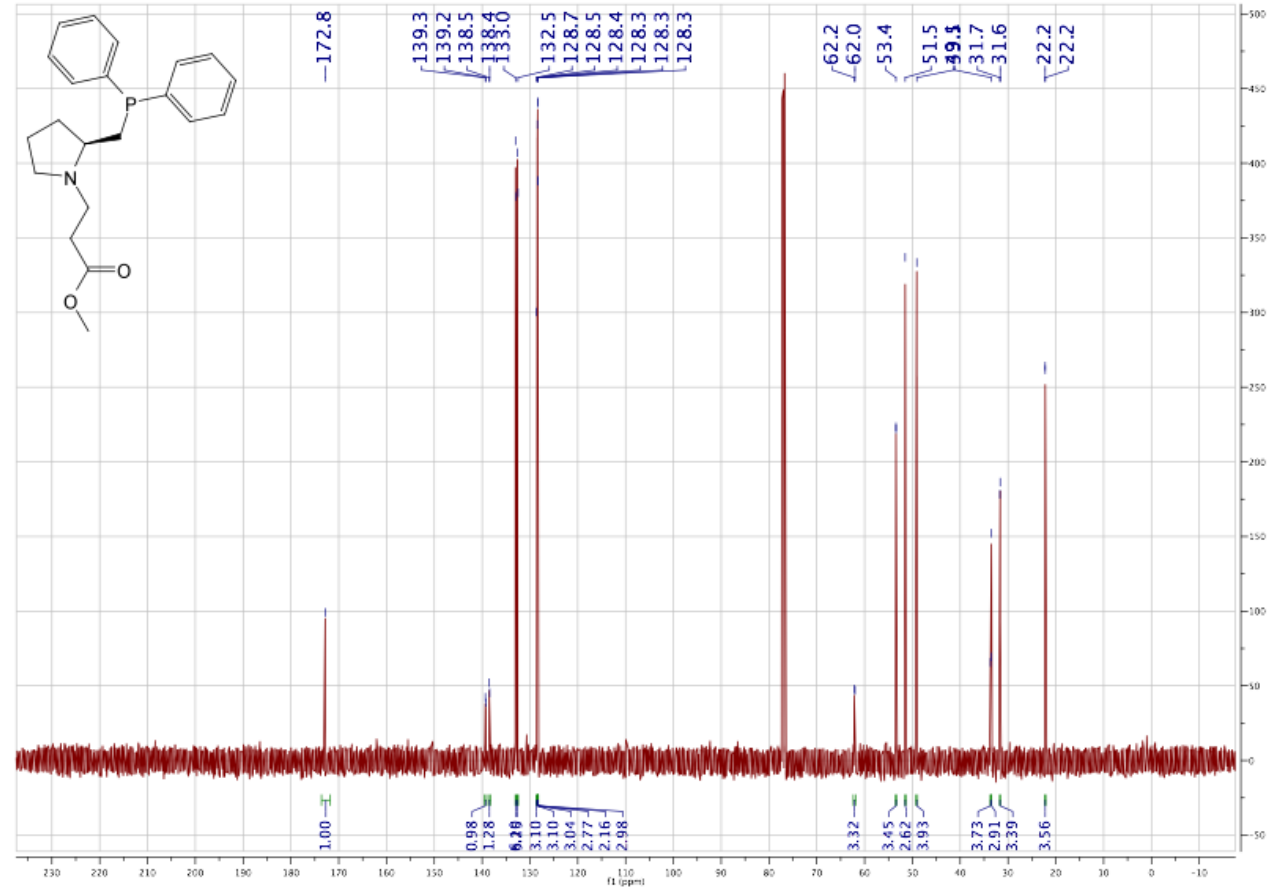

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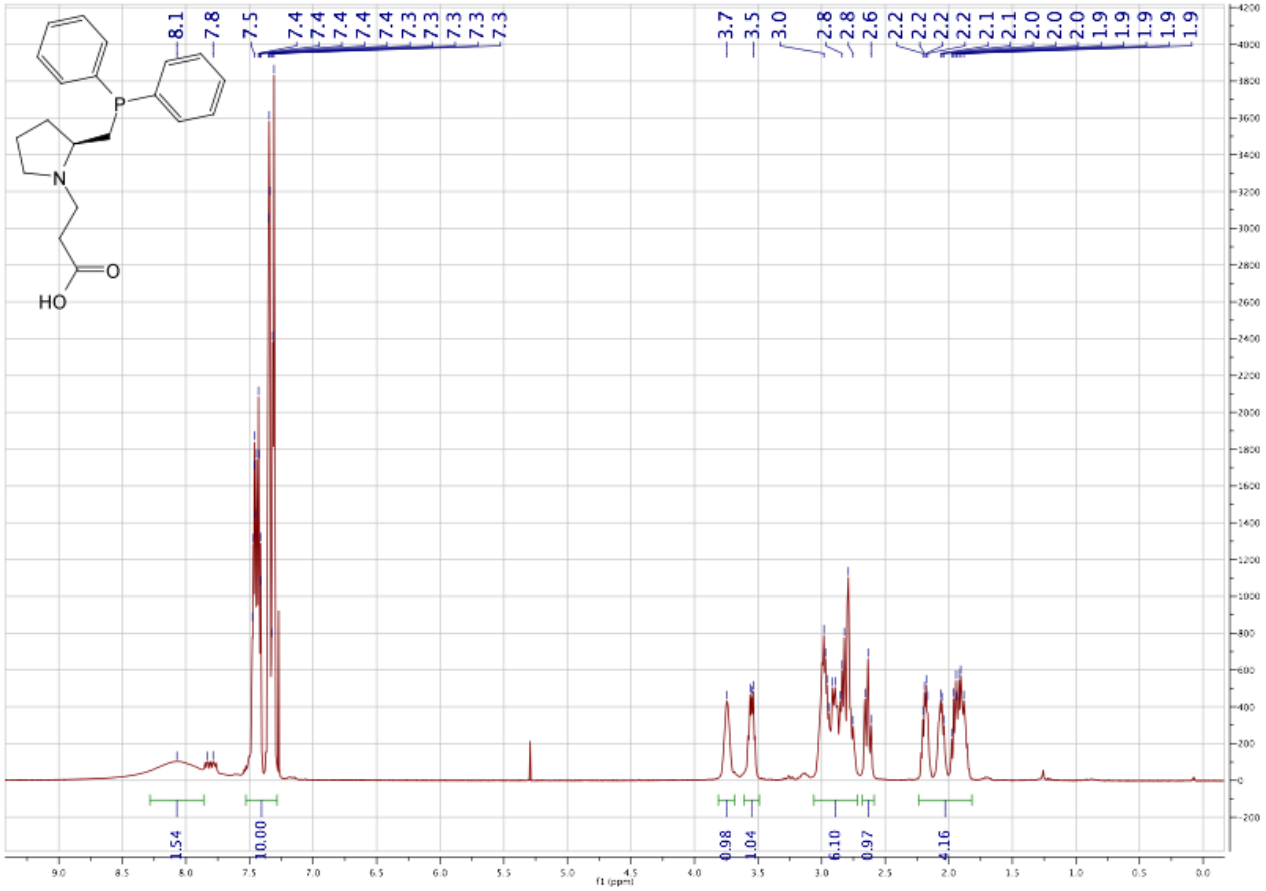
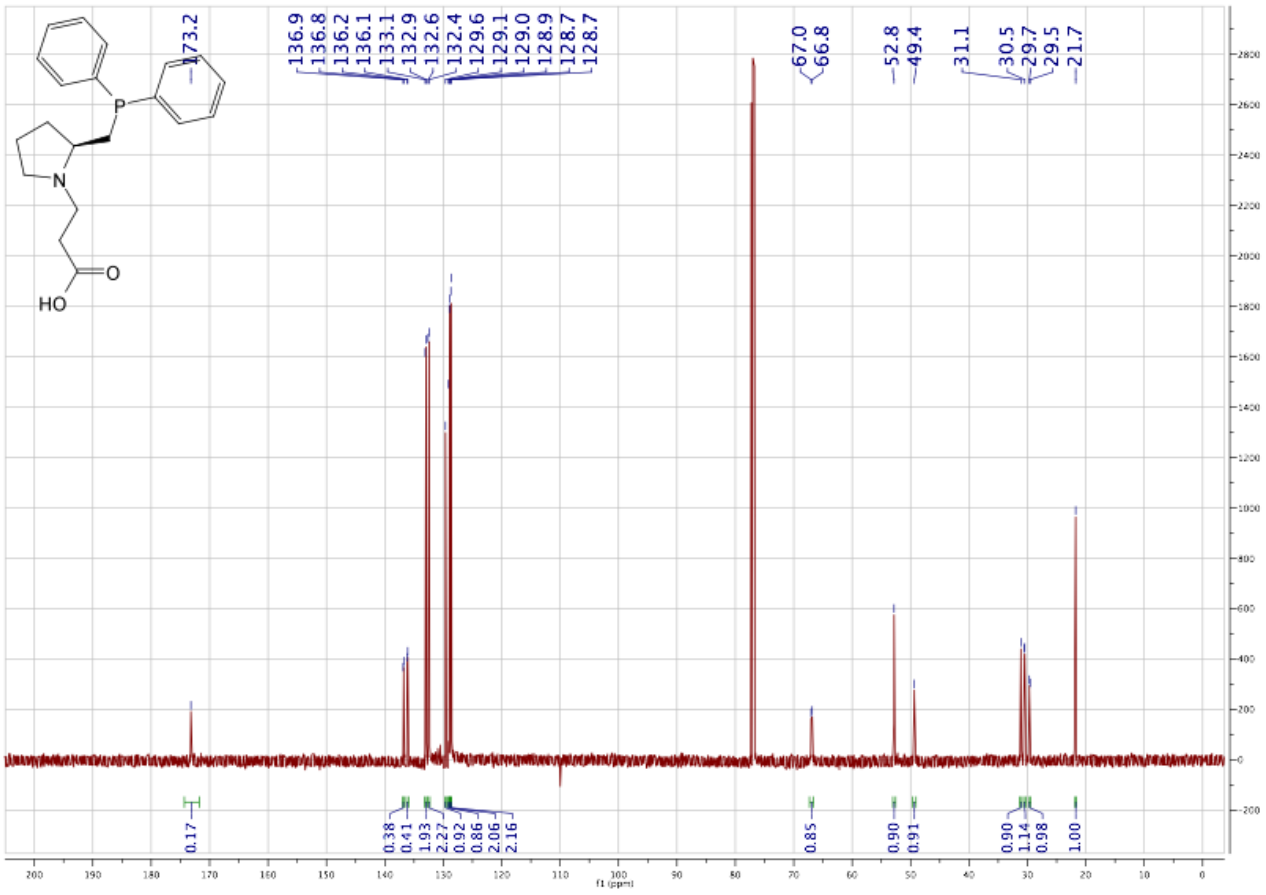
3-{(2*S*)-2-[(diphenylphosphino)methyl]pyrrolidin-1-yl}propanoic acid





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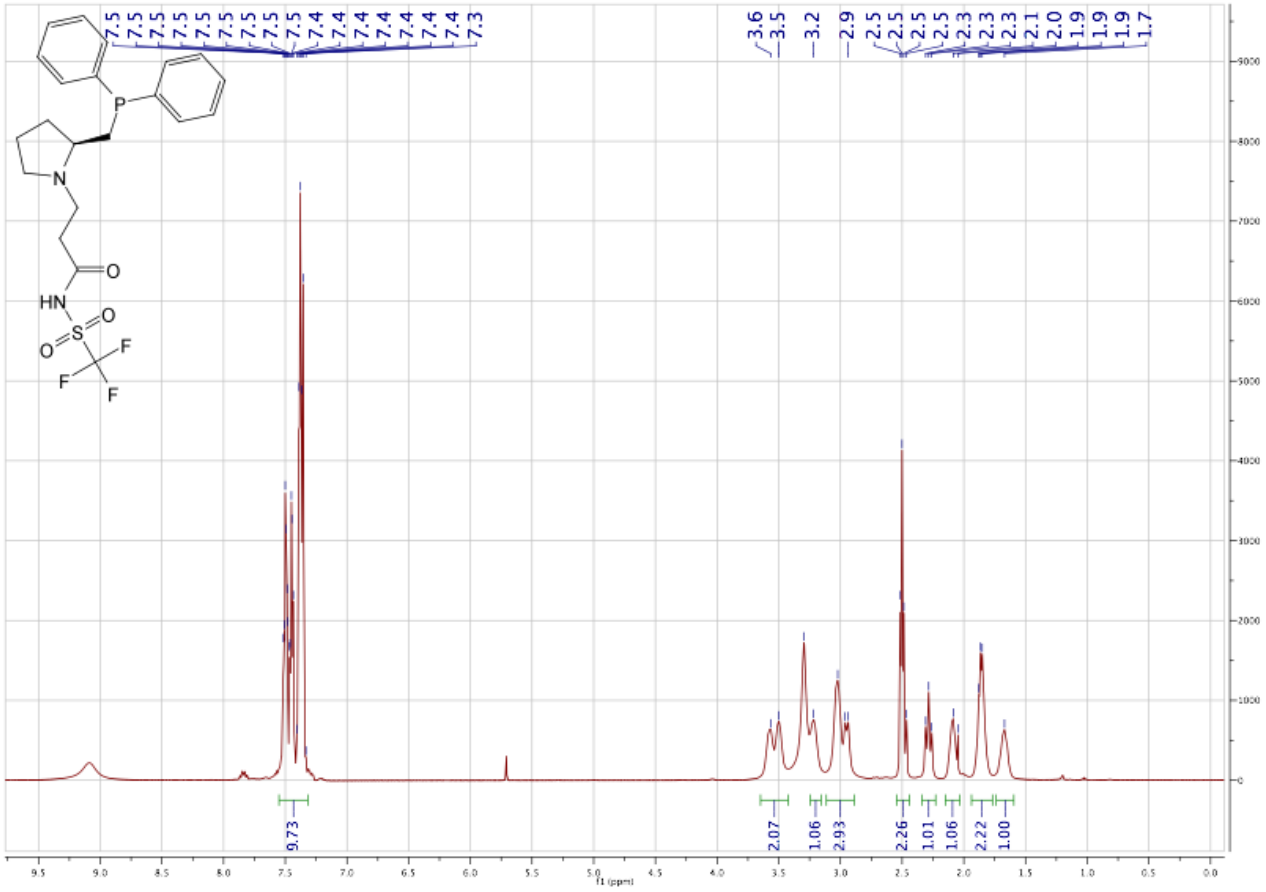
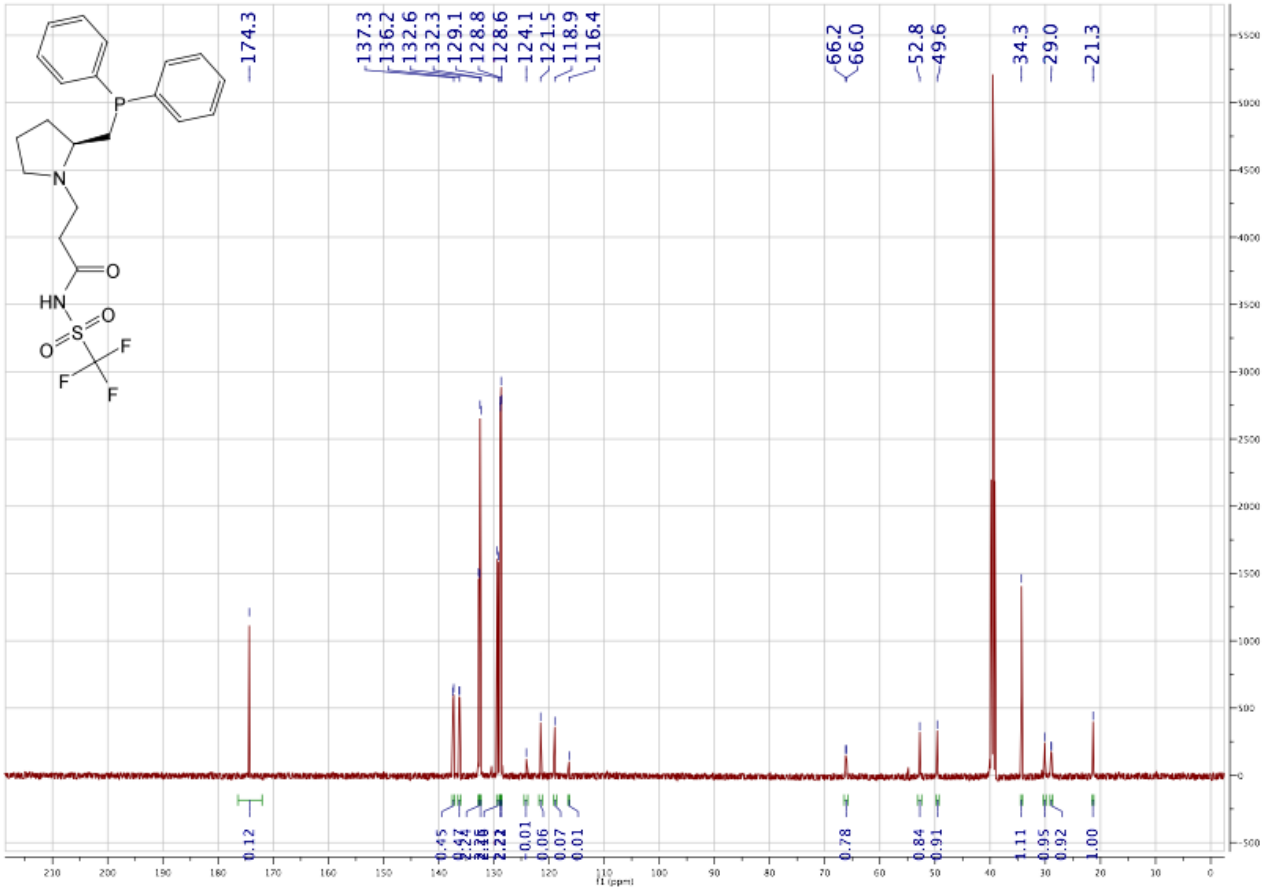
3-{(2*S*)-2-[(diphenylphosphino)methyl]pyrrolidin-1-yl}-*N*-[(trifluoromethyl)sulfonyl]propanamide





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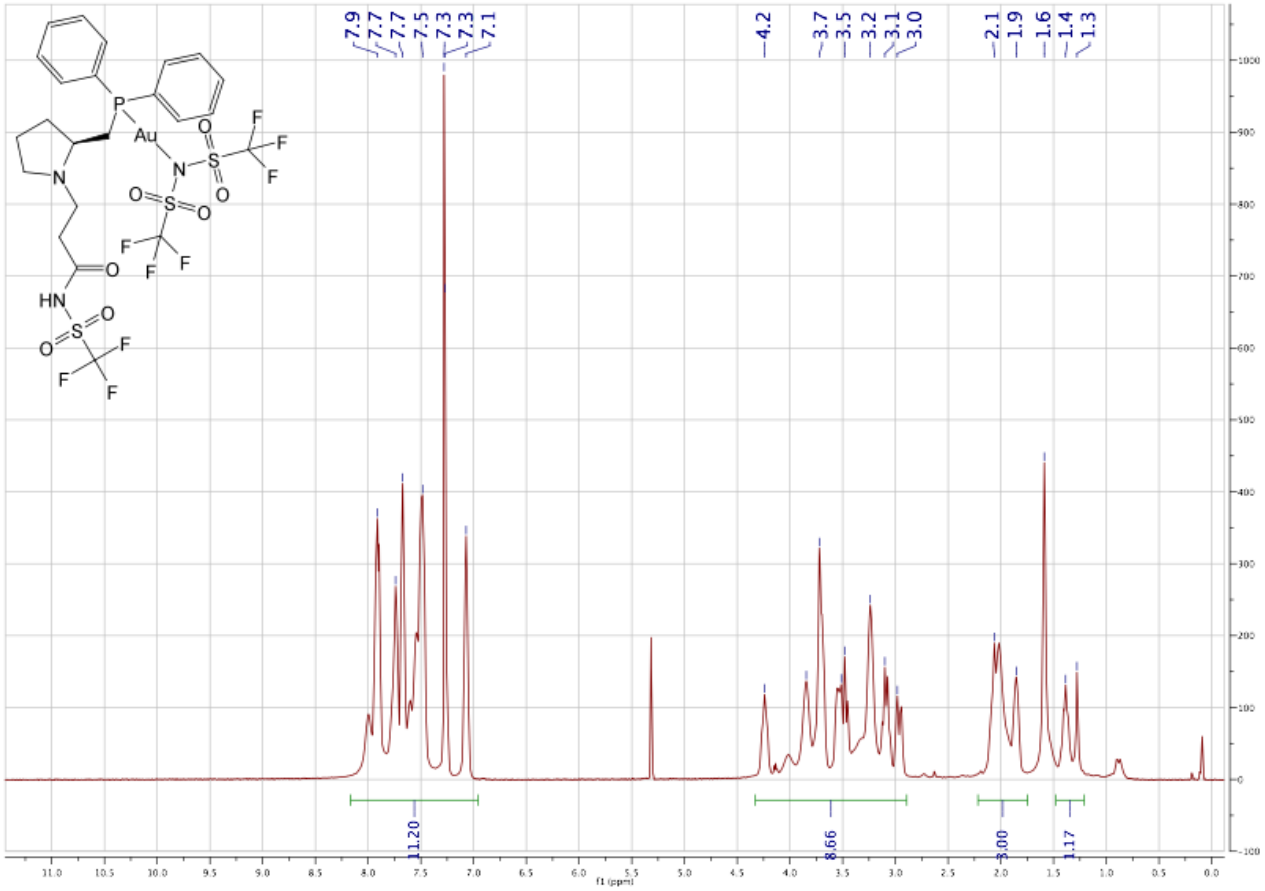
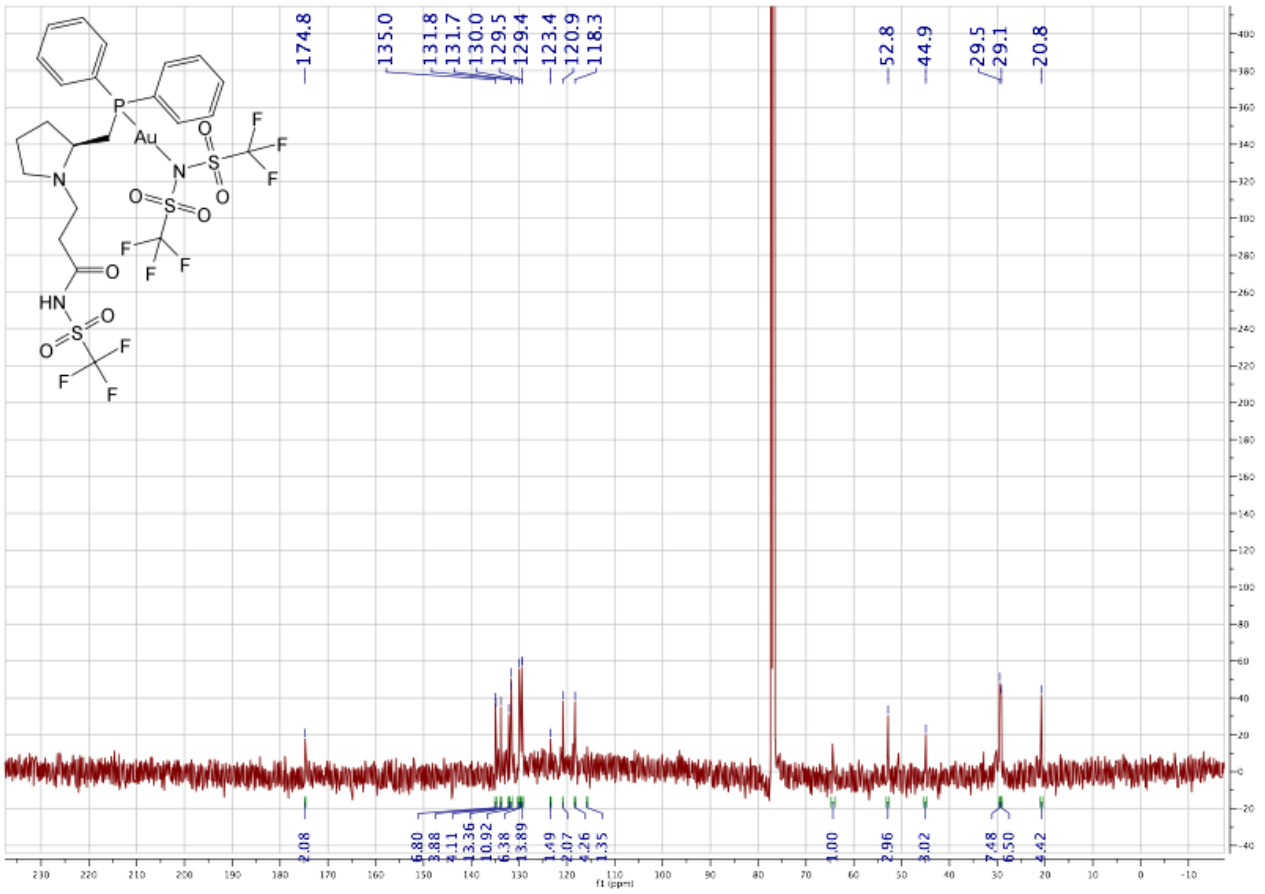
3-{(2*S*)-2-[(diphenylphosphino)methyl]pyrrolidin-1-yl}-*N*-[(trifluoromethyl)sulfonyl]propanamide gold bis(trifluoromethanesulfonate).





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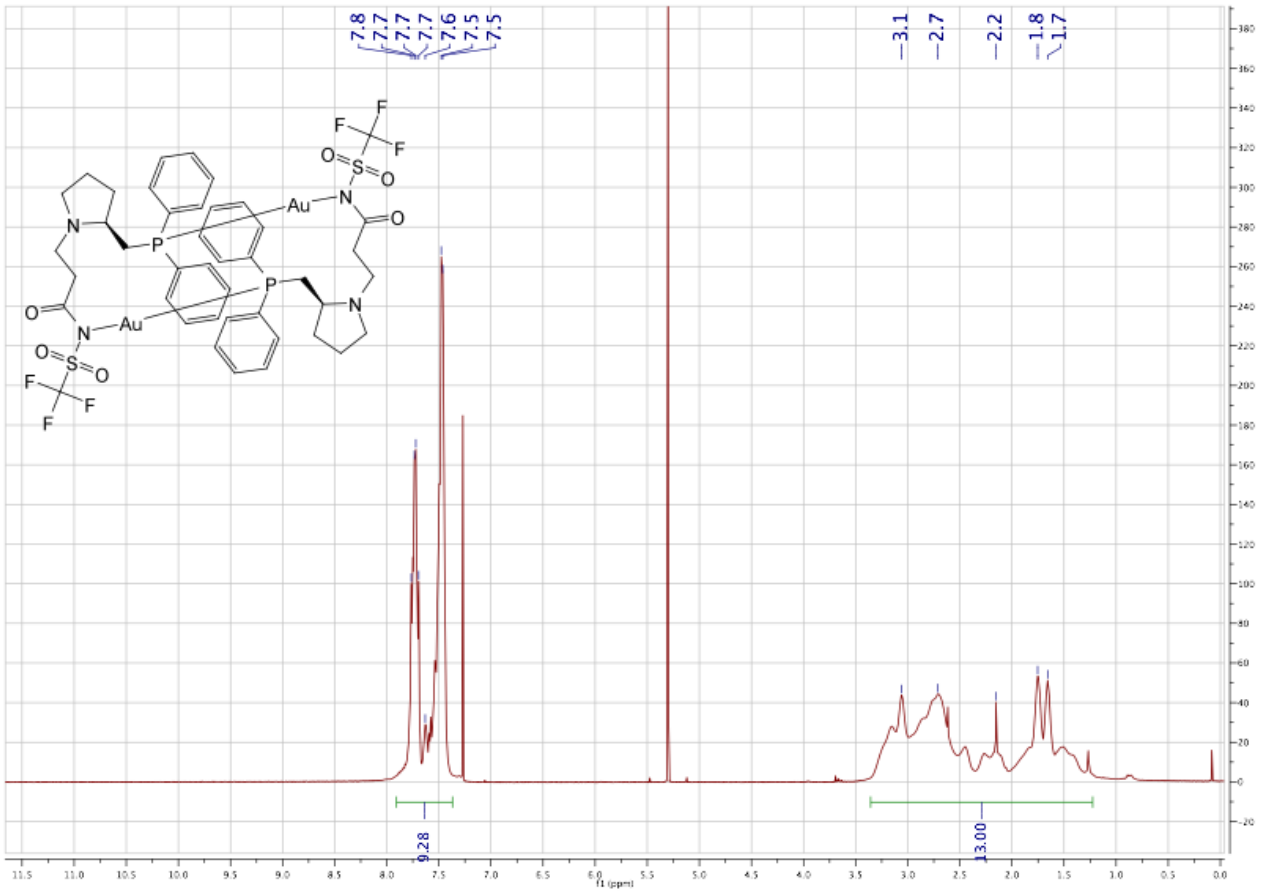
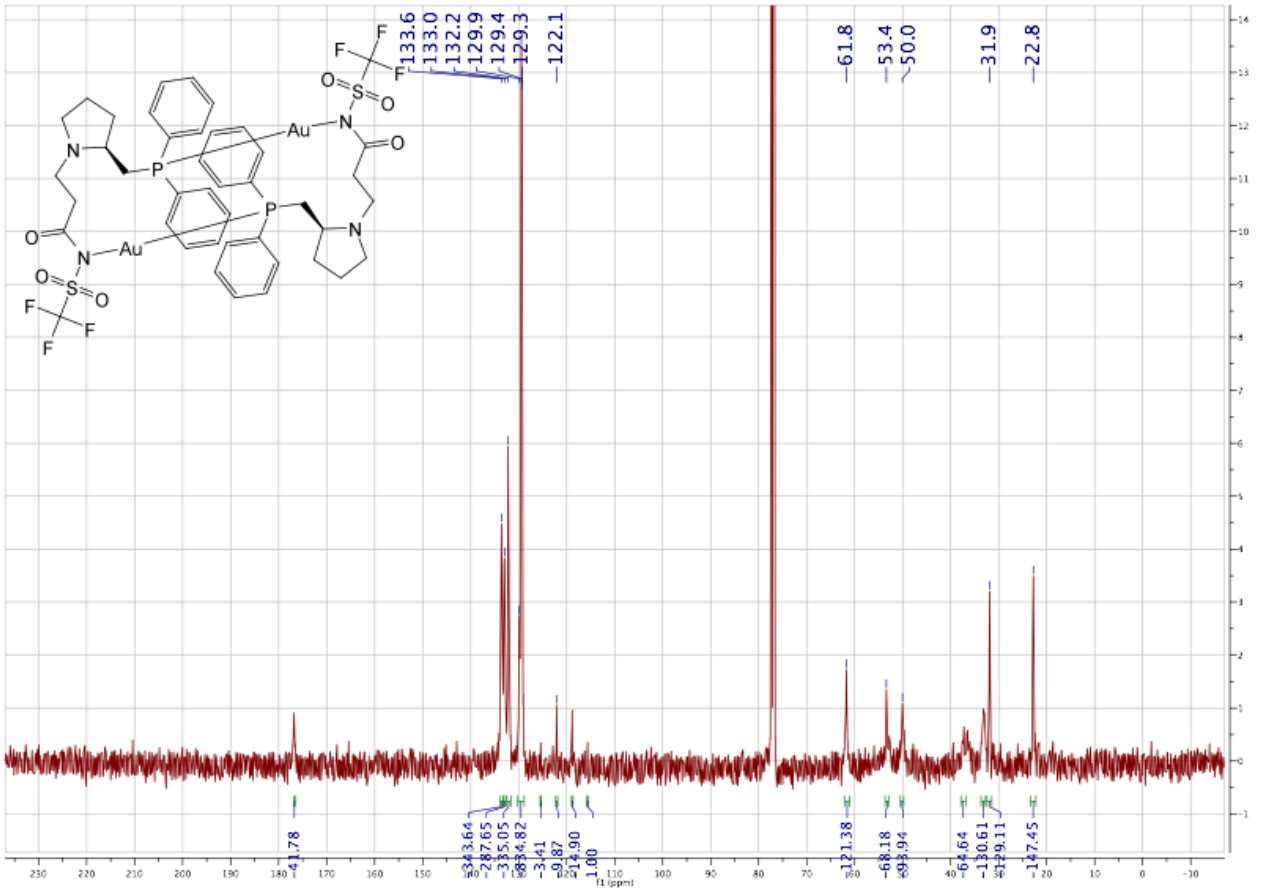
bis(3-{(2*S*)-2-[(diphenylphosphino)methyl]pyrrolidin-1-yl}-*N*-[(trifluoromethyl)sulfonyl]propanamide) di-gold





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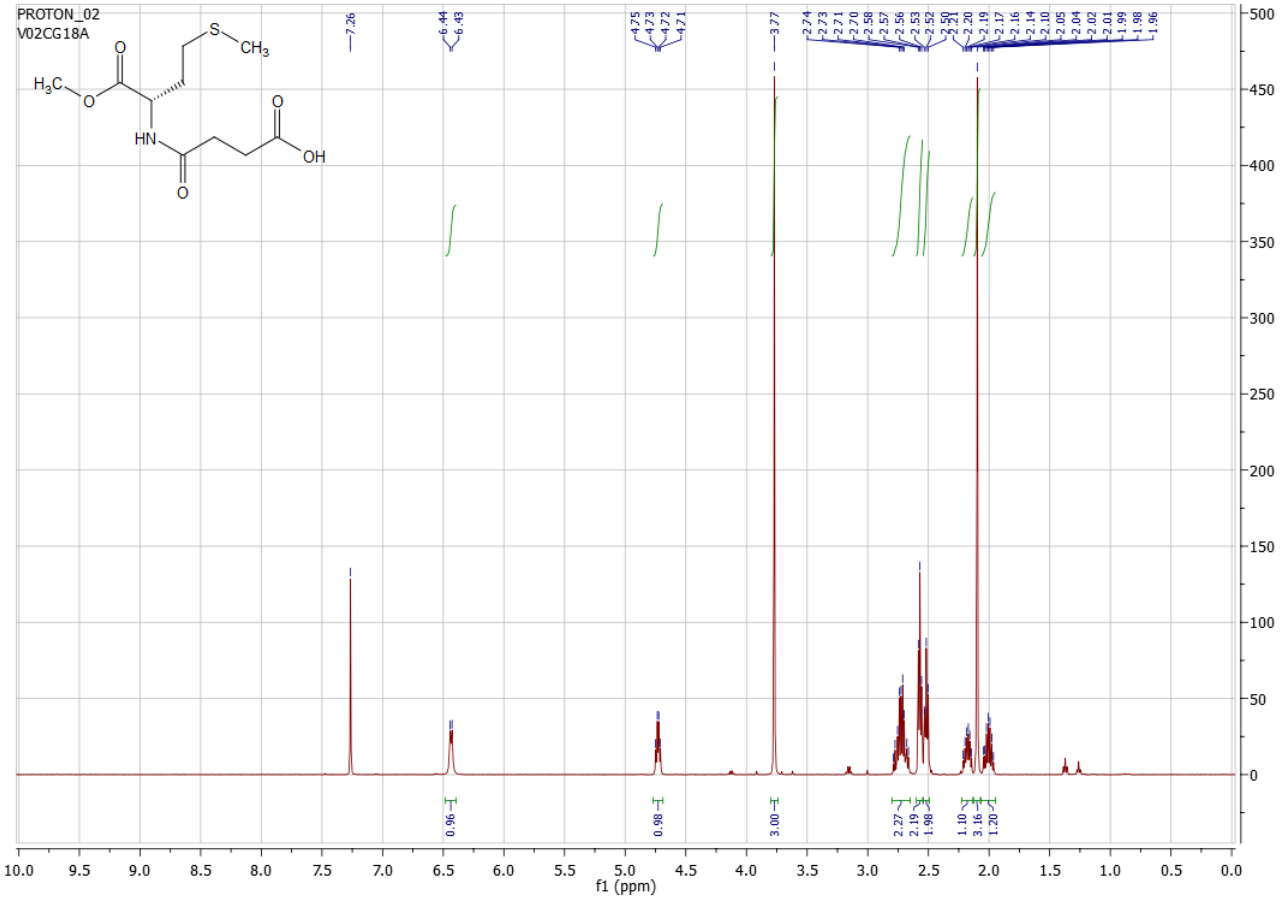
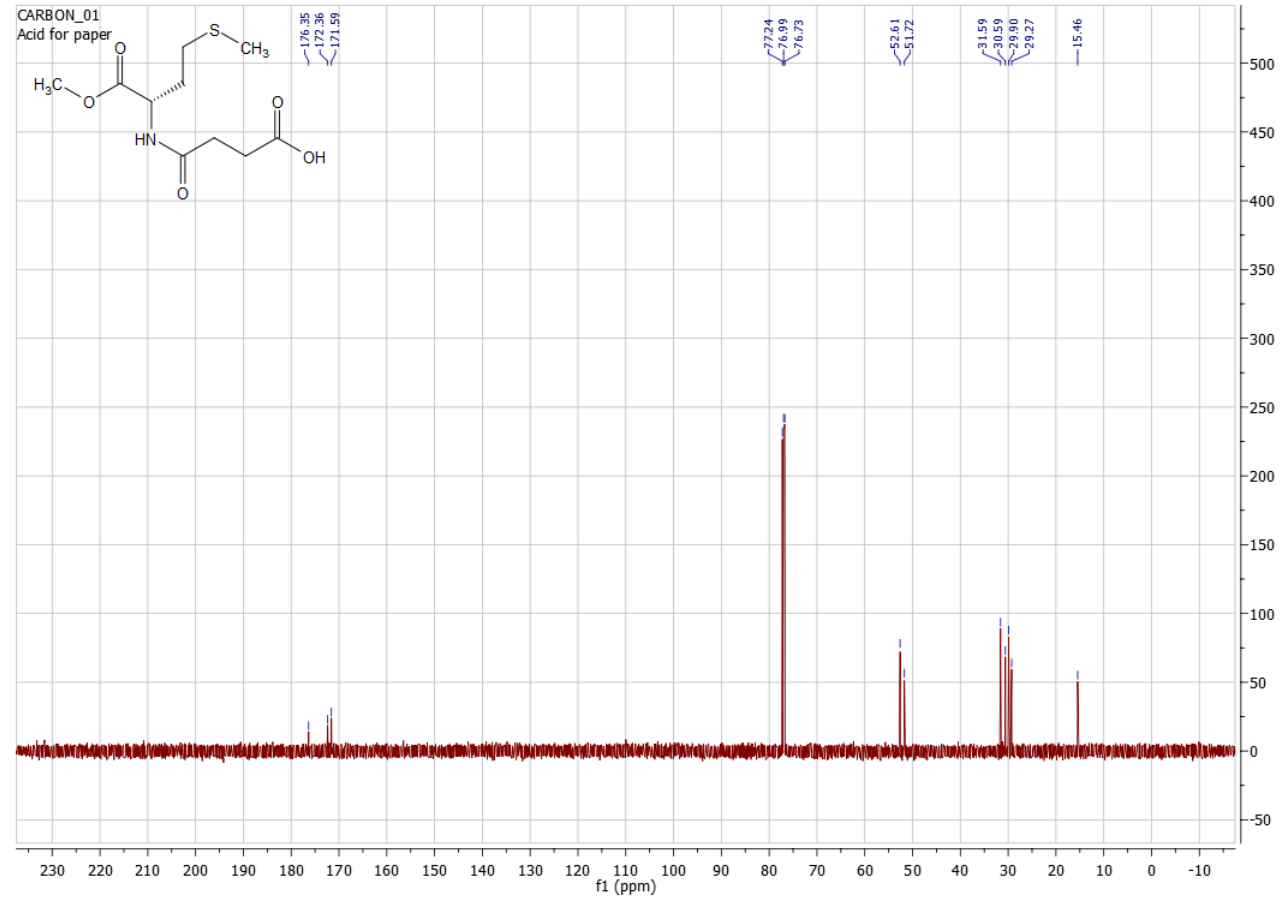
(*S*)-4-((1-methoxy-4-(methylthio)-1-oxobutan-2-yl)amino)-4-oxobutanoic acid





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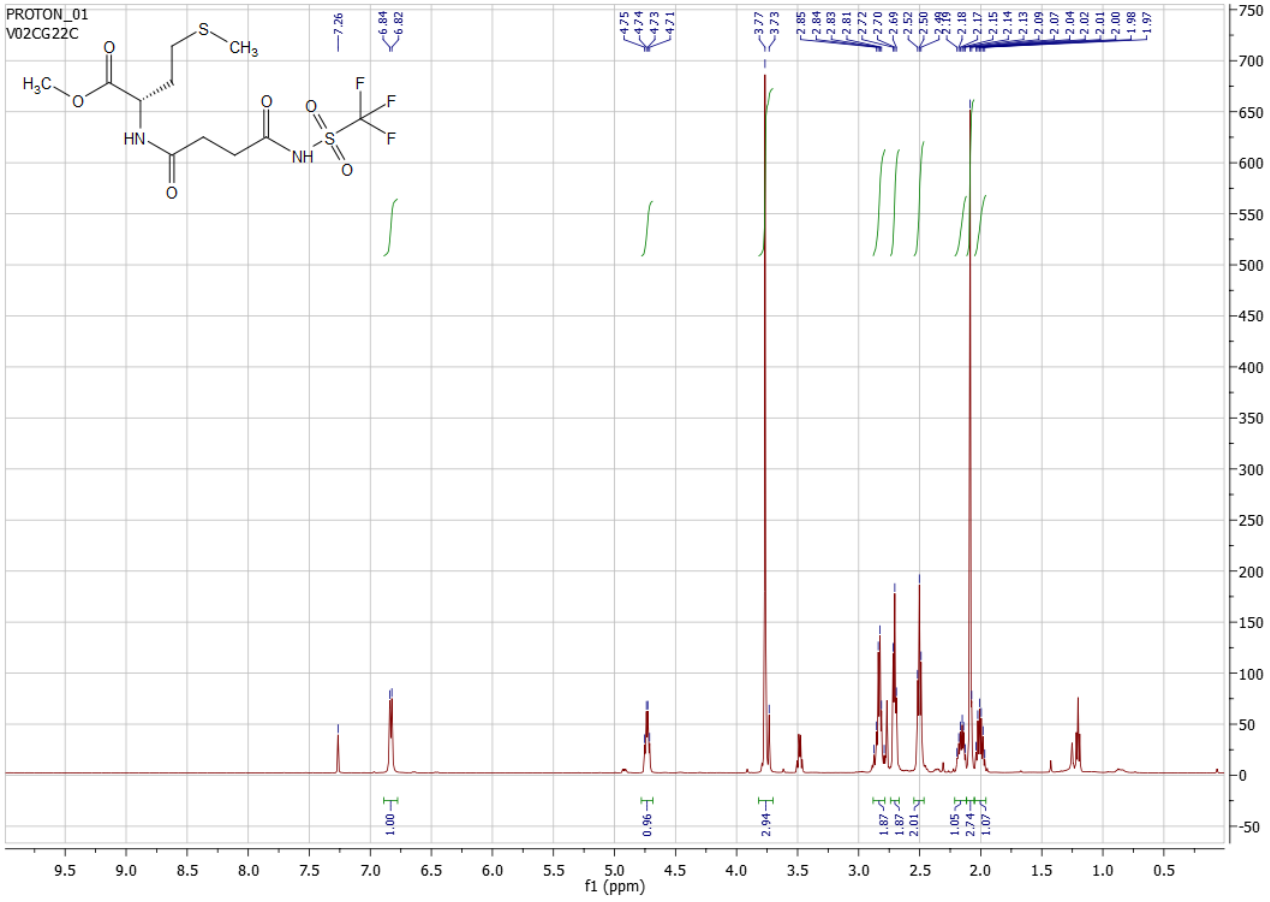
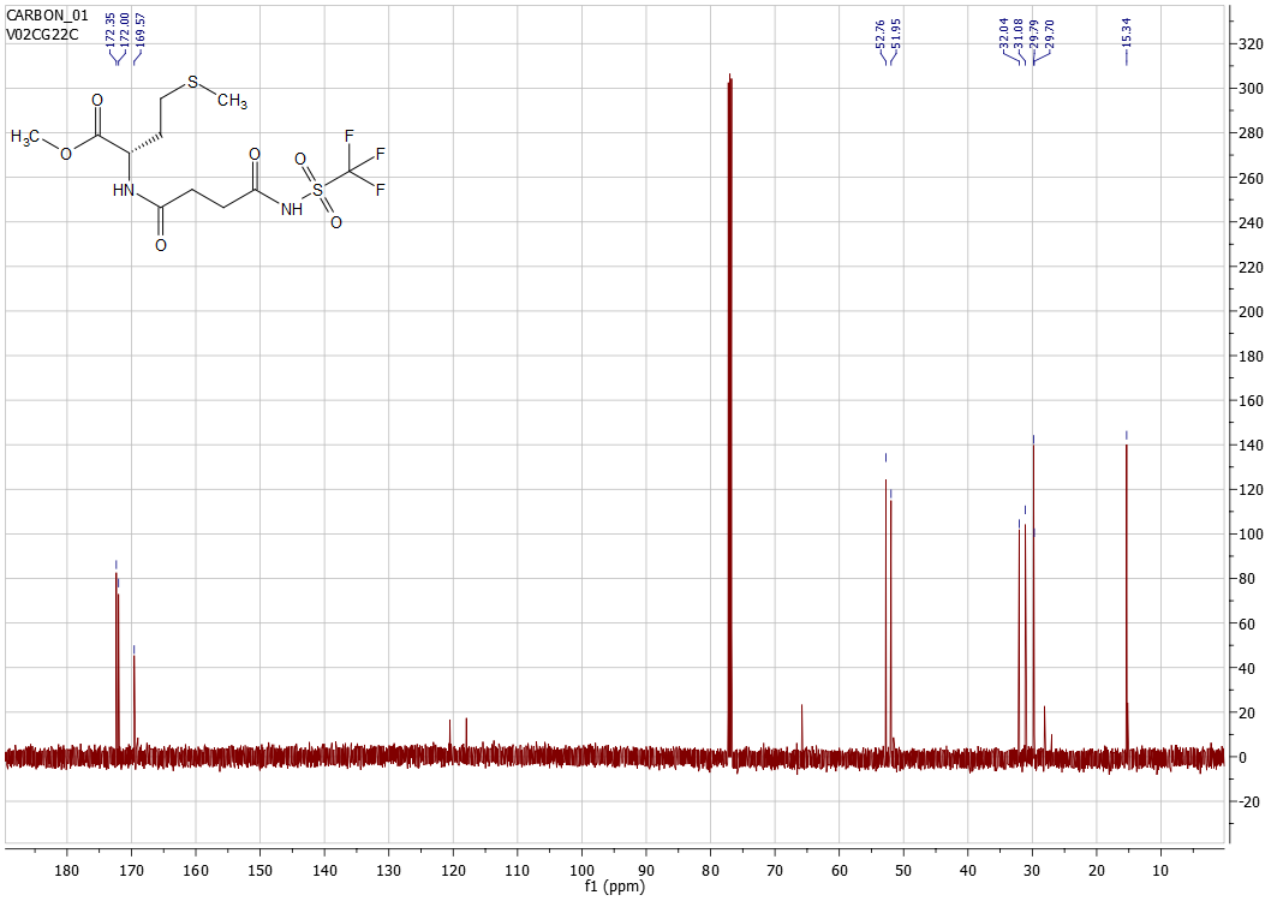
(*S*)-methyl 4-(methylthio)-2-(4-oxo-4 (trifluoromethylsulfonamido)butanamido)butanoate





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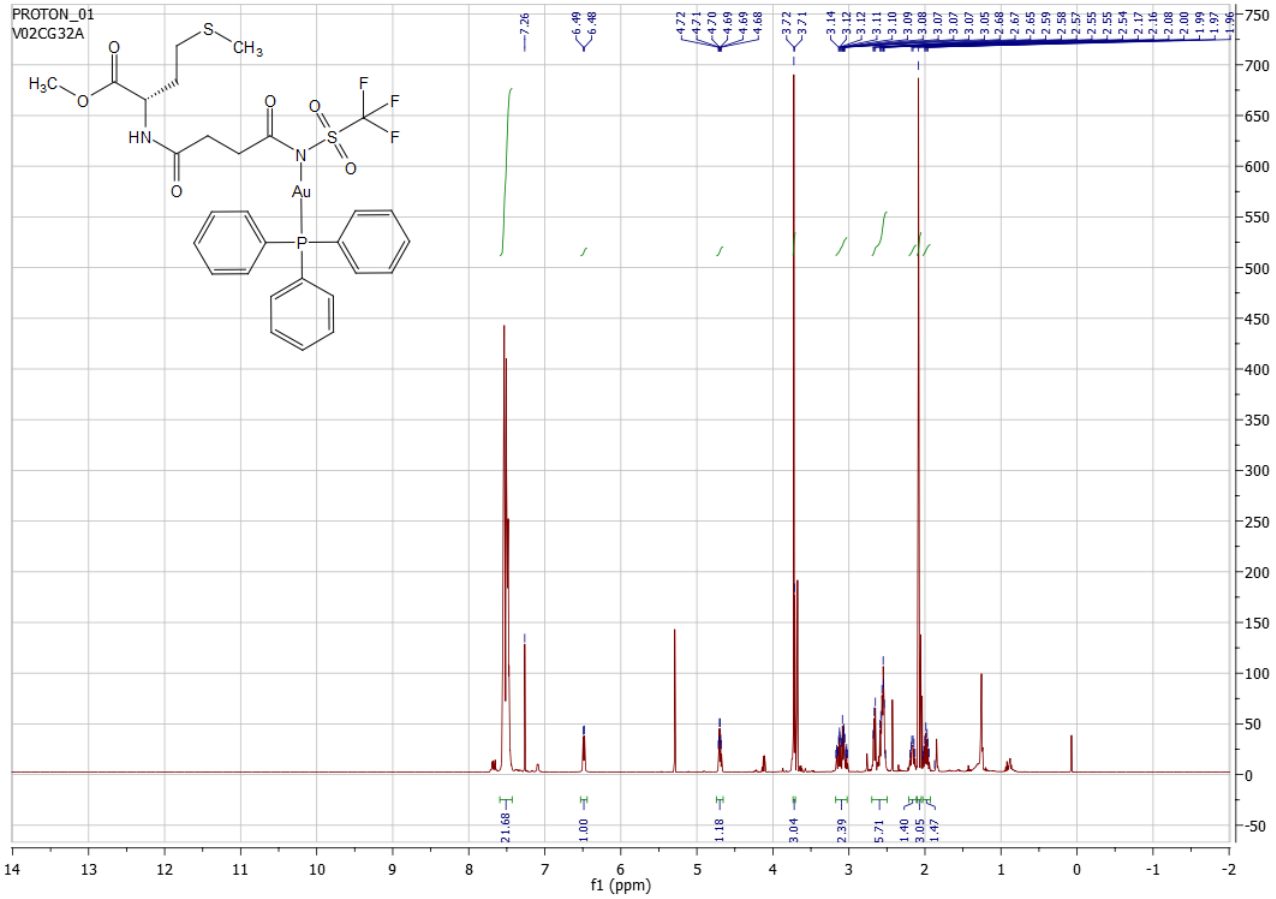
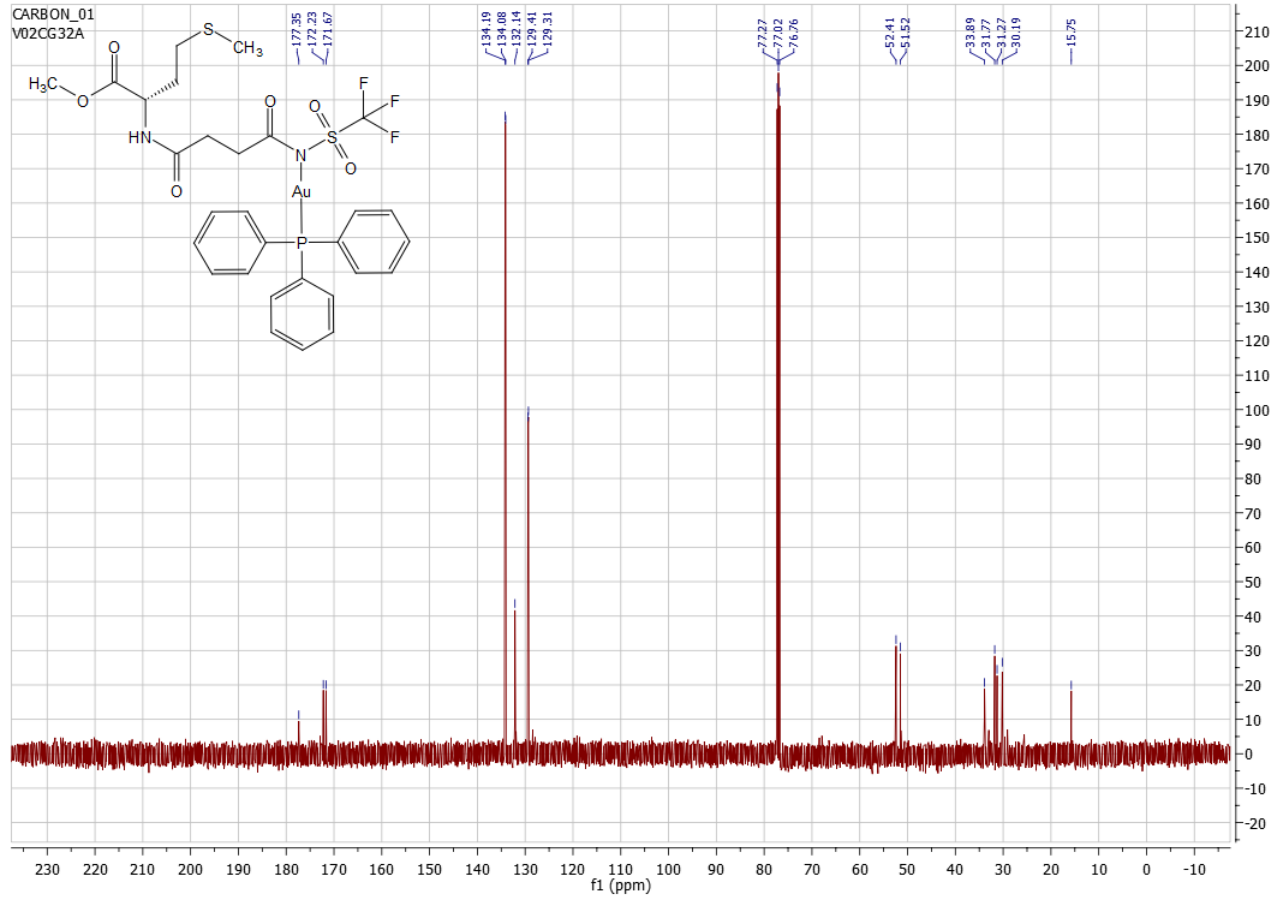
Triphenylphosphine gold (*S*)-methyl 4-(methylthio)-2-(4-oxo-4 (trifluoromethylsulfonamido)butanamido)butanoate





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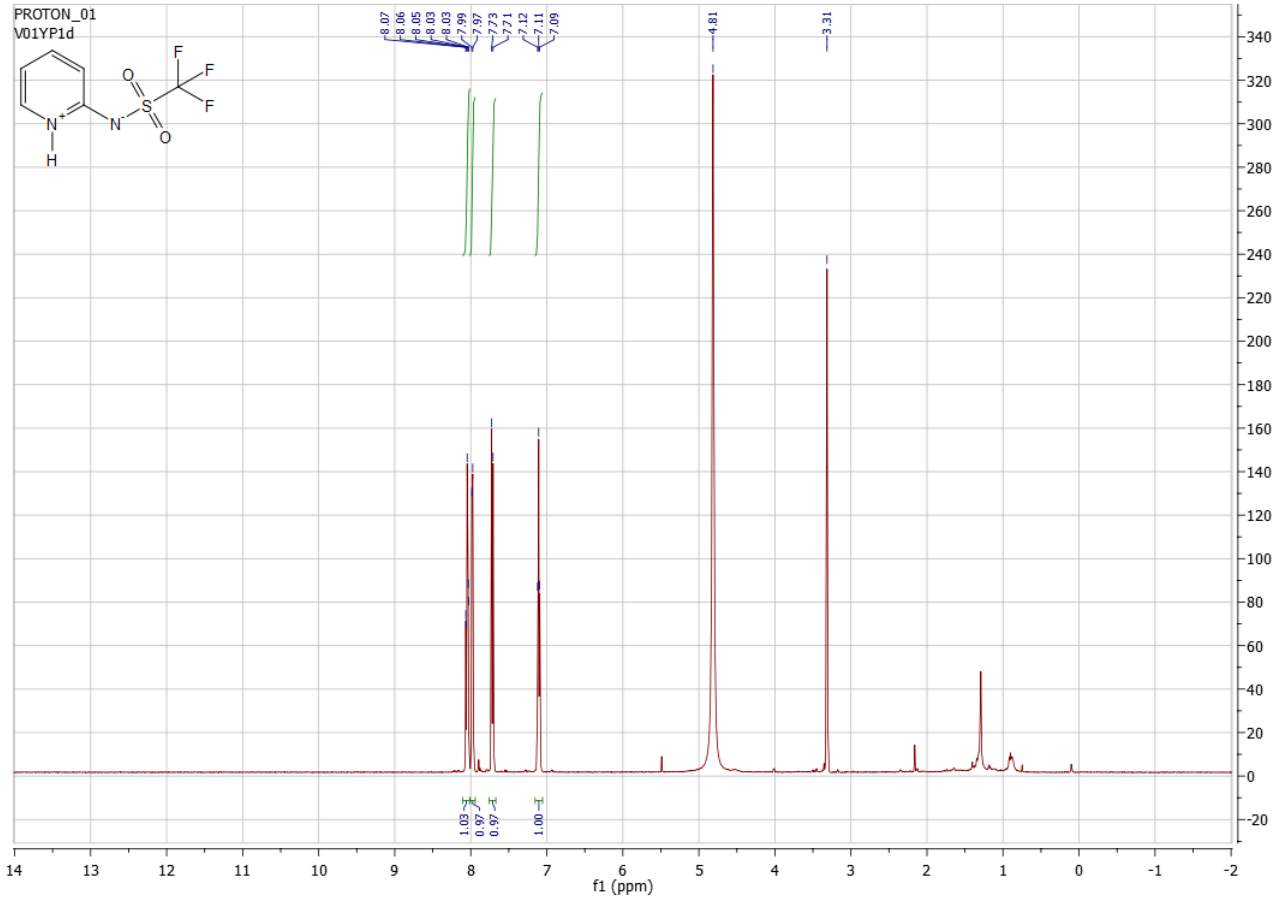
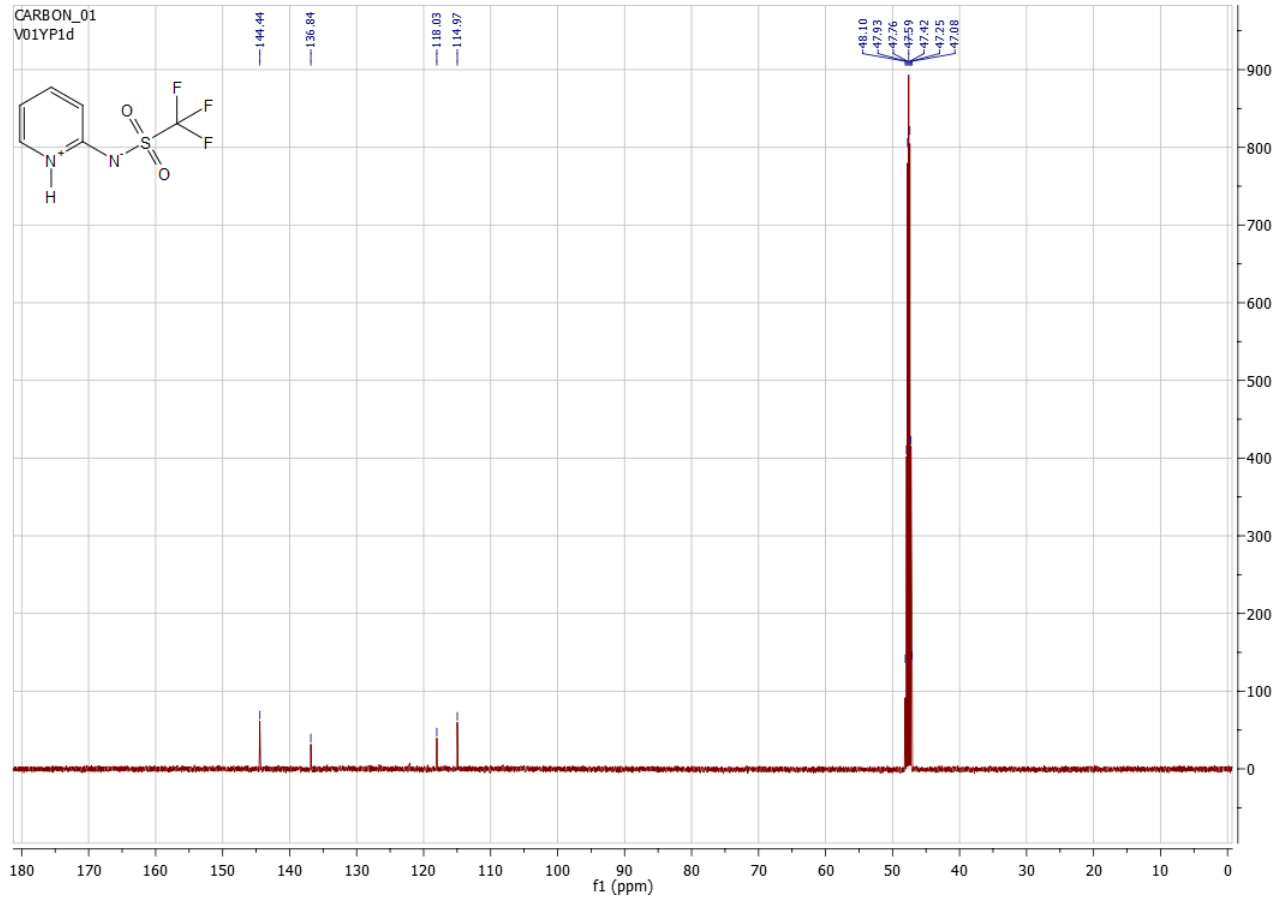
Pyridinium-2-yl(trifluoromethylsulfonyl)amide





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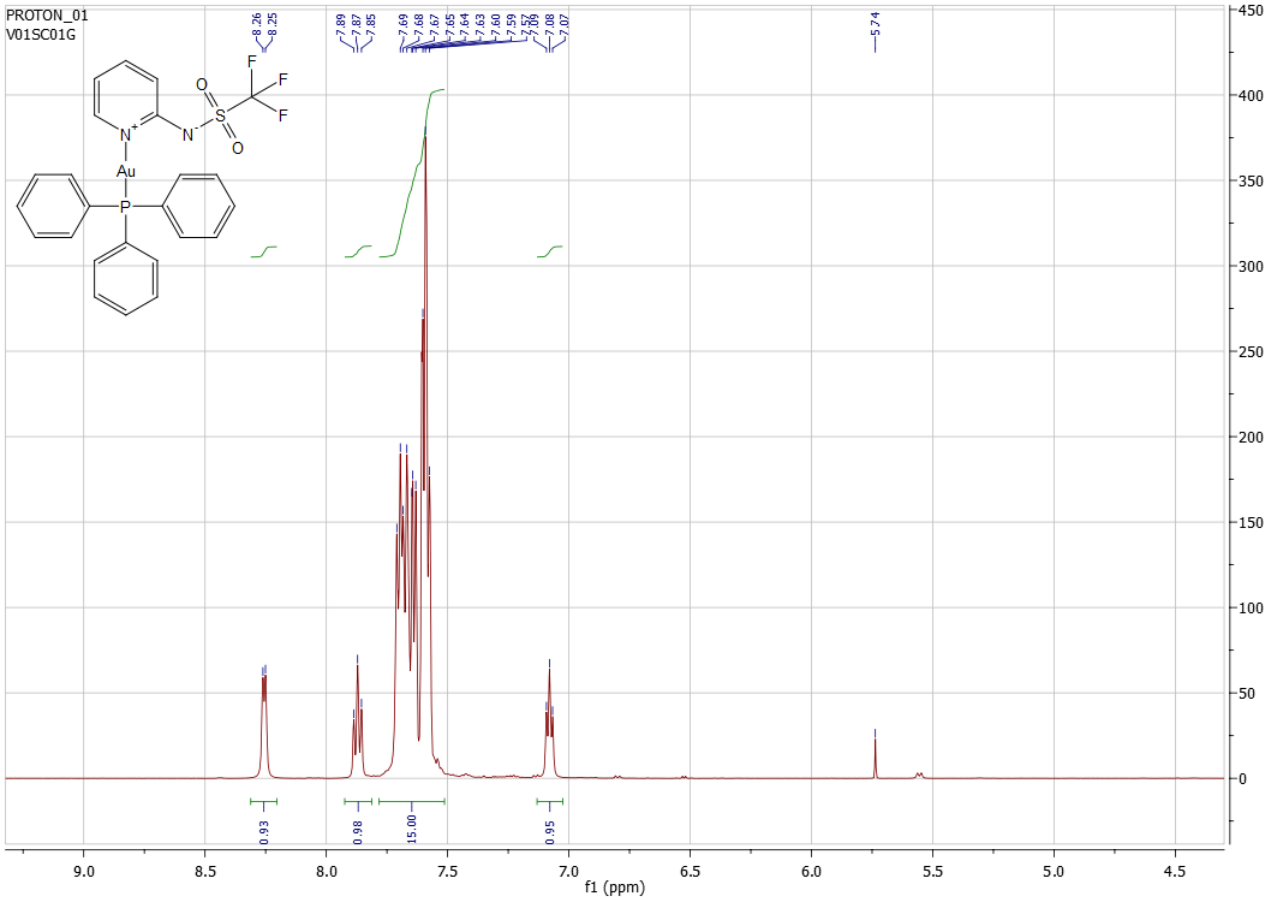
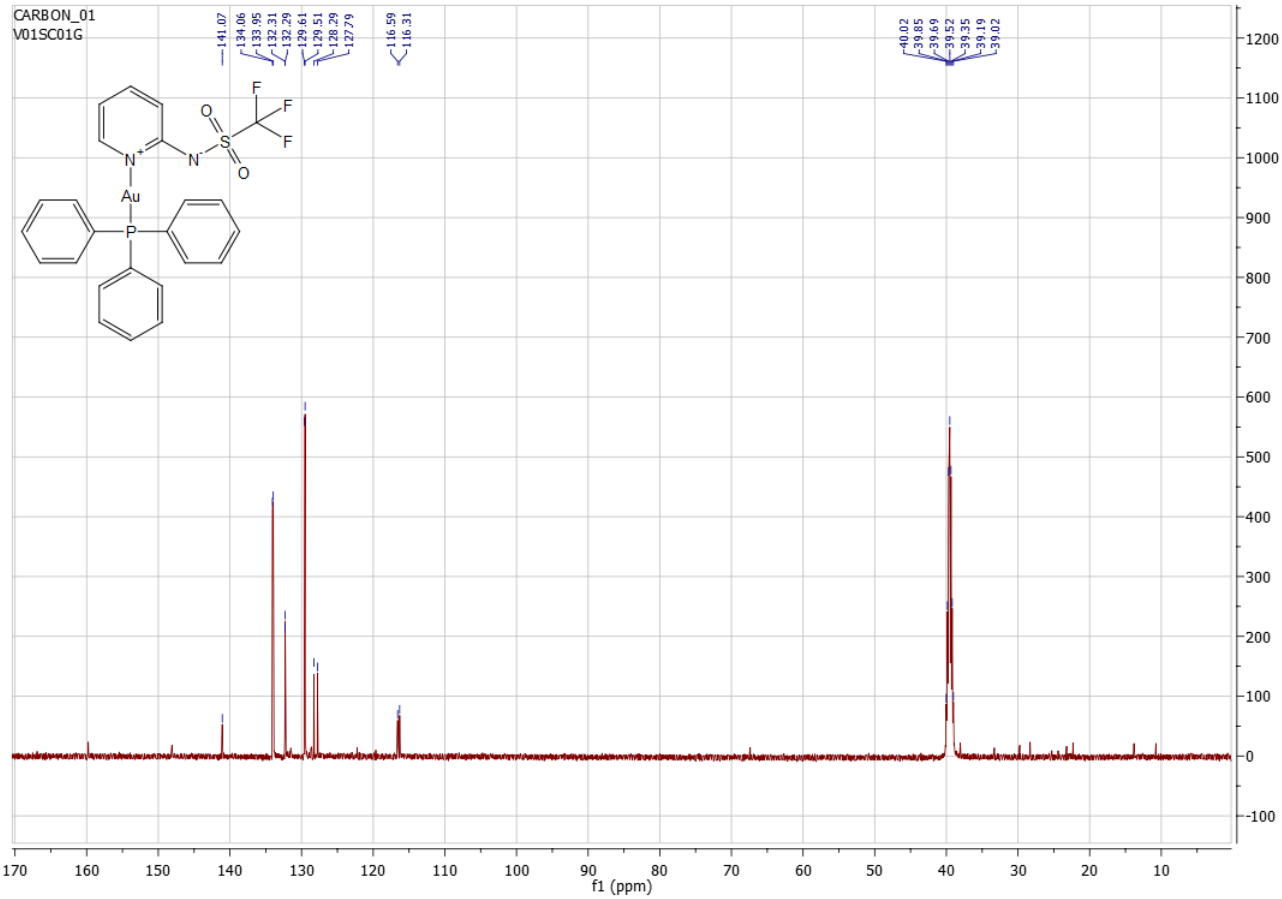
Triphenylphosphine gold pyridinium-2-yl(trifluoromethylsulfonyl)amide





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III. X-Ray Data

Triphenylphosphine gold methyl *N*-[(trifluoromethyl)sulfonyl]-*D*-tryptophanate

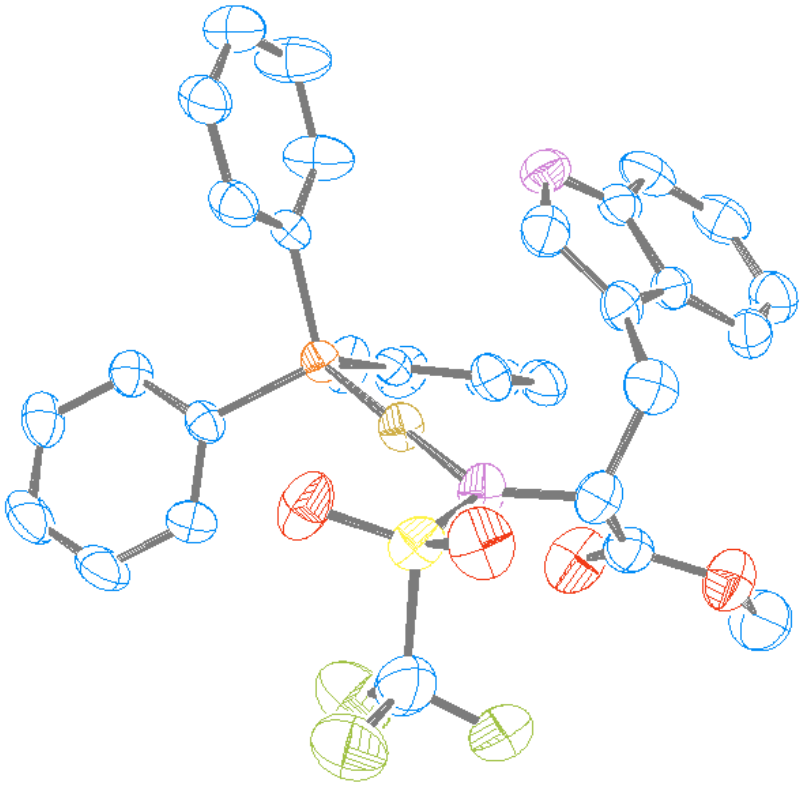

Table 1. Crystal data and structure refinement for import.

Identification code	shelxl
Empirical formula	C37 H33 Au F3 N2 O4 P S
Formula weight	886.65
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P 21
Unit cell dimensions	a = 11.5810(2) A alpha = 90 deg. b = 13.0950(3) A beta = 114.4260(10) deg. c = 13.0305(3) A gamma = 90 deg.
Volume	1799.25(7) A^3
Z, Calculated density	2, 1.637 Mg/m^3
Absorption coefficient	4.248 mm^-1
F(000)	876
Crystal size	0.30 x 0.30 x 0.06 mm
Theta range for data collection	3.43 to 27.26 deg.
Limiting indices	-14<=h<=14, -16<=k<=16, -16<=l<=16
Reflections collected / unique	22995 / 7832 [R(int) = 0.0473]
Completeness to theta = 27.26	98.8 %
Max. and min. transmission	0.7847 and 0.3622
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7832 / 1 / 443
Goodness-of-fit on F^2	1.064
Final R indices [I>2sigma(I)]	R1 = 0.0460, wR2 = 0.1194
R indices (all data)	R1 = 0.0519, wR2 = 0.1249
Absolute structure parameter	0.124(9)
Largest diff. peak and hole	2.021 and -2.166 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for import.

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	903(6)	2412(6)	8357(5)	48(1)
C(2)	-15(7)	2873(8)	7392(7)	76(3)
C(3)	-1254(6)	2477(13)	6963(7)	81(2)
C(4)	-1543(8)	1659(9)	7459(9)	83(3)
C(5)	-630(10)	1218(7)	8425(11)	81(3)

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C(6)	587(8)	1613(6)	8863(7)	64(2)
C(7)	3314(5)	2424(6)	8144(5)	49(1)
C(8)	4562(7)	2686(7)	8478(8)	71(2)
C(9)	5230(9)	2336(7)	7865(10)	82(3)
C(10)	4637(11)	1736(10)	6927(11)	92(3)
C(11)	3383(10)	1453(12)	6613(11)	111(5)
C(12)	2727(9)	1805(10)	7206(10)	95(4)
C(13)	2369(6)	4288(5)	8707(6)	52(2)
C(14)	2251(7)	4701(6)	7697(7)	61(2)
C(15)	2187(9)	5756(7)	7521(9)	77(2)
C(16)	2187(11)	6394(7)	8365(12)	92(3)
C(17)	2259(12)	5996(8)	9349(14)	94(4)
C(18)	2353(9)	4943(7)	9539(8)	69(2)
C(19)	4190(7)	1265(7)	12929(7)	62(2)
C(20)	4547(8)	266(8)	12529(8)	71(2)
C(21)	3962(7)	68(6)	11287(7)	59(2)
C(22)	2778(7)	-444(5)	10628(6)	55(2)
C(23)	2682(9)	-488(7)	9502(7)	60(2)
C(24)	4500(8)	278(7)	10560(9)	73(2)
C(25)	1826(9)	-853(6)	10869(8)	70(2)
C(26)	790(11)	-1291(8)	10006(12)	86(3)
C(27)	689(11)	-1315(8)	8898(10)	88(3)
C(28)	1605(11)	-923(7)	8638(9)	83(3)
C(29)	4950(15)	3708(12)	13902(12)	106(4)
C(30)	2795(9)	1338(7)	12665(8)	68(2)
C(31)	1129(13)	664(12)	13018(14)	116(5)
C(101)	-630(40)	10122(15)	5477(18)	175(12)
C(102)	-1600(20)	9490(20)	5463(19)	152(8)
C(103)	-1450(20)	8470(20)	5410(20)	160(9)
C(104)	-440(30)	8081(17)	5397(17)	156(8)
C(105)	549(16)	8710(30)	5451(14)	187(15)
C(106)	320(30)	9730(30)	5462(18)	174(12)
Au(1)	3547(1)	2531(1)	10771(1)	56(1)
F(1)	4389(12)	3224(7)	14457(9)	150(4)
F(2)	5766(12)	4367(8)	14603(8)	156(4)
F(3)	4029(12)	4275(8)	13141(12)	151(4)
N(1)	4555(6)	2151(5)	12462(4)	62(2)
N(2)	3735(8)	-52(6)	9493(7)	73(2)
O(1)	6550(5)	2309(8)	14176(5)	92(3)
O(2)	6057(7)	3525(7)	12596(6)	94(2)
O(3)	2492(8)	687(7)	13303(8)	95(2)
O(4)	2029(7)	1858(8)	11976(7)	101(2)
P(1)	2500(2)	2931(1)	8963(1)	47(1)
S(5)	5636(2)	2865(2)	13239(2)	67(1)

Table 3. Bond lengths [A] and angles [deg] for import.

C(1)-C(6)	1.365(11)
C(1)-C(2)	1.404(10)
C(1)-P(1)	1.816(7)
C(2)-C(3)	1.406(11)
C(2)-H(2)	0.9300
C(3)-C(4)	1.362(18)
C(3)-H(3)	0.9300
C(4)-C(5)	1.391(16)
C(4)-H(4)	0.9300
C(5)-C(6)	1.383(13)
C(5)-H(5)	0.9300
C(6)-H(6)	0.9300
C(7)-C(8)	1.370(10)
C(7)-C(12)	1.388(11)
C(7)-P(1)	1.817(6)
C(8)-C(9)	1.399(12)
C(8)-H(8)	0.9300
C(9)-C(10)	1.374(16)
C(9)-H(9)	0.9300
C(10)-C(11)	1.387(16)
C(10)-H(10)	0.9300
C(11)-C(12)	1.368(15)
C(11)-H(11)	0.9300
C(12)-H(12)	0.9300
C(13)-C(14)	1.376(11)
C(13)-C(18)	1.388(11)
C(13)-P(1)	1.803(7)
C(14)-C(15)	1.397(12)
C(14)-H(14)	0.9300
C(15)-C(16)	1.382(16)
C(15)-H(15)	0.9300

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C(16)-C(17)	1.354(19)
C(16)-H(16)	0.9300
C(17)-C(18)	1.398(15)
C(17)-H(17)	0.9300
C(18)-H(18)	0.9300
C(19)-N(1)	1.452(11)
C(19)-C(30)	1.509(13)
C(19)-C(20)	1.528(14)
C(19)-H(19)	0.9800
C(20)-C(21)	1.496(12)
C(20)-H(20A)	0.9700
C(20)-H(20B)	0.9700
C(21)-C(24)	1.360(12)
C(21)-C(22)	1.447(12)
C(22)-C(25)	1.374(11)
C(22)-C(23)	1.425(11)
C(23)-N(2)	1.351(13)
C(23)-C(28)	1.410(15)
C(24)-N(2)	1.374(13)
C(24)-H(24)	0.9300
C(25)-C(26)	1.385(15)
C(25)-H(25)	0.9300
C(26)-C(27)	1.399(17)
C(26)-H(26)	0.9300
C(27)-C(28)	1.342(17)
C(27)-H(27)	0.9300
C(28)-H(28)	0.9300
C(29)-F(1)	1.317(15)
C(29)-F(2)	1.327(16)
C(29)-F(3)	1.341(19)
C(29)-S(5)	1.778(15)
C(30)-O(4)	1.183(12)
C(30)-O(3)	1.334(12)
C(31)-O(3)	1.465(16)
C(31)-H(31A)	0.9600
C(31)-H(31B)	0.9600
C(31)-H(31C)	0.9600
C(101)-C(106)	1.23(4)
C(101)-C(102)	1.38(4)
C(101)-H(101)	0.9300
C(102)-C(103)	1.35(4)
C(102)-H(102)	0.9300
C(103)-C(104)	1.28(3)
C(103)-H(103)	0.9300
C(104)-C(105)	1.39(4)
C(104)-H(104)	0.9300
C(105)-C(106)	1.35(4)
C(105)-H(105)	0.9300
C(106)-H(106)	0.9300
Au(1)-N(1)	2.084(5)
Au(1)-P(1)	2.2201(16)
N(1)-S(5)	1.555(6)
N(2)-H(2A)	0.8600
O(1)-S(5)	1.440(7)
O(2)-S(5)	1.423(7)
C(6)-C(1)-C(2)	120.5(7)
C(6)-C(1)-P(1)	120.3(5)
C(2)-C(1)-P(1)	119.1(6)
C(1)-C(2)-C(3)	117.9(9)
C(1)-C(2)-H(2)	121.1
C(3)-C(2)-H(2)	121.1
C(4)-C(3)-C(2)	120.8(9)
C(4)-C(3)-H(3)	119.6
C(2)-C(3)-H(3)	119.6
C(3)-C(4)-C(5)	120.8(8)
C(3)-C(4)-H(4)	119.6
C(5)-C(4)-H(4)	119.6
C(6)-C(5)-C(4)	118.8(10)
C(6)-C(5)-H(5)	120.6
C(4)-C(5)-H(5)	120.6
C(1)-C(6)-C(5)	121.2(8)
C(1)-C(6)-H(6)	119.4
C(5)-C(6)-H(6)	119.4
C(8)-C(7)-C(12)	119.6(7)
C(8)-C(7)-P(1)	117.2(6)
C(12)-C(7)-P(1)	123.2(6)
C(7)-C(8)-C(9)	119.7(8)
C(7)-C(8)-H(8)	120.1

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C(9)-C(8)-H(8)	120.1
C(10)-C(9)-C(8)	120.3(9)
C(10)-C(9)-H(9)	119.8
C(8)-C(9)-H(9)	119.8
C(9)-C(10)-C(11)	119.5(10)
C(9)-C(10)-H(10)	120.3
C(11)-C(10)-H(10)	120.3
C(12)-C(11)-C(10)	120.1(10)
C(12)-C(11)-H(11)	119.9
C(10)-C(11)-H(11)	119.9
C(11)-C(12)-C(7)	120.7(9)
C(11)-C(12)-H(12)	119.7
C(7)-C(12)-H(12)	119.7
C(14)-C(13)-C(18)	118.5(7)
C(14)-C(13)-P(1)	122.1(6)
C(18)-C(13)-P(1)	119.4(6)
C(13)-C(14)-C(15)	121.5(9)
C(13)-C(14)-H(14)	119.2
C(15)-C(14)-H(14)	119.2
C(16)-C(15)-C(14)	119.0(9)
C(16)-C(15)-H(15)	120.5
C(14)-C(15)-H(15)	120.5
C(17)-C(16)-C(15)	120.0(9)
C(17)-C(16)-H(16)	120.0
C(15)-C(16)-H(16)	120.0
C(16)-C(17)-C(18)	121.2(10)
C(16)-C(17)-H(17)	119.4
C(18)-C(17)-H(17)	119.4
C(13)-C(18)-C(17)	119.7(10)
C(13)-C(18)-H(18)	120.1
C(17)-C(18)-H(18)	120.1
N(1)-C(19)-C(30)	108.9(7)
N(1)-C(19)-C(20)	111.9(7)
C(30)-C(19)-C(20)	113.1(7)
N(1)-C(19)-H(19)	107.6
C(30)-C(19)-H(19)	107.6
C(20)-C(19)-H(19)	107.6
C(21)-C(20)-C(19)	116.9(6)
C(21)-C(20)-H(20A)	108.1
C(19)-C(20)-H(20A)	108.1
C(21)-C(20)-H(20B)	108.1
C(19)-C(20)-H(20B)	108.1
H(20A)-C(20)-H(20B)	107.3
C(24)-C(21)-C(22)	105.9(8)
C(24)-C(21)-C(20)	125.8(8)
C(22)-C(21)-C(20)	128.1(7)
C(25)-C(22)-C(23)	119.4(8)
C(25)-C(22)-C(21)	134.2(8)
C(23)-C(22)-C(21)	106.4(7)
N(2)-C(23)-C(28)	131.9(9)
N(2)-C(23)-C(22)	107.8(8)
C(28)-C(23)-C(22)	120.3(9)
C(21)-C(24)-N(2)	110.6(8)
C(21)-C(24)-H(24)	124.7
N(2)-C(24)-H(24)	124.7
C(22)-C(25)-C(26)	118.8(9)
C(22)-C(25)-H(25)	120.6
C(26)-C(25)-H(25)	120.6
C(25)-C(26)-C(27)	121.5(9)
C(25)-C(26)-H(26)	119.3
C(27)-C(26)-H(26)	119.3
C(28)-C(27)-C(26)	121.0(10)
C(28)-C(27)-H(27)	119.5
C(26)-C(27)-H(27)	119.5
C(27)-C(28)-C(23)	118.9(10)
C(27)-C(28)-H(28)	120.6
C(23)-C(28)-H(28)	120.6
F(1)-C(29)-F(2)	107.9(12)
F(1)-C(29)-F(3)	104.6(14)
F(2)-C(29)-F(3)	105.7(14)
F(1)-C(29)-S(5)	112.9(11)
F(2)-C(29)-S(5)	113.8(11)
F(3)-C(29)-S(5)	111.3(10)
O(4)-C(30)-O(3)	122.2(9)
O(4)-C(30)-C(19)	127.2(9)
O(3)-C(30)-C(19)	110.5(8)
O(3)-C(31)-H(31A)	109.5
O(3)-C(31)-H(31B)	109.5

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H(31A)-C(31)-H(31B)	109.5
O(3)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(106)-C(101)-C(102)	118(2)
C(106)-C(101)-H(101)	120.9
C(102)-C(101)-H(101)	120.9
C(103)-C(102)-C(101)	118(2)
C(103)-C(102)-H(102)	120.9
C(101)-C(102)-H(102)	120.9
C(104)-C(103)-C(102)	122(2)
C(104)-C(103)-H(103)	119.0
C(102)-C(103)-H(103)	119.0
C(103)-C(104)-C(105)	120(2)
C(103)-C(104)-H(104)	120.0
C(105)-C(104)-H(104)	120.0
C(106)-C(105)-C(104)	115.1(18)
C(106)-C(105)-H(105)	122.4
C(104)-C(105)-H(105)	122.4
C(101)-C(106)-C(105)	126(2)
C(101)-C(106)-H(106)	116.8
C(105)-C(106)-H(106)	116.8
N(1)-Au(1)-P(1)	179.1(2)
C(19)-N(1)-S(5)	120.2(5)
C(19)-N(1)-Au(1)	120.1(5)
S(5)-N(1)-Au(1)	119.5(4)
C(23)-N(2)-C(24)	109.3(7)
C(23)-N(2)-H(2A)	125.4
C(24)-N(2)-H(2A)	125.4
C(30)-O(3)-C(31)	112.9(10)
C(13)-P(1)-C(1)	107.2(3)
C(13)-P(1)-C(7)	106.0(4)
C(1)-P(1)-C(7)	106.8(3)
C(13)-P(1)-Au(1)	113.3(3)
C(1)-P(1)-Au(1)	112.6(2)
C(7)-P(1)-Au(1)	110.4(2)
O(2)-S(5)-O(1)	119.7(5)
O(2)-S(5)-N(1)	111.2(4)
O(1)-S(5)-N(1)	111.1(5)
O(2)-S(5)-C(29)	103.9(6)
O(1)-S(5)-C(29)	102.8(6)
N(1)-S(5)-C(29)	106.7(6)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for import.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

–

	U11	U22	U33	U23	U13	U12
C(1)	50(3)	43(4)	46(3)	-3(3)	17(2)	0(3)
C(2)	47(3)	102(7)	58(4)	19(4)	2(3)	-7(4)
C(3)	44(3)	116(7)	66(4)	-7(8)	6(3)	-15(7)
C(4)	50(4)	112(7)	81(6)	-33(6)	22(4)	-10(4)
C(5)	75(5)	64(5)	114(8)	-12(5)	50(6)	-8(4)
C(6)	63(4)	53(4)	67(5)	6(3)	18(4)	2(3)
C(7)	49(3)	39(3)	51(3)	-3(3)	14(2)	3(3)
C(8)	61(4)	60(6)	89(5)	-18(4)	29(4)	-9(4)
C(9)	65(4)	68(7)	120(7)	-24(5)	46(5)	-13(4)
C(10)	84(7)	102(7)	94(8)	-19(6)	42(6)	6(6)
C(11)	70(6)	152(12)	105(9)	-65(9)	28(6)	-6(6)
C(12)	51(4)	127(9)	90(7)	-54(6)	12(4)	-5(5)
C(13)	43(3)	44(3)	65(4)	-1(3)	18(3)	1(2)
C(14)	56(4)	59(4)	62(4)	11(3)	18(3)	10(3)
C(15)	67(5)	62(5)	97(7)	25(5)	29(5)	12(4)
C(16)	100(7)	45(4)	134(10)	5(5)	50(7)	17(4)
C(17)	96(8)	60(5)	146(12)	-26(7)	70(8)	5(5)
C(18)	71(5)	66(5)	73(5)	-7(4)	31(4)	8(4)
C(19)	57(4)	76(5)	45(4)	12(3)	12(3)	3(3)
C(20)	60(4)	76(5)	61(5)	12(4)	9(3)	18(4)
C(21)	61(4)	53(3)	56(4)	17(3)	19(3)	14(3)
C(22)	65(4)	49(3)	52(4)	13(3)	25(3)	16(3)
C(23)	77(5)	50(4)	55(4)	8(3)	29(4)	17(4)
C(24)	63(4)	69(5)	93(7)	20(4)	39(5)	19(4)
C(25)	75(5)	62(4)	74(5)	9(4)	34(4)	2(4)

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C(26)	87(6)	66(5)	116(9)	-12(5)	53(6)	-18(5)
C(27)	81(6)	73(6)	97(8)	-29(5)	24(6)	-8(5)
C(28)	102(8)	63(5)	70(6)	-16(4)	23(5)	14(5)
C(29)	125(10)	112(9)	89(8)	-17(7)	51(8)	-28(8)
C(30)	74(5)	68(4)	64(5)	-9(4)	30(4)	-6(4)
C(31)	98(9)	119(10)	155(14)	-20(10)	77(10)	-26(8)
C(101)	330(40)	98(11)	116(14)	-25(10)	110(20)	-17(18)
C(102)	180(20)	170(20)	111(12)	-1(15)	63(12)	48(17)
C(103)	180(20)	140(17)	210(20)	-47(16)	131(19)	-47(15)
C(104)	220(30)	130(13)	118(13)	15(11)	67(16)	63(16)
C(105)	77(9)	380(50)	68(8)	-43(16)	-2(7)	55(16)
C(106)	210(30)	220(30)	130(16)	-75(19)	111(19)	-110(20)
Au(1)	53(1)	61(1)	38(1)	3(1)	4(1)	-3(1)
F(1)	228(12)	120(6)	176(9)	-19(6)	158(10)	-19(7)
F(2)	223(11)	131(7)	108(6)	-62(6)	62(7)	-64(7)
F(3)	152(9)	111(7)	182(11)	-12(7)	60(8)	19(6)
N(1)	59(3)	76(4)	26(2)	4(2)	-6(2)	-16(3)
N(2)	90(5)	74(4)	64(4)	10(3)	43(4)	18(4)
O(1)	68(3)	105(10)	61(4)	4(3)	-15(3)	-5(3)
O(2)	83(4)	129(6)	65(4)	-5(4)	24(3)	-46(4)
O(3)	91(5)	104(5)	101(5)	15(4)	50(4)	-7(4)
O(4)	60(4)	138(7)	96(5)	25(5)	24(3)	14(4)
P(1)	47(1)	47(1)	37(1)	3(1)	7(1)	1(1)
S(5)	52(1)	92(2)	47(1)	-9(1)	9(1)	-15(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for import.

	x	y	z	U(eq)
H(2)	190	3423	7047	91
H(3)	-1884	2778	6333	97
H(4)	-2360	1393	7149	99
H(5)	-834	667	8770	97
H(6)	1200	1329	9515	77
H(8)	4964	3095	9110	85
H(9)	6078	2511	8093	98
H(10)	5074	1521	6507	110
H(11)	2987	1023	5998	134
H(12)	1879	1628	6977	114
H(14)	2214	4267	7119	73
H(15)	2145	6024	6845	93
H(16)	2138	7098	8258	111
H(17)	2246	6431	9908	113
H(18)	2405	4681	10221	83
H(19)	4656	1295	13751	75
H(20A)	5461	253	12784	85
H(20B)	4320	-293	12897	85
H(24)	5278	600	10758	88
H(25)	1877	-836	11600	84
H(26)	147	-1575	10166	103
H(27)	-24	-1606	8334	106
H(28)	1530	-938	7899	99
H(31A)	965	197	13509	174
H(31B)	680	445	12251	174
H(31C)	848	1335	13105	174
H(101)	-705	10828	5497	210
H(102)	-2327	9759	5486	183
H(103)	-2094	8038	5391	192
H(104)	-372	7377	5349	187
H(105)	1310	8458	5477	224
H(106)	953	10165	5459	209
H(2A)	3900	9	8910	87

Table 6. Torsion angles [deg] for import.

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(*S*)-methyl 3-(4-(((trifluoromethyl)sulfonyl)oxy)phenyl)-2-(trifluoromethylsulfonamido)propanoate

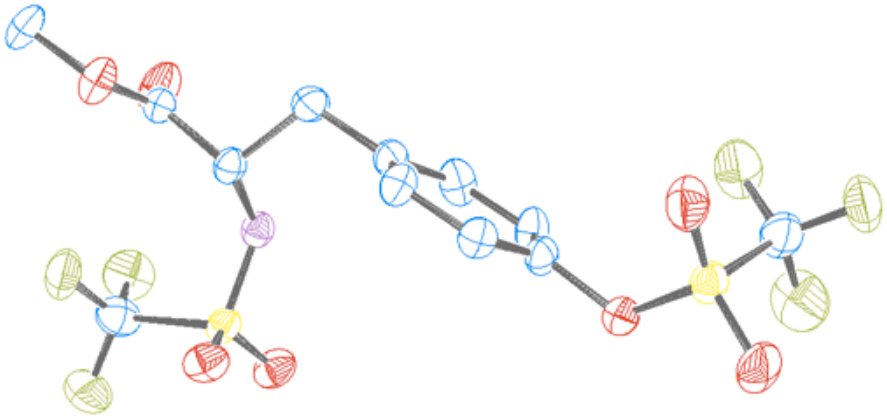

Table 1. Crystal data and structure refinement for import.

Identification code	shelxl
Empirical formula	C12 H10 F6 N O7 S2
Formula weight	458.33
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	triclinic, P1
Unit cell dimensions	a = 8.6306(4) A alpha = 75.784(2) deg. b = 10.5975(6) A beta = 68.397(3) deg. c = 11.0234(6) A gamma = 84.028(3) deg.
Volume	908.60(8) A^3
Z, Calculated density	2, 1.675 Mg/m^3
Absorption coefficient	0.388 mm^-1
F(000)	462
Crystal size	0.14 x 0.14 x 0.08 mm

Theta range for data collection	2.04 to 27.55 deg.
Limiting indices	-10<=h<=11, -13<=k<=13, -14<=l<=14
Reflections collected / unique	12584 / 7333 [R(int) = 0.0400]
Completeness to theta = 27.55	97.8 %
Max. and min. transmission	0.9696 and 0.9476
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7333 / 3 / 505
Goodness-of-fit on F^2	1.050
Final R indices [I>2sigma(I)]	R1 = 0.0547, wR2 = 0.1157
R indices (all data)	R1 = 0.0905, wR2 = 0.1342
Absolute structure parameter	0.03(8)
Largest diff. peak and hole	0.314 and -0.272 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for import.

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	-2206(8)	-1629(8)	3049(7)	74(2)
C(2)	-672(6)	415(5)	4338(5)	49(1)
C(3)	-259(6)	228(5)	5422(5)	52(1)
C(4)	1293(7)	696(5)	5260(5)	56(1)
C(5)	2312(6)	1358(5)	4020(5)	51(1)
C(6)	1785(8)	1536(6)	2957(5)	64(2)
C(7)	272(7)	1101(6)	3077(5)	60(1)
C(8)	3993(7)	1835(5)	3864(6)	58(1)
C(9)	3815(6)	3178(4)	4263(4)	46(1)
C(10)	5594(6)	3614(5)	3967(6)	51(1)
C(11)	7604(7)	3688(7)	4922(7)	81(2)
C(12)	3050(9)	6507(6)	4017(7)	73(2)
C(51)	13702(10)	9638(8)	9908(7)	83(2)
C(52)	12253(6)	7432(5)	8778(5)	51(1)
C(53)	11231(7)	6831(6)	10005(5)	62(2)
C(54)	9701(7)	6398(6)	10128(5)	64(2)
C(55)	9227(6)	6606(5)	9021(5)	49(1)

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C(56)	10333(7)	7204(5)	7789(5)	55(1)
C(57)	11848(7)	7608(6)	7644(5)	59(1)
C(58)	7578(7)	6141(5)	9151(6)	57(1)
C(59)	7408(5)	4667(4)	9487(4)	47(1)
C(60)	5688(6)	4386(5)	9562(5)	51(1)
C(61)	4101(7)	4078(7)	8316(7)	79(2)
C(62)	8500(9)	1493(6)	9068(7)	73(2)
F(1)	-633(5)	-1420(5)	2369(4)	111(2)
F(2)	-2540(5)	-2805(4)	3086(4)	96(1)
F(3)	-3111(7)	-847(5)	2458(4)	122(2)
F(4)	3834(5)	6031(4)	4861(4)	94(1)
F(5)	4159(5)	6869(4)	2811(4)	102(1)
F(6)	2119(5)	7497(4)	4374(5)	106(1)
F(51)	14023(7)	10863(5)	9791(5)	120(2)
F(52)	14506(11)	8958(7)	10619(5)	187(3)
F(53)	12143(7)	9475(7)	10517(6)	185(3)
F(54)	7051(5)	1560(4)	10066(4)	104(1)
F(55)	8163(6)	1616(4)	7975(5)	114(2)
F(56)	9188(6)	370(4)	9344(6)	139(2)
N(1)	3024(4)	4134(4)	3464(3)	49(1)
N(51)	8780(4)	4106(4)	8491(4)	48(1)
O(1)	-1719(6)	-2263(4)	5314(4)	79(1)
O(2)	-4509(5)	-1459(5)	5290(4)	89(1)
O(3)	-2307(4)	45(3)	4472(4)	58(1)
O(4)	5978(5)	3277(4)	5057(4)	71(1)
O(5)	6456(5)	4206(5)	2910(4)	85(1)
O(6)	774(4)	4745(4)	5401(3)	64(1)
O(7)	985(4)	5799(4)	3084(3)	69(1)
O(51)	16131(5)	9270(5)	7834(5)	89(1)
O(52)	13476(6)	10084(4)	7558(5)	86(1)
O(53)	13880(4)	7801(4)	8651(4)	59(1)
O(54)	5682(4)	4291(4)	8394(3)	61(1)
O(55)	4477(4)	4304(4)	10556(3)	69(1)
O(56)	9814(5)	2702(4)	10189(4)	86(1)
O(57)	11239(4)	2724(4)	7779(4)	76(1)
S(1)	-2753(2)	-1405(1)	4739(1)	56(1)
S(2)	1741(1)	5215(1)	4032(1)	50(1)
S(51)	14387(2)	9270(1)	8284(1)	58(1)
S(52)	9793(2)	2820(1)	8896(1)	56(1)

Table 3. Bond lengths [A] and angles [deg] for import.

C(1)-F(2)	1.296(8)
C(1)-F(1)	1.298(7)
C(1)-F(3)	1.303(8)
C(1)-S(1)	1.815(7)
C(2)-C(3)	1.333(7)
C(2)-C(7)	1.385(7)
C(2)-O(3)	1.450(6)
C(3)-C(4)	1.410(7)
C(3)-H(3)	0.9300
C(4)-C(5)	1.381(7)
C(4)-H(4)	0.9300
C(5)-C(6)	1.373(8)
C(5)-C(8)	1.521(7)
C(6)-C(7)	1.379(8)
C(6)-H(6)	0.9300
C(7)-H(7)	0.9300
C(8)-C(9)	1.567(7)
C(8)-H(8A)	0.9700
C(8)-H(8B)	0.9700
C(9)-N(1)	1.459(6)
C(9)-C(10)	1.543(7)
C(9)-H(9)	0.9800
C(10)-O(5)	1.184(6)
C(10)-O(4)	1.319(6)
C(11)-O(4)	1.457(7)
C(11)-H(11A)	0.9600
C(11)-H(11B)	0.9600
C(11)-H(11C)	0.9600
C(12)-F(6)	1.302(7)
C(12)-F(5)	1.311(7)
C(12)-F(4)	1.319(7)
C(12)-S(2)	1.857(7)
C(51)-F(53)	1.271(9)
C(51)-F(52)	1.279(9)
C(51)-F(51)	1.321(9)
C(51)-S(51)	1.795(7)

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C(52)-C(53)	1.352(7)
C(52)-C(57)	1.384(7)
C(52)-O(53)	1.444(6)
C(53)-C(54)	1.391(8)
C(53)-H(53)	0.9300
C(54)-C(55)	1.386(7)
C(54)-H(54)	0.9300
C(55)-C(56)	1.381(7)
C(55)-C(58)	1.500(7)
C(56)-C(57)	1.360(8)
C(56)-H(56)	0.9300
C(57)-H(57)	0.9300
C(58)-C(59)	1.524(7)
C(58)-H(58A)	0.9700
C(58)-H(58B)	0.9700
C(59)-N(51)	1.476(6)
C(59)-C(60)	1.514(6)
C(59)-H(59)	0.9800
C(60)-O(55)	1.195(6)
C(60)-O(54)	1.317(5)
C(61)-O(54)	1.442(6)
C(61)-H(61A)	0.9600
C(61)-H(61B)	0.9600
C(61)-H(61C)	0.9600
C(62)-F(56)	1.292(7)
C(62)-F(55)	1.314(8)
C(62)-F(54)	1.337(8)
C(62)-S(52)	1.817(7)
N(1)-S(2)	1.584(4)
N(51)-S(52)	1.600(4)
O(1)-S(1)	1.411(4)
O(2)-S(1)	1.411(4)
O(3)-S(1)	1.554(4)
O(6)-S(2)	1.418(3)
O(7)-S(2)	1.415(4)
O(51)-S(51)	1.400(4)
O(52)-S(51)	1.409(4)
O(53)-S(51)	1.575(4)
O(56)-S(52)	1.407(4)
O(57)-S(52)	1.409(4)
F(2)-C(1)-F(1)	109.1(6)
F(2)-C(1)-F(3)	106.9(6)
F(1)-C(1)-F(3)	110.3(6)
F(2)-C(1)-S(1)	110.0(5)
F(1)-C(1)-S(1)	111.0(5)
F(3)-C(1)-S(1)	109.5(5)
C(3)-C(2)-C(7)	124.6(5)
C(3)-C(2)-O(3)	119.7(5)
C(7)-C(2)-O(3)	115.1(5)
C(2)-C(3)-C(4)	117.8(5)
C(2)-C(3)-H(3)	121.1
C(4)-C(3)-H(3)	121.1
C(5)-C(4)-C(3)	120.4(5)
C(5)-C(4)-H(4)	119.8
C(3)-C(4)-H(4)	119.8
C(6)-C(5)-C(4)	118.4(5)
C(6)-C(5)-C(8)	122.1(5)
C(4)-C(5)-C(8)	119.5(5)
C(5)-C(6)-C(7)	122.9(5)
C(5)-C(6)-H(6)	118.5
C(7)-C(6)-H(6)	118.5
C(6)-C(7)-C(2)	115.8(5)
C(6)-C(7)-H(7)	122.1
C(2)-C(7)-H(7)	122.1
C(5)-C(8)-C(9)	111.3(4)
C(5)-C(8)-H(8A)	109.4
C(9)-C(8)-H(8A)	109.4
C(5)-C(8)-H(8B)	109.4
C(9)-C(8)-H(8B)	109.4
H(8A)-C(8)-H(8B)	108.0
N(1)-C(9)-C(10)	109.7(4)
N(1)-C(9)-C(8)	110.0(4)
C(10)-C(9)-C(8)	106.9(4)
N(1)-C(9)-H(9)	110.1
C(10)-C(9)-H(9)	110.1
C(8)-C(9)-H(9)	110.1
O(5)-C(10)-O(4)	125.6(5)

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O(5)-C(10)-C(9)	123.9(5)
O(4)-C(10)-C(9)	110.5(4)
O(4)-C(11)-H(11A)	109.5
O(4)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
O(4)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
F(6)-C(12)-F(5)	110.3(5)
F(6)-C(12)-F(4)	109.7(6)
F(5)-C(12)-F(4)	108.8(6)
F(6)-C(12)-S(2)	110.0(5)
F(5)-C(12)-S(2)	109.2(5)
F(4)-C(12)-S(2)	108.9(4)
F(53)-C(51)-F(52)	110.3(7)
F(53)-C(51)-F(51)	108.0(7)
F(52)-C(51)-F(51)	105.5(7)
F(53)-C(51)-S(51)	111.7(6)
F(52)-C(51)-S(51)	111.2(6)
F(51)-C(51)-S(51)	110.0(5)
C(53)-C(52)-C(57)	122.5(5)
C(53)-C(52)-O(53)	117.8(5)
C(57)-C(52)-O(53)	119.5(5)
C(52)-C(53)-C(54)	118.5(5)
C(52)-C(53)-H(53)	120.8
C(54)-C(53)-H(53)	120.8
C(55)-C(54)-C(53)	120.5(5)
C(55)-C(54)-H(54)	119.7
C(53)-C(54)-H(54)	119.7
C(56)-C(55)-C(54)	118.6(5)
C(56)-C(55)-C(58)	120.7(5)
C(54)-C(55)-C(58)	120.7(5)
C(57)-C(56)-C(55)	121.7(5)
C(57)-C(56)-H(56)	119.1
C(55)-C(56)-H(56)	119.1
C(56)-C(57)-C(52)	118.2(5)
C(56)-C(57)-H(57)	120.9
C(52)-C(57)-H(57)	120.9
C(55)-C(58)-C(59)	115.0(4)
C(55)-C(58)-H(58A)	108.5
C(59)-C(58)-H(58A)	108.5
C(55)-C(58)-H(58B)	108.5
C(59)-C(58)-H(58B)	108.5
H(58A)-C(58)-H(58B)	107.5
N(51)-C(59)-C(60)	114.1(4)
N(51)-C(59)-C(58)	109.6(4)
C(60)-C(59)-C(58)	107.5(4)
N(51)-C(59)-H(59)	108.5
C(60)-C(59)-H(59)	108.5
C(58)-C(59)-H(59)	108.5
O(55)-C(60)-O(54)	124.5(5)
O(55)-C(60)-C(59)	123.6(4)
O(54)-C(60)-C(59)	111.9(4)
O(54)-C(61)-H(61A)	109.5
O(54)-C(61)-H(61B)	109.5
H(61A)-C(61)-H(61B)	109.5
O(54)-C(61)-H(61C)	109.5
H(61A)-C(61)-H(61C)	109.5
H(61B)-C(61)-H(61C)	109.5
F(56)-C(62)-F(55)	110.2(7)
F(56)-C(62)-F(54)	108.5(6)
F(55)-C(62)-F(54)	107.3(6)
F(56)-C(62)-S(52)	111.9(5)
F(55)-C(62)-S(52)	110.5(5)
F(54)-C(62)-S(52)	108.3(5)
C(9)-N(1)-S(2)	123.5(3)
C(59)-N(51)-S(52)	122.7(3)
C(2)-O(3)-S(1)	121.4(3)
C(10)-O(4)-C(11)	115.8(4)
C(52)-O(53)-S(51)	121.9(3)
C(60)-O(54)-C(61)	117.4(4)
O(1)-S(1)-O(2)	122.7(3)
O(1)-S(1)-O(3)	112.4(2)
O(2)-S(1)-O(3)	106.2(3)
O(1)-S(1)-C(1)	106.6(3)
O(2)-S(1)-C(1)	105.0(3)
O(3)-S(1)-C(1)	101.7(3)
O(7)-S(2)-O(6)	121.3(2)

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O(7)-S(2)-N(1)	108.4(2)
O(6)-S(2)-N(1)	110.8(2)
O(7)-S(2)-C(12)	104.9(3)
O(6)-S(2)-C(12)	105.1(3)
N(1)-S(2)-C(12)	104.9(3)
O(51)-S(51)-O(52)	122.4(3)
O(51)-S(51)-O(53)	106.0(3)
O(52)-S(51)-O(53)	111.9(2)
O(51)-S(51)-C(51)	105.3(4)
O(52)-S(51)-C(51)	107.4(4)
O(53)-S(51)-C(51)	101.6(3)
O(56)-S(52)-O(57)	123.3(3)
O(56)-S(52)-N(51)	110.3(2)
O(57)-S(52)-N(51)	108.2(2)
O(56)-S(52)-C(62)	104.6(3)
O(57)-S(52)-C(62)	104.5(3)
N(51)-S(52)-C(62)	104.2(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for import.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	62(4)	93(5)	68(4)	-29(4)	-17(3)	-7(4)
C(2)	43(3)	51(3)	51(3)	-12(2)	-12(2)	-12(2)
C(3)	51(3)	56(3)	45(3)	-6(2)	-13(2)	-8(3)
C(4)	55(3)	61(3)	59(3)	-10(3)	-28(3)	-5(3)
C(5)	45(3)	52(3)	51(3)	-14(2)	-9(2)	-10(3)
C(6)	71(4)	66(4)	46(3)	-12(3)	-3(3)	-26(3)
C(7)	72(4)	66(4)	47(3)	-5(3)	-25(3)	-23(3)
C(8)	42(3)	58(4)	73(4)	-22(3)	-13(3)	-3(3)
C(9)	40(2)	52(3)	44(3)	-8(2)	-12(2)	-10(2)
C(10)	44(3)	53(3)	63(3)	-22(2)	-22(3)	0(2)
C(11)	58(4)	102(5)	107(5)	-28(4)	-54(4)	0(3)
C(12)	74(5)	56(4)	78(4)	-11(3)	-17(4)	-1(3)
C(51)	93(6)	98(6)	51(4)	-15(4)	-9(4)	-32(4)
C(52)	46(3)	52(3)	58(3)	-11(2)	-23(3)	-2(3)
C(53)	73(4)	68(4)	45(3)	-2(3)	-24(3)	-16(3)
C(54)	64(4)	79(4)	43(3)	-11(3)	-8(3)	-27(3)
C(55)	45(3)	48(3)	56(3)	-23(2)	-14(2)	0(2)
C(56)	60(4)	63(3)	44(3)	-6(2)	-20(3)	-14(3)
C(57)	59(4)	68(4)	44(3)	-9(2)	-11(2)	-19(3)
C(58)	41(3)	63(4)	65(3)	-17(3)	-15(3)	0(3)
C(59)	42(2)	57(3)	43(2)	-12(2)	-14(2)	-8(2)
C(60)	51(3)	57(3)	43(3)	-12(2)	-13(2)	-8(2)
C(61)	58(4)	113(5)	82(4)	-32(4)	-35(3)	-10(4)
C(62)	72(5)	61(4)	83(5)	-12(3)	-25(4)	-7(3)
F(1)	85(3)	139(4)	86(3)	-56(2)	26(2)	-46(3)
F(2)	92(3)	99(3)	106(3)	-59(2)	-15(2)	-29(2)
F(3)	165(5)	138(4)	93(3)	-32(3)	-82(3)	19(3)
F(4)	99(3)	97(3)	120(3)	-38(2)	-68(3)	-4(2)
F(5)	90(3)	82(3)	103(3)	2(2)	-6(2)	-35(2)
F(6)	104(3)	75(3)	149(4)	-54(2)	-44(3)	15(2)
F(51)	133(4)	108(3)	129(4)	-64(3)	-27(3)	-26(3)
F(52)	318(10)	177(6)	96(4)	-31(4)	-114(5)	12(6)
F(53)	123(4)	251(7)	151(5)	-143(5)	74(4)	-100(5)
F(54)	83(3)	89(3)	113(3)	-7(2)	-5(2)	-30(2)
F(55)	148(4)	109(3)	113(3)	-49(2)	-58(3)	-21(3)
F(56)	136(4)	59(3)	186(5)	-9(3)	-31(4)	1(2)
N(1)	46(2)	57(2)	44(2)	-11(2)	-15(2)	-7(2)
N(51)	41(2)	55(2)	45(2)	-11(2)	-12(2)	0(2)
O(1)	94(3)	63(3)	93(3)	-11(2)	-50(3)	-12(2)
O(2)	47(2)	129(4)	85(3)	-50(3)	8(2)	-31(2)
O(3)	47(2)	56(2)	74(2)	-21(2)	-20(2)	-4(2)
O(4)	62(2)	90(3)	72(3)	-12(2)	-35(2)	-14(2)
O(5)	58(2)	132(4)	55(2)	-3(2)	-10(2)	-41(2)
O(6)	52(2)	82(3)	44(2)	-5(2)	-5(2)	-2(2)
O(7)	63(2)	90(3)	55(2)	-7(2)	-30(2)	6(2)
O(51)	43(2)	100(3)	108(3)	-34(3)	1(2)	-19(2)
O(52)	110(4)	64(3)	95(3)	2(2)	-60(3)	-1(2)
O(53)	45(2)	62(2)	73(2)	-12(2)	-26(2)	-7(2)
O(54)	41(2)	97(3)	52(2)	-28(2)	-14(2)	-9(2)
O(55)	44(2)	115(3)	47(2)	-25(2)	-7(2)	-12(2)
O(56)	105(3)	100(3)	64(2)	-14(2)	-52(2)	17(2)
O(57)	48(2)	93(3)	73(3)	-18(2)	-9(2)	14(2)

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S(1)	46(1)	68(1)	50(1)	-18(1)	-8(1)	-12(1)
S(2)	43(1)	64(1)	42(1)	-10(1)	-14(1)	-4(1)
S(51)	48(1)	63(1)	60(1)	-15(1)	-12(1)	-9(1)
S(52)	51(1)	64(1)	55(1)	-11(1)	-23(1)	2(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for import.

	x	y	z	U(eq)
H(3)	-970	-197	6257	63
H(4)	1631	557	5992	68
H(6)	2478	1969	2118	77
H(7)	-91	1259	2356	72
H(8A)	4738	1923	2941	70
H(8B)	4479	1198	4424	70
H(9)	3155	3081	5218	55
H(11A)	7766	3395	5764	121
H(11B)	7658	4620	4661	121
H(11C)	8460	3319	4254	121
H(53)	11543	6709	10748	74
H(54)	8990	5966	10960	76
H(56)	10033	7334	7038	66
H(57)	12592	7992	6805	70
H(58A)	7393	6496	8316	68
H(58B)	6708	6489	9844	68
H(59)	7493	4317	10371	56
H(61A)	4261	4026	7421	118
H(61B)	3351	4787	8549	118
H(61C)	3639	3279	8927	118

Table 6. Torsion angles [deg] for import.

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Triphenylphosphine gold (*S*)-methyl 3-(4-(((trifluoromethyl)sulfonyl)oxy)phenyl)-2-(trifluoromethylsulfonamido)propanoate

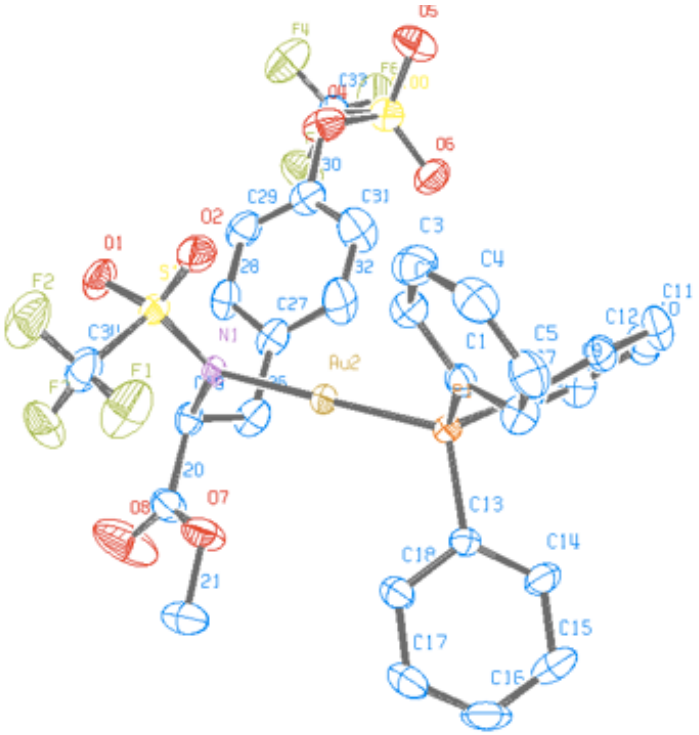

Table 1. Crystal data and structure refinement for import.

Identification code	shelxl
Empirical formula	C30 H25 Au F6 N O7 P S2
Formula weight	917.57
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	monoclinic, P 21
Unit cell dimensions	a = 8.69020(10) A alpha = 90 deg.
	b = 34.9283(3) A beta = 103.15 deg.
	c = 11.4932(2) A gamma = 90 deg.
Volume	3397.14(8) A^3
Z, Calculated density	4, 1.794 Mg/m^3
Absorption coefficient	4.579 mm^-1
F(000)	1792
Crystal size	0.20 x 0.20 x 0.10 mm
Theta range for data collection	3.44 to 27.11 deg.
Limiting indices	-11<=h<=11, -44<=k<=44, -14<=l<=14
Reflections collected / unique	32544 / 13530 [R(int) = 0.0551]
Completeness to theta = 27.11	97.7 %
Max. and min. transmission	0.6574 and 0.4611
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	13530 / 1 / 865
Goodness-of-fit on F^2	1.003
Final R indices [I>2sigma(I)]	R1 = 0.0375, wR2 = 0.0789
R indices (all data)	R1 = 0.0479, wR2 = 0.0832
Absolute structure parameter	0.050(4)
Largest diff. peak and hole	0.670 and -0.521 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for import.

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	7842(8)	7092(2)	9324(6)	42(2)
C(2)	6798(9)	7291(2)	9831(7)	53(2)
C(3)	6300(11)	7662(3)	9428(9)	75(3)
C(4)	6914(10)	7822(3)	8530(8)	68(2)
C(5)	7951(11)	7628(2)	8025(7)	65(2)
C(6)	8439(9)	7263(2)	8422(7)	53(2)
C(7)	7424(7)	6266(2)	8903(6)	39(1)

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C(8)	7489(9)	5893(2)	9290(7)	51(2)
C(9)	6697(11)	5602(3)	8581(9)	68(2)
C(10)	5777(11)	5695(3)	7477(8)	72(2)
C(11)	5699(11)	6063(3)	7063(7)	70(2)
C(12)	6525(9)	6348(2)	7768(6)	52(2)
C(13)	10527(7)	6572(2)	9790(5)	42(1)
C(14)	10953(9)	6408(2)	8824(7)	57(2)
C(15)	12512(11)	6374(3)	8772(9)	73(3)
C(16)	13643(9)	6500(4)	9704(9)	82(3)
C(17)	13259(9)	6670(4)	10664(8)	85(3)
C(18)	11687(8)	6700(3)	10715(7)	62(2)
C(19)	8653(8)	6152(2)	14238(6)	45(2)
C(20)	10448(9)	6200(3)	14579(7)	59(2)
C(21)	12674(9)	6478(3)	14100(9)	82(3)
C(26)	8251(10)	5770(2)	13604(8)	63(2)
C(27)	6499(10)	5677(2)	13297(7)	55(2)
C(28)	5727(11)	5557(2)	14158(7)	61(2)
C(29)	4117(10)	5466(3)	13886(8)	68(2)
C(30)	3321(10)	5506(2)	12755(8)	61(2)
C(31)	4021(12)	5636(3)	11863(9)	84(3)
C(32)	5605(12)	5716(3)	12146(8)	81(3)
C(33)	627(10)	4760(3)	12860(7)	65(2)
C(34)	8509(12)	7125(3)	14760(9)	75(3)
C(51)	2720(8)	8822(2)	6816(6)	44(2)
C(52)	2222(10)	9039(3)	5805(8)	66(2)
C(53)	3076(13)	9367(3)	5641(11)	90(4)
C(54)	4392(13)	9466(3)	6514(13)	91(4)
C(55)	4907(13)	9247(3)	7460(9)	81(3)
C(56)	4088(10)	8922(3)	7638(7)	62(2)
C(57)	2583(8)	7985(2)	6796(6)	45(2)
C(58)	3381(9)	7988(3)	5860(7)	57(2)
C(59)	4090(11)	7655(3)	5569(8)	77(3)
C(60)	4012(12)	7328(3)	6200(10)	78(3)
C(61)	3230(11)	7325(3)	7100(10)	79(3)
C(62)	2512(9)	7653(3)	7420(8)	61(2)
C(63)	-306(8)	8426(2)	6155(6)	45(1)
C(64)	-1565(8)	8590(2)	6541(7)	52(2)
C(65)	-3017(9)	8611(3)	5746(9)	75(3)
C(66)	-3250(9)	8458(3)	4620(8)	73(2)
C(67)	-2015(10)	8293(3)	4266(8)	78(3)
C(68)	-568(10)	8273(3)	5015(7)	68(2)
C(69)	653(9)	8860(2)	11229(6)	55(2)
C(70)	1195(11)	9241(3)	10782(8)	65(2)
C(71)	2905(11)	9342(2)	11230(8)	61(2)
C(72)	3708(12)	9296(3)	12373(9)	81(3)
C(73)	5285(14)	9392(3)	12759(9)	90(3)
C(74)	6047(12)	9547(3)	11932(10)	76(3)
C(75)	5256(12)	9595(3)	10771(9)	78(3)
C(76)	3696(12)	9499(3)	10396(8)	71(2)
C(77)	-1066(10)	8794(3)	10700(7)	62(2)
C(78)	1116(11)	7840(3)	11831(9)	68(2)
C(84)	8876(18)	10291(4)	12186(12)	103(4)
C(89)	-3492(10)	8610(3)	11082(9)	82(3)
Au(2)	8166(1)	6547(1)	11760(1)	41(1)
Au(51)	1562(1)	8452(1)	9108(1)	46(1)
F(1)	9225(8)	7273(2)	13976(7)	117(3)
F(2)	7878(9)	7409(2)	15234(7)	113(2)
F(3)	9552(7)	6953(2)	15600(6)	115(2)
F(4)	-280(8)	4909(2)	13503(6)	108(2)
F(5)	1941(7)	4662(2)	13578(6)	101(2)
F(6)	-75(9)	4447(2)	12366(6)	105(2)
F(51)	-186(8)	7955(2)	12105(8)	124(3)
F(52)	1763(8)	7577(2)	12607(6)	101(2)
F(53)	767(9)	7678(2)	10766(6)	106(2)
F(54)	7515(13)	10402(3)	11548(9)	159(4)
F(55)	9743(11)	10153(3)	11491(7)	149(3)
F(56)	9700(13)	10558(3)	12806(9)	171(4)
N(1)	7830(6)	6470(2)	13482(4)	37(1)
N(51)	1561(7)	8536(2)	10898(4)	47(2)
O(1)	6401(7)	6646(2)	15026(5)	67(2)
O(2)	5973(7)	7004(2)	13125(5)	73(2)
O(4)	1655(7)	5440(2)	12472(7)	76(2)
O(5)	-591(8)	5190(2)	11078(6)	90(2)
O(6)	2025(7)	4901(2)	11150(6)	75(2)
O(7)	10994(6)	6410(2)	13832(5)	74(2)
O(8)	11252(9)	6060(3)	15440(8)	141(4)
O(51)	3722(7)	8076(2)	11450(7)	88(2)
O(52)	2685(8)	8393(2)	13038(5)	88(2)

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O(53)	7747(8)	9605(2)	12245(7)	92(2)
O(54)	10033(11)	9774(3)	13718(9)	143(4)
O(55)	7496(10)	10059(3)	13838(7)	103(3)
O(57)	-1862(6)	8716(2)	11507(5)	70(2)
O(58)	-1673(8)	8804(3)	9654(6)	118(3)
P(1)	8484(2)	6624(1)	9897(2)	38(1)
P(51)	1618(2)	8410(1)	7174(2)	40(1)
S(1)	6971(2)	6784(1)	14034(2)	46(1)
S(51)	2465(2)	8246(1)	11841(2)	55(1)
S(52)	8535(3)	9907(1)	13192(2)	79(1)
S(100)	928(3)	5082(1)	11710(2)	60(1)

Table 3. Bond lengths [A] and angles [deg] for import.

C(1)-C(2)	1.372(10)
C(1)-C(6)	1.394(10)
C(1)-P(1)	1.805(7)
C(2)-C(3)	1.413(12)
C(2)-H(2)	0.9300
C(3)-C(4)	1.382(14)
C(3)-H(3)	0.9300
C(4)-C(5)	1.359(13)
C(4)-H(4)	0.9300
C(5)-C(6)	1.388(11)
C(5)-H(5)	0.9300
C(6)-H(6)	0.9300
C(7)-C(8)	1.376(10)
C(7)-C(12)	1.389(9)
C(7)-P(1)	1.798(7)
C(8)-C(9)	1.384(12)
C(8)-H(8)	0.9300
C(9)-C(10)	1.376(13)
C(9)-H(9)	0.9300
C(10)-C(11)	1.366(13)
C(10)-H(10)	0.9300
C(11)-C(12)	1.379(11)
C(11)-H(11)	0.9300
C(12)-H(12)	0.9300
C(13)-C(18)	1.363(9)
C(13)-C(14)	1.374(9)
C(13)-P(1)	1.817(6)
C(14)-C(15)	1.374(11)
C(14)-H(14)	0.9300
C(15)-C(16)	1.353(13)
C(15)-H(15)	0.9300
C(16)-C(17)	1.360(14)
C(16)-H(16)	0.9300
C(17)-C(18)	1.385(11)
C(17)-H(17)	0.9300
C(18)-H(18)	0.9300
C(19)-N(1)	1.488(9)
C(19)-C(26)	1.523(11)
C(19)-C(20)	1.528(11)
C(19)-H(19)	0.9800
C(20)-O(8)	1.180(10)
C(20)-O(7)	1.297(9)
C(21)-O(7)	1.442(9)
C(21)-H(21A)	0.9600
C(21)-H(21B)	0.9600
C(21)-H(21C)	0.9600
C(26)-C(27)	1.518(12)
C(26)-H(26A)	0.9700
C(26)-H(26B)	0.9700
C(27)-C(32)	1.380(12)
C(27)-C(28)	1.381(11)
C(28)-C(29)	1.398(12)
C(28)-H(28)	0.9300
C(29)-C(30)	1.334(12)
C(29)-H(29)	0.9300
C(30)-C(31)	1.382(12)
C(30)-O(4)	1.429(10)
C(31)-C(32)	1.369(13)
C(31)-H(31)	0.9300
C(32)-H(32)	0.9300
C(33)-F(5)	1.294(10)
C(33)-F(4)	1.307(10)
C(33)-F(6)	1.315(10)
C(33)-S(100)	1.800(9)

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C(34)-F(3)	1.311(13)
C(34)-F(2)	1.310(11)
C(34)-F(1)	1.313(11)
C(34)-S(1)	1.842(9)
C(51)-C(52)	1.372(11)
C(51)-C(56)	1.384(10)
C(51)-P(51)	1.828(7)
C(52)-C(53)	1.402(14)
C(52)-H(52)	0.9300
C(53)-C(54)	1.383(17)
C(53)-H(53)	0.9300
C(54)-C(55)	1.323(15)
C(54)-H(54)	0.9300
C(55)-C(56)	1.380(12)
C(55)-H(55)	0.9300
C(56)-H(56)	0.9300
C(57)-C(62)	1.373(11)
C(57)-C(58)	1.407(10)
C(57)-P(51)	1.805(7)
C(58)-C(59)	1.393(12)
C(58)-H(58)	0.9300
C(59)-C(60)	1.363(15)
C(59)-H(59)	0.9300
C(60)-C(61)	1.361(14)
C(60)-H(60)	0.9300
C(61)-C(62)	1.394(13)
C(61)-H(61)	0.9300
C(62)-H(62)	0.9300
C(63)-C(68)	1.385(10)
C(63)-C(64)	1.394(10)
C(63)-P(51)	1.811(7)
C(64)-C(65)	1.381(11)
C(64)-H(64)	0.9300
C(65)-C(66)	1.372(13)
C(65)-H(65)	0.9300
C(66)-C(67)	1.360(12)
C(66)-H(66)	0.9300
C(67)-C(68)	1.355(11)
C(67)-H(67)	0.9300
C(68)-H(68)	0.9300
C(69)-N(51)	1.478(10)
C(69)-C(77)	1.497(11)
C(69)-C(70)	1.536(12)
C(69)-H(69)	0.9800
C(70)-C(71)	1.499(13)
C(70)-H(70A)	0.9700
C(70)-H(70B)	0.9700
C(71)-C(72)	1.349(13)
C(71)-C(76)	1.411(13)
C(72)-C(73)	1.382(15)
C(72)-H(72)	0.9300
C(73)-C(74)	1.387(13)
C(73)-H(73)	0.9300
C(74)-C(75)	1.366(13)
C(74)-O(53)	1.453(12)
C(75)-C(76)	1.368(13)
C(75)-H(75)	0.9300
C(76)-H(76)	0.9300
C(77)-O(58)	1.198(10)
C(77)-O(57)	1.307(10)
C(78)-F(51)	1.306(11)
C(78)-F(52)	1.312(11)
C(78)-F(53)	1.320(11)
C(78)-S(51)	1.839(9)
C(84)-F(56)	1.289(14)
C(84)-F(54)	1.302(16)
C(84)-F(55)	1.308(14)
C(84)-S(52)	1.837(14)
C(89)-O(57)	1.437(10)
C(89)-H(89A)	0.9600
C(89)-H(89B)	0.9600
C(89)-H(89C)	0.9600
Au(2)-N(1)	2.083(4)
Au(2)-P(1)	2.2367(17)
Au(51)-N(51)	2.077(5)
Au(51)-P(51)	2.2390(17)
N(1)-S(1)	1.544(6)

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N(51)-S(51)	1.559(6)
O(1)-S(1)	1.426(5)
O(2)-S(1)	1.422(6)
O(4)-S(100)	1.572(6)
O(5)-S(100)	1.405(7)
O(6)-S(100)	1.416(6)
O(51)-S(51)	1.405(7)
O(52)-S(51)	1.439(6)
O(53)-S(52)	1.557(7)
O(54)-S(52)	1.384(8)
O(55)-S(52)	1.399(8)
C(2)-C(1)-C(6)	119.7(7)
C(2)-C(1)-P(1)	118.8(6)
C(6)-C(1)-P(1)	121.4(6)
C(1)-C(2)-C(3)	120.5(8)
C(1)-C(2)-H(2)	119.8
C(3)-C(2)-H(2)	119.8
C(4)-C(3)-C(2)	118.2(8)
C(4)-C(3)-H(3)	120.9
C(2)-C(3)-H(3)	120.9
C(5)-C(4)-C(3)	121.7(8)
C(5)-C(4)-H(4)	119.2
C(3)-C(4)-H(4)	119.2
C(4)-C(5)-C(6)	120.0(8)
C(4)-C(5)-H(5)	120.0
C(6)-C(5)-H(5)	120.0
C(5)-C(6)-C(1)	119.9(8)
C(5)-C(6)-H(6)	120.0
C(1)-C(6)-H(6)	120.0
C(8)-C(7)-C(12)	118.1(6)
C(8)-C(7)-P(1)	118.4(5)
C(12)-C(7)-P(1)	123.5(5)
C(7)-C(8)-C(9)	121.9(7)
C(7)-C(8)-H(8)	119.1
C(9)-C(8)-H(8)	119.1
C(8)-C(9)-C(10)	118.4(8)
C(8)-C(9)-H(9)	120.8
C(10)-C(9)-H(9)	120.8
C(11)-C(10)-C(9)	121.1(8)
C(11)-C(10)-H(10)	119.4
C(9)-C(10)-H(10)	119.4
C(10)-C(11)-C(12)	119.8(8)
C(10)-C(11)-H(11)	120.1
C(12)-C(11)-H(11)	120.1
C(11)-C(12)-C(7)	120.7(7)
C(11)-C(12)-H(12)	119.7
C(7)-C(12)-H(12)	119.7
C(18)-C(13)-C(14)	118.7(6)
C(18)-C(13)-P(1)	118.4(5)
C(14)-C(13)-P(1)	122.9(5)
C(13)-C(14)-C(15)	121.3(8)
C(13)-C(14)-H(14)	119.3
C(15)-C(14)-H(14)	119.3
C(16)-C(15)-C(14)	118.9(8)
C(16)-C(15)-H(15)	120.5
C(14)-C(15)-H(15)	120.5
C(15)-C(16)-C(17)	121.1(7)
C(15)-C(16)-H(16)	119.4
C(17)-C(16)-H(16)	119.4
C(16)-C(17)-C(18)	119.6(8)
C(16)-C(17)-H(17)	120.2
C(18)-C(17)-H(17)	120.2
C(13)-C(18)-C(17)	120.2(8)
C(13)-C(18)-H(18)	119.9
C(17)-C(18)-H(18)	119.9
N(1)-C(19)-C(26)	110.3(6)
N(1)-C(19)-C(20)	113.3(6)
C(26)-C(19)-C(20)	109.2(6)
N(1)-C(19)-H(19)	108.0
C(26)-C(19)-H(19)	108.0
C(20)-C(19)-H(19)	108.0
O(8)-C(20)-O(7)	123.6(8)
O(8)-C(20)-C(19)	123.0(8)
O(7)-C(20)-C(19)	113.4(6)
O(7)-C(21)-H(21A)	109.5
O(7)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
O(7)-C(21)-H(21C)	109.5

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H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(27)-C(26)-C(19)	114.1(7)
C(27)-C(26)-H(26A)	108.7
C(19)-C(26)-H(26A)	108.7
C(27)-C(26)-H(26B)	108.7
C(19)-C(26)-H(26B)	108.7
H(26A)-C(26)-H(26B)	107.6
C(32)-C(27)-C(28)	117.3(8)
C(32)-C(27)-C(26)	121.2(7)
C(28)-C(27)-C(26)	121.6(8)
C(27)-C(28)-C(29)	122.2(8)
C(27)-C(28)-H(28)	118.9
C(29)-C(28)-H(28)	118.9
C(30)-C(29)-C(28)	117.7(8)
C(30)-C(29)-H(29)	121.2
C(28)-C(29)-H(29)	121.2
C(29)-C(30)-C(31)	122.6(8)
C(29)-C(30)-O(4)	118.6(8)
C(31)-C(30)-O(4)	118.6(9)
C(32)-C(31)-C(30)	118.7(9)
C(32)-C(31)-H(31)	120.7
C(30)-C(31)-H(31)	120.7
C(31)-C(32)-C(27)	121.6(8)
C(31)-C(32)-H(32)	119.2
C(27)-C(32)-H(32)	119.2
F(5)-C(33)-F(4)	107.7(8)
F(5)-C(33)-F(6)	108.1(8)
F(4)-C(33)-F(6)	107.2(8)
F(5)-C(33)-S(100)	112.3(6)
F(4)-C(33)-S(100)	111.9(7)
F(6)-C(33)-S(100)	109.5(6)
F(3)-C(34)-F(2)	109.0(8)
F(3)-C(34)-F(1)	109.3(9)
F(2)-C(34)-F(1)	107.3(9)
F(3)-C(34)-S(1)	110.3(7)
F(2)-C(34)-S(1)	110.4(7)
F(1)-C(34)-S(1)	110.6(7)
C(52)-C(51)-C(56)	119.7(7)
C(52)-C(51)-P(51)	123.0(6)
C(56)-C(51)-P(51)	117.2(6)
C(51)-C(52)-C(53)	119.4(9)
C(51)-C(52)-H(52)	120.3
C(53)-C(52)-H(52)	120.3
C(54)-C(53)-C(52)	118.9(10)
C(54)-C(53)-H(53)	120.6
C(52)-C(53)-H(53)	120.6
C(55)-C(54)-C(53)	121.4(10)
C(55)-C(54)-H(54)	119.3
C(53)-C(54)-H(54)	119.3
C(54)-C(55)-C(56)	120.6(10)
C(54)-C(55)-H(55)	119.7
C(56)-C(55)-H(55)	119.7
C(55)-C(56)-C(51)	119.9(9)
C(55)-C(56)-H(56)	120.1
C(51)-C(56)-H(56)	120.1
C(62)-C(57)-C(58)	119.7(7)
C(62)-C(57)-P(51)	119.3(6)
C(58)-C(57)-P(51)	121.0(6)
C(59)-C(58)-C(57)	119.9(9)
C(59)-C(58)-H(58)	120.0
C(57)-C(58)-H(58)	120.0
C(60)-C(59)-C(58)	119.7(9)
C(60)-C(59)-H(59)	120.2
C(58)-C(59)-H(59)	120.2
C(61)-C(60)-C(59)	120.3(8)
C(61)-C(60)-H(60)	119.9
C(59)-C(60)-H(60)	119.9
C(60)-C(61)-C(62)	121.7(9)
C(60)-C(61)-H(61)	119.1
C(62)-C(61)-H(61)	119.1
C(57)-C(62)-C(61)	118.7(8)
C(57)-C(62)-H(62)	120.6
C(61)-C(62)-H(62)	120.6
C(68)-C(63)-C(64)	119.2(7)
C(68)-C(63)-P(51)	121.9(6)
C(64)-C(63)-P(51)	118.9(5)
C(65)-C(64)-C(63)	118.5(7)

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C(65)-C(64)-H(64)	120.7
C(63)-C(64)-H(64)	120.7
C(66)-C(65)-C(64)	121.3(8)
C(66)-C(65)-H(65)	119.3
C(64)-C(65)-H(65)	119.3
C(67)-C(66)-C(65)	119.3(7)
C(67)-C(66)-H(66)	120.3
C(65)-C(66)-H(66)	120.3
C(68)-C(67)-C(66)	120.9(8)
C(68)-C(67)-H(67)	119.5
C(66)-C(67)-H(67)	119.5
C(67)-C(68)-C(63)	120.7(8)
C(67)-C(68)-H(68)	119.7
C(63)-C(68)-H(68)	119.7
N(51)-C(69)-C(77)	108.6(6)
N(51)-C(69)-C(70)	110.7(6)
C(77)-C(69)-C(70)	110.5(7)
N(51)-C(69)-H(69)	109.0
C(77)-C(69)-H(69)	109.0
C(70)-C(69)-H(69)	109.0
C(71)-C(70)-C(69)	116.3(7)
C(71)-C(70)-H(70A)	108.2
C(69)-C(70)-H(70A)	108.2
C(71)-C(70)-H(70B)	108.2
C(69)-C(70)-H(70B)	108.2
H(70A)-C(70)-H(70B)	107.4
C(72)-C(71)-C(76)	118.9(9)
C(72)-C(71)-C(70)	124.0(9)
C(76)-C(71)-C(70)	117.1(8)
C(71)-C(72)-C(73)	122.7(10)
C(71)-C(72)-H(72)	118.7
C(73)-C(72)-H(72)	118.7
C(72)-C(73)-C(74)	117.9(10)
C(72)-C(73)-H(73)	121.1
C(74)-C(73)-H(73)	121.1
C(75)-C(74)-C(73)	120.3(9)
C(75)-C(74)-O(53)	118.8(9)
C(73)-C(74)-O(53)	120.2(10)
C(76)-C(75)-C(74)	121.3(9)
C(76)-C(75)-H(75)	119.3
C(74)-C(75)-H(75)	119.3
C(75)-C(76)-C(71)	118.9(9)
C(75)-C(76)-H(76)	120.6
C(71)-C(76)-H(76)	120.6
O(58)-C(77)-O(57)	122.3(8)
O(58)-C(77)-C(69)	125.0(8)
O(57)-C(77)-C(69)	112.6(7)
F(51)-C(78)-F(52)	108.2(8)
F(51)-C(78)-F(53)	109.1(9)
F(52)-C(78)-F(53)	107.7(9)
F(51)-C(78)-S(51)	110.2(7)
F(52)-C(78)-S(51)	111.1(7)
F(53)-C(78)-S(51)	110.4(6)
F(56)-C(84)-F(54)	114.4(13)
F(56)-C(84)-F(55)	106.2(12)
F(54)-C(84)-F(55)	110.0(13)
F(56)-C(84)-S(52)	109.3(10)
F(54)-C(84)-S(52)	108.5(10)
F(55)-C(84)-S(52)	108.3(10)
O(57)-C(89)-H(89A)	109.5
O(57)-C(89)-H(89B)	109.5
H(89A)-C(89)-H(89B)	109.5
O(57)-C(89)-H(89C)	109.5
H(89A)-C(89)-H(89C)	109.5
H(89B)-C(89)-H(89C)	109.5
N(1)-Au(2)-P(1)	178.86(16)
N(51)-Au(51)-P(51)	175.51(19)
C(19)-N(1)-S(1)	120.2(4)
C(19)-N(1)-Au(2)	119.9(4)
S(1)-N(1)-Au(2)	118.9(3)
C(69)-N(51)-S(51)	122.2(4)
C(69)-N(51)-Au(51)	118.9(4)
S(51)-N(51)-Au(51)	118.9(3)
C(30)-O(4)-S(100)	120.9(5)
C(20)-O(7)-C(21)	117.2(7)
C(74)-O(53)-S(52)	122.0(6)
C(77)-O(57)-C(89)	116.9(7)

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C(7)-P(1)-C(1)	109.1(3)
C(7)-P(1)-C(13)	104.8(3)
C(1)-P(1)-C(13)	106.9(3)
C(7)-P(1)-Au(2)	111.6(2)
C(1)-P(1)-Au(2)	111.2(2)
C(13)-P(1)-Au(2)	112.8(2)
C(57)-P(51)-C(63)	106.3(4)
C(57)-P(51)-C(51)	107.3(3)
C(63)-P(51)-C(51)	106.5(3)
C(57)-P(51)-Au(51)	114.2(2)
C(63)-P(51)-Au(51)	114.5(2)
C(51)-P(51)-Au(51)	107.6(2)
O(2)-S(1)-O(1)	120.4(4)
O(2)-S(1)-N(1)	110.7(3)
O(1)-S(1)-N(1)	112.1(3)
O(2)-S(1)-C(34)	104.0(5)
O(1)-S(1)-C(34)	101.8(4)
N(1)-S(1)-C(34)	106.1(4)
O(51)-S(51)-O(52)	120.8(5)
O(51)-S(51)-N(51)	110.9(4)
O(52)-S(51)-N(51)	111.7(4)
O(51)-S(51)-C(78)	102.3(5)
O(52)-S(51)-C(78)	103.1(4)
N(51)-S(51)-C(78)	106.1(4)
O(54)-S(52)-O(55)	123.5(6)
O(54)-S(52)-O(53)	107.4(6)
O(55)-S(52)-O(53)	113.2(4)
O(54)-S(52)-C(84)	104.4(7)
O(55)-S(52)-C(84)	105.9(6)
O(53)-S(52)-C(84)	99.3(5)
O(5)-S(100)-O(6)	122.4(5)
O(5)-S(100)-O(4)	106.6(4)
O(6)-S(100)-O(4)	112.5(4)
O(5)-S(100)-C(33)	105.7(4)
O(6)-S(100)-C(33)	106.2(4)
O(4)-S(100)-C(33)	101.2(4)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for import.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	42(4)	42(4)	41(4)	-5(3)	5(3)	-2(3)
C(2)	55(4)	48(5)	58(5)	-2(3)	15(3)	-4(4)
C(3)	64(5)	72(6)	89(7)	-20(5)	17(5)	8(5)
C(4)	73(6)	47(5)	74(6)	1(4)	-1(4)	6(4)
C(5)	80(6)	53(5)	55(5)	7(4)	3(4)	-2(4)
C(6)	62(5)	43(4)	56(4)	3(3)	17(4)	2(3)
C(7)	35(3)	45(4)	41(3)	-2(3)	13(3)	-7(3)
C(8)	61(5)	46(4)	44(4)	4(3)	10(3)	-7(4)
C(9)	88(7)	50(5)	68(6)	-1(4)	19(5)	-10(4)
C(10)	73(6)	79(7)	63(5)	-22(5)	13(4)	-25(5)
C(11)	83(6)	81(7)	39(4)	2(4)	-1(4)	-9(5)
C(12)	57(4)	58(5)	40(4)	5(3)	6(3)	3(4)
C(13)	34(3)	46(4)	45(3)	-3(3)	10(2)	-2(3)
C(14)	46(4)	68(6)	62(4)	-10(4)	25(3)	-5(4)
C(15)	68(6)	69(6)	99(7)	-9(5)	54(5)	1(4)
C(16)	33(4)	115(8)	99(7)	16(7)	19(4)	0(5)
C(17)	43(4)	136(10)	67(6)	-5(6)	-5(4)	-15(5)
C(18)	42(4)	98(7)	44(4)	1(4)	7(3)	-7(4)
C(19)	56(4)	44(4)	37(3)	4(3)	15(3)	0(3)
C(20)	50(4)	71(6)	53(5)	5(4)	4(4)	-4(4)
C(21)	44(4)	96(8)	100(7)	-1(6)	8(4)	-1(5)
C(26)	75(6)	50(5)	74(6)	-9(4)	34(4)	-9(4)
C(27)	77(5)	33(4)	64(5)	-6(3)	31(4)	-9(4)
C(28)	86(6)	51(5)	50(4)	-7(3)	25(4)	-14(4)
C(29)	74(6)	69(6)	73(6)	-6(4)	39(5)	-11(5)
C(30)	61(5)	43(4)	83(6)	-15(4)	25(4)	-15(4)
C(31)	91(7)	92(8)	67(6)	21(5)	16(5)	-33(6)
C(32)	94(7)	98(8)	56(5)	7(5)	26(5)	-44(6)
C(33)	66(5)	70(6)	55(5)	3(4)	9(4)	1(4)
C(34)	84(7)	70(6)	79(6)	-29(5)	36(6)	-21(5)
C(51)	50(4)	45(4)	40(4)	-5(3)	17(3)	-2(3)
C(52)	54(5)	77(6)	72(5)	19(4)	22(4)	-3(4)
C(53)	79(7)	87(8)	115(9)	51(7)	47(6)	11(6)
C(54)	73(7)	55(6)	156(11)	21(6)	49(7)	-11(5)

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C(55)	92(7)	82(7)	75(6)	-17(5)	30(5)	-35(6)
C(56)	63(5)	65(5)	60(5)	-4(4)	19(4)	-17(4)
C(57)	43(4)	44(4)	49(4)	0(3)	12(3)	7(3)
C(58)	52(5)	66(5)	54(5)	-4(4)	15(4)	3(4)
C(59)	77(6)	94(8)	61(5)	-21(5)	17(4)	24(5)
C(60)	75(6)	56(6)	99(7)	-24(5)	11(5)	13(5)
C(61)	79(6)	43(5)	106(8)	9(5)	2(6)	-1(4)
C(62)	60(5)	59(5)	63(5)	14(4)	11(4)	7(4)
C(63)	47(4)	45(4)	47(3)	4(3)	17(3)	0(3)
C(64)	49(4)	60(5)	51(4)	-5(3)	18(3)	2(3)
C(65)	40(4)	89(7)	97(7)	-1(5)	19(4)	17(4)
C(66)	44(4)	95(7)	72(5)	9(6)	-2(4)	5(5)
C(67)	59(5)	117(9)	53(5)	-16(5)	-1(4)	5(5)
C(68)	59(5)	93(7)	51(4)	-8(4)	12(4)	11(4)
C(69)	59(5)	67(5)	40(4)	-5(3)	17(3)	7(4)
C(70)	74(6)	53(5)	69(5)	-5(4)	18(4)	7(4)
C(71)	74(5)	54(5)	58(5)	-12(4)	20(4)	4(4)
C(72)	86(7)	90(8)	65(6)	3(5)	15(5)	-29(6)
C(73)	109(8)	94(8)	62(6)	-5(5)	10(6)	-33(6)
C(74)	77(6)	56(6)	101(8)	-3(5)	33(6)	-10(5)
C(75)	84(7)	87(7)	70(6)	-8(5)	32(5)	-11(6)
C(76)	91(7)	68(6)	57(5)	2(4)	22(5)	-2(5)
C(77)	58(5)	74(6)	53(5)	-8(4)	12(4)	2(4)
C(78)	75(6)	60(6)	72(6)	7(5)	25(5)	-7(5)
C(84)	121(10)	89(9)	102(9)	-20(7)	32(8)	-8(8)
C(89)	62(6)	99(8)	91(7)	-13(6)	27(5)	-7(5)
Au(2)	39(1)	53(1)	32(1)	-2(1)	10(1)	-1(1)
Au(51)	51(1)	53(1)	35(1)	2(1)	16(1)	-1(1)
F(1)	138(6)	94(5)	147(6)	-39(4)	89(5)	-58(4)
F(2)	138(5)	80(4)	136(6)	-57(4)	62(5)	-22(4)
F(3)	83(4)	140(6)	101(5)	-50(4)	-21(3)	-12(4)
F(4)	134(5)	87(4)	126(5)	5(4)	80(4)	7(4)
F(5)	94(4)	107(5)	91(4)	22(4)	-2(3)	6(4)
F(6)	146(6)	72(4)	98(4)	-4(3)	31(4)	-46(4)
F(51)	97(4)	103(5)	198(8)	19(5)	87(5)	-14(4)
F(52)	132(5)	75(4)	93(4)	31(3)	17(4)	-11(4)
F(53)	143(6)	78(4)	87(4)	-14(3)	5(4)	-31(4)
F(54)	190(9)	130(8)	154(8)	47(6)	33(7)	12(7)
F(55)	197(8)	148(7)	138(7)	-59(5)	114(6)	-54(6)
F(56)	241(10)	120(7)	173(9)	-68(6)	89(8)	-80(7)
N(1)	40(3)	51(4)	22(2)	2(2)	11(2)	-5(2)
N(51)	59(3)	58(5)	23(2)	0(2)	10(2)	-2(3)
O(1)	74(4)	81(5)	58(3)	-10(3)	40(3)	-14(3)
O(2)	70(4)	83(4)	63(4)	3(3)	13(3)	30(3)
O(4)	62(4)	54(4)	118(6)	-20(4)	31(3)	-6(3)
O(5)	70(4)	95(5)	95(5)	23(4)	-3(3)	10(4)
O(6)	72(4)	81(5)	78(4)	-12(3)	34(3)	0(3)
O(7)	41(3)	104(5)	71(4)	18(3)	2(3)	-14(3)
O(8)	84(5)	188(10)	128(7)	98(7)	-26(5)	-17(5)
O(51)	53(3)	100(5)	116(5)	41(4)	29(3)	12(3)
O(52)	113(5)	97(5)	43(3)	8(3)	-6(3)	-14(4)
O(53)	83(5)	80(5)	116(6)	-32(4)	30(4)	-12(4)
O(54)	98(6)	183(11)	129(7)	22(7)	-15(5)	35(6)
O(55)	107(6)	134(7)	76(5)	-27(5)	41(4)	-25(5)
O(57)	59(4)	90(5)	67(4)	-2(3)	28(3)	-4(3)
O(58)	76(5)	217(11)	59(4)	8(5)	11(3)	-16(5)
P(1)	34(1)	45(1)	35(1)	0(1)	11(1)	1(1)
P(51)	43(1)	46(1)	34(1)	0(1)	12(1)	1(1)
S(1)	43(1)	57(1)	42(1)	-5(1)	17(1)	-2(1)
S(51)	49(1)	67(1)	45(1)	9(1)	1(1)	-11(1)
S(52)	76(2)	94(2)	64(1)	-1(1)	8(1)	2(1)
S(100)	60(1)	52(1)	67(1)	1(1)	14(1)	-4(1)

Table 5. Torsion angles [deg] for import

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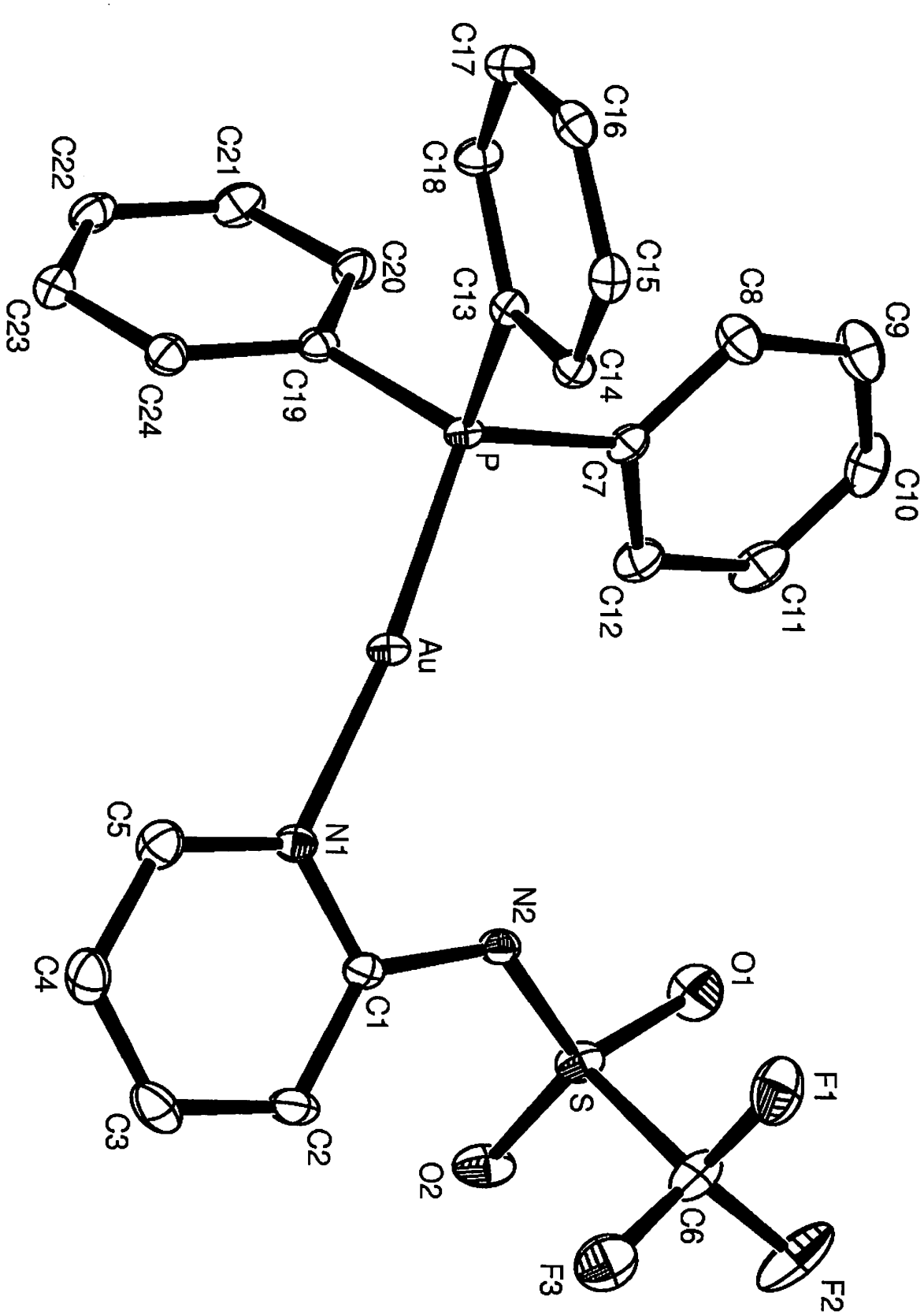

Triphenylphosphine gold pyridinium-2-yl(trifluoromethylsulfonyl)amide

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Table 1. Crystal data and structure refinement for $Au(C_6H_4N\text{-}2\text{-}NTf)(PPh_3)$.

Identification code	apr411 / src20110454	
Empirical formula	C24 H19 Au F3 N2 O2 P S	
Formula weight	684.41	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P\ 2_1/c$ (No.14)	
Unit cell dimensions	a = 10.9430(2) Å	α= 90°.
	b = 13.1579(2) Å	β= 102.532(1)°.
	c = 16.8166(4) Å	γ = 90°.
Volume	2363.68(8) $Å^3$	
Z	4	
Density (calculated)	1.92 Mg/m^3	
Absorption coefficient	6.43 mm^{-1}	
F(000)	1320	
Crystal size	0.25 x 0.25 x 0.12 mm^3	
Theta range for data collection	2.93 to 27.50°.	
Index ranges	-14<=h<=14, -17<=k<=16, -21<=l<=21	
Reflections collected	30402	
Independent reflections	5408 [R(int) = 0.037]	
Reflections with I>2sigma(I)	4887	
Completeness to theta = 27.50°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Tmax. and Tmin.	0.7456 and 0.5147	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5408 / 0 / 307	
Goodness-of-fit on F^2	1.185	
Final R indices [I>2sigma(I)]	R1 = 0.024, wR2 = 0.062	
R indices (all data)	R1 = 0.029, wR2 = 0.072	
Largest diff. peak and hole	1.30 and -1.48 e.$Å^{-3}$	

Data collection Bruker-Nonius Roper CCD camera on \k-goniostat , Program package WinGX , Abs correction MULTISCAN (sadabs); refinement using SHELXL-97 , Drawing using ORTEP-3 for Windows

NOTE: ANY PUBLICATION THAT INCLUDES THIS DATA MUST ACKNOWLEDGE SERVICE COLLECTION BY THE UK NATIONAL CRYSTALLOGRAPHY SERVICE (NCS) AT THE UNIVERSITY OF SOUTHAMPTON

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Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for apr411. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Au	11218(1)	1797(1)	7871(1)	19(1)
S	13437(1)	2779(1)	10172(1)	25(1)
P	9241(1)	2261(1)	7361(1)	18(1)
F(1)	12989(3)	1193(2)	11018(2)	48(1)
F(2)	14081(4)	2349(2)	11745(2)	70(1)
F(3)	14935(3)	1383(2)	10990(2)	50(1)
O(1)	12403(3)	3308(2)	10381(2)	37(1)
O(2)	14575(3)	3334(2)	10179(2)	35(1)
N(1)	13071(3)	1338(2)	8225(2)	20(1)
N(2)	12954(3)	2100(2)	9413(2)	21(1)
C(1)	13715(3)	1652(2)	8958(2)	19(1)
C(2)	15012(3)	1475(3)	9180(2)	27(1)
C(3)	15584(4)	965(3)	8645(3)	34(1)
C(4)	14913(4)	630(3)	7907(3)	34(1)
C(5)	13652(4)	836(3)	7708(2)	29(1)
C(6)	13890(5)	1884(3)	11029(3)	36(1)
C(7)	8549(3)	3019(3)	8048(2)	21(1)
C(8)	7308(4)	2921(3)	8096(3)	29(1)
C(9)	6804(4)	3533(3)	8626(3)	39(1)
C(10)	7545(4)	4256(3)	9090(3)	38(1)
C(11)	8768(4)	4379(3)	9037(3)	39(1)
C(12)	9290(4)	3753(3)	8528(2)	32(1)
C(13)	8277(3)	1136(2)	7097(2)	18(1)
C(14)	8575(3)	277(2)	7590(2)	20(1)
C(15)	7898(3)	-609(2)	7407(2)	24(1)
C(16)	6932(3)	-657(3)	6722(2)	24(1)
C(17)	6628(3)	193(3)	6226(2)	25(1)
C(18)	7288(3)	1091(3)	6415(2)	23(1)
C(19)	9091(3)	2999(2)	6432(2)	19(1)
C(20)	8263(3)	3826(3)	6262(2)	24(1)
C(21)	8185(4)	4366(3)	5540(2)	29(1)

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C(22)	8900(4)	4088(3)	4997(2)	29(1)
C(23)	9717(4)	3273(3)	5159(3)	29(1)
C(24)	9818(3)	2730(3)	5880(2)	25(1)

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Table 3. Bond lengths [Å] and angles [°] for apr411.

Au-N(1)	2.076(3)
Au-P	2.2317(8)
S-O(1)	1.436(3)
S-O(2)	1.442(3)
S-N(2)	1.553(3)
S-C(6)	1.844(4)
P-C(7)	1.812(4)
P-C(13)	1.815(3)
P-C(19)	1.817(4)
F(1)-C(6)	1.338(5)
F(2)-C(6)	1.325(5)
F(3)-C(6)	1.335(5)
N(1)-C(1)	1.346(5)
N(1)-C(5)	1.354(4)
N(2)-C(1)	1.380(4)
C(1)-C(2)	1.406(5)
C(2)-C(3)	1.377(6)
C(3)-C(4)	1.371(6)
C(4)-C(5)	1.374(5)
C(7)-C(8)	1.384(5)
C(7)-C(12)	1.399(5)
C(8)-C(9)	1.399(5)
C(9)-C(10)	1.377(6)
C(10)-C(11)	1.370(6)
C(11)-C(12)	1.396(6)
C(13)-C(18)	1.397(5)
C(13)-C(14)	1.399(5)
C(14)-C(15)	1.380(5)
C(15)-C(16)	1.386(5)
C(16)-C(17)	1.392(5)
C(17)-C(18)	1.385(5)
C(19)-C(24)	1.393(5)
C(19)-C(20)	1.405(5)
C(20)-C(21)	1.392(5)

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C(21)-C(22)	1.375(5)
C(22)-C(23)	1.385(5)
C(23)-C(24)	1.392(5)

N(1)-Au-P	174.24(8)
O(1)-S-O(2)	118.55(17)
O(1)-S-N(2)	109.49(18)
O(2)-S-N(2)	115.99(18)
O(1)-S-C(6)	102.1(2)
O(2)-S-C(6)	103.4(2)
N(2)-S-C(6)	105.13(17)
C(7)-P-C(13)	107.71(16)
C(7)-P-C(19)	106.39(17)
C(13)-P-C(19)	106.56(16)
C(7)-P-Au	114.22(13)
C(13)-P-Au	109.54(11)
C(19)-P-Au	112.05(12)
C(1)-N(1)-C(5)	120.8(3)
C(1)-N(1)-Au	117.3(2)
C(5)-N(1)-Au	121.6(2)
C(1)-N(2)-S	124.2(2)
N(1)-C(1)-N(2)	112.3(3)
N(1)-C(1)-C(2)	119.4(3)
N(2)-C(1)-C(2)	128.3(3)
C(3)-C(2)-C(1)	118.8(4)
C(4)-C(3)-C(2)	121.2(4)
C(3)-C(4)-C(5)	117.9(4)
N(1)-C(5)-C(4)	121.8(4)
F(2)-C(6)-F(3)	107.8(4)
F(2)-C(6)-F(1)	107.3(4)
F(3)-C(6)-F(1)	107.4(3)
F(2)-C(6)-S	112.2(3)
F(3)-C(6)-S	111.4(3)
F(1)-C(6)-S	110.5(3)
C(8)-C(7)-C(12)	119.0(3)
C(8)-C(7)-P	122.5(3)

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C(12)-C(7)-P	118.5(3)
C(7)-C(8)-C(9)	120.7(4)
C(10)-C(9)-C(8)	119.6(4)
C(11)-C(10)-C(9)	120.5(4)
C(10)-C(11)-C(12)	120.3(4)
C(11)-C(12)-C(7)	119.9(4)
C(18)-C(13)-C(14)	119.4(3)
C(18)-C(13)-P	122.8(2)
C(14)-C(13)-P	117.7(3)
C(15)-C(14)-C(13)	120.4(3)
C(14)-C(15)-C(16)	120.0(3)
C(15)-C(16)-C(17)	120.1(3)
C(18)-C(17)-C(16)	120.2(3)
C(17)-C(18)-C(13)	119.8(3)
C(24)-C(19)-C(20)	119.8(3)
C(24)-C(19)-P	118.6(3)
C(20)-C(19)-P	121.5(3)
C(21)-C(20)-C(19)	119.2(3)
C(22)-C(21)-C(20)	120.5(3)
C(21)-C(22)-C(23)	120.7(4)
C(22)-C(23)-C(24)	119.7(4)
C(23)-C(24)-C(19)	120.1(3)

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BIOLOGY

Materials and methods

Cell culture

The breast cancer cell lines MDA-MB-231 and MDA-MB-468 as well as green monkey kidney epithelial cells (CV1) were obtained from Cancer Research UK. Cells were grown in 25 ml Dulbecco's modified medium (DMEM, 21969; Gibco) supplemented with 12% fetal calf serum (16010-159; lot 1014583; PAA), 1% penicillin/streptomycin and 1% L-glutamate in 75 cm^3 cell culture flasks (Corning). The media and supplements were obtained from Gibco/invitrogen. Cell cultures were maintained at 37°C and 5% CO_2. Cells were split every 3-4 days, cells never reached a confluency greater than 95% to avoid cells growing on top of each other. Prior to trypsinization of cells in preparation for splitting, cells were inspected on a standard light microscope and only propagated further or used in assays if they appeared 'normal' (not floating) and were not contaminated (*e.g.* by bacteria or yeast). A maximum of 25 passages were carried out.

Trypsinization.

Cells were washed twice in 13 mls of phosphate buffered saline (pH 7.25). Cells were trypsinized with 2.5 mg trypsin (27250-018; GIBCO)/ml phosphate buffered saline (pH 7.25) for 5 min. at 37°C and 5% CO_2. The trypsin was removed from the cells adding 10 ml of DMEM, supplemented as above ("Cell Culture") to the culture flask and then adding the cell suspension to a 30 ml tube (201150, Greiner Bio One). The cells were centrifuged at 1500 rpm in a Rotina 38R (Hettich) for 5 min. (room temperature, ~21 °C) and the supernatant was aspirated before cells were resuspended in 10mls of DMEM, supplemented as above. Haemocytometer counts were carried out at this stage to determine 'cell concentration'.

Cell viability assay

Cell viability was determined using the CellTiter-Blue® Cell Viability Assay (G8080, Promega) following the instructions by the supplier. It was found that confluency of the cells prior to incubation with the gold(I) complexes influenced cell viability. Therefore, cells were initially grown to a 'cell concentration' between 2×10^5 to $5 \times$

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10^5 cells/ml, as determined by haemocytometer counts after trypsinization of the cells (see above). At this 'cell concentration', cells were healthy and no substantial level of 'floating', detached cells were noticed. Moreover, cell viability was substantially higher after treatment with the gold(I) complexes within this range, compared to higher, commonly-used concentrations (or confluencies leading to higher concentrations using the cell concentration measure defined above).

After trypsinization, cells were resuspended in phenol red free DMEM (VX1053028; Fisher) to prevent interactions of the gold compounds and phenol red. This was supplemented as described above for the standard DMEM. ~ 5000 cells were then seeded into wells of 96-well black-walled, clear bottomed plates (655090; Greiner). The plates were incubated for 24 hours, as described above, to allow cells to adhere to the well. The gold(I) compounds were prepared from powder immediately prior to use by dissolving the compound in undiluted (~100%) DMSO to give a stock concentration of 100 mM. This stock was further diluted with 10% (v/v, diluted in sterile, distilled water) DMSO to yield a 1 mM solution in 10.9% DMSO. Gold compounds were added to each well in the indicated concentrations, keeping the final concentration of DMSO constant at 0.109% (v/v), except for the [Bis(trifluoromethanesulfonyl)imidate](triphenylphosphine)gold(I) experiments where the final concentration was 0.209% (v/v) DMSO. 3-8 replicates were made each time. A DMSO-only control (0.1% v/v), a medium-only control (no DMSO and no drug), and no-cells control (media only) were added to the plate. The final volume of each well was 100 µl.

The plates were incubated for a further 44 hours, at 37°C and 5% CO_2 (in the dark). After 44 hours, 20 µl of CellTiter-Blue® was added to each well of the plate and the plate incubated for a further 4 hours at 37°C and 5% CO_2 (in the dark). Fluorescence readings from each well were then measured at 560nm/590nm using a Promega Glomax multi detection system. Cell viability was determined as follows. Fluorescence of each well was recorded as 'total fluorescence'. 'Background fluorescence' (determined by the mean value of the 'no-cells' control) was subtracted from 'total fluorescence' to yield 'adjusted fluorescence'. 'Normalized fluorescence' was calculated as 'adjusted fluorescence' divided by the 'adjusted fluorescence' of the mean of the DMSO-only (no drug, or 0 µM) treated cells. We observed no significant

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differences between DMSO-only treated cells (0.1% or 0.2% v/v) and media-only treated cells (Figures 2 and Figure 4).

Curve fitting and IC_{50} determination.

IC_{50} concentrations for complexes 1 and 2 were determined using GraphPad Prism. The nonlinear regression curve fit model was chosen using the log(inhibitor) vs. response-variable response (four parameter) equation. Outliers were identified using the Grubbs test.

Treatment with nigericin.

Cell viability in response to nigericin (N7143, Sigma) and treatment with compounds 1 and 2 were carried out as above, except the cells were treated with nigericin at the indicated final concentration or ethanol-only (CV1 0.1%, MDA-MB-231 0.3-1% ethanol) for 30 min. prior to the addition of compound 1 or 2 (final concentration 4.28 μM or 5 μM respectively, or DMSO-only).

Thioredoxin reductase and Glutathione reductase assays

The *in vitro* thioredoxin reductase and glutathione reductase activity were measured using abcam thioredoxin reductase and glutathione reductase assay kits (ab83463 and ab83461, respectively) following the instructions by the supplier. Briefly, thioredoxin reductase (T9698, Sigma) or glutathione reductase (G9297, sigma) both at concentrations of 0.0005 units/μl were treated with increasing concentrations of compound 1, compound 2, or the indicated ligands. The absorbance was measured on a BIO-TEK synergy HT plate reader at 405 nm, every 30 seconds for up to 20 min. TrxR and GR activities were calculated as nmol TNB $\cdot$ min^{-1} $\cdot$ ml^{-1} sample volume.

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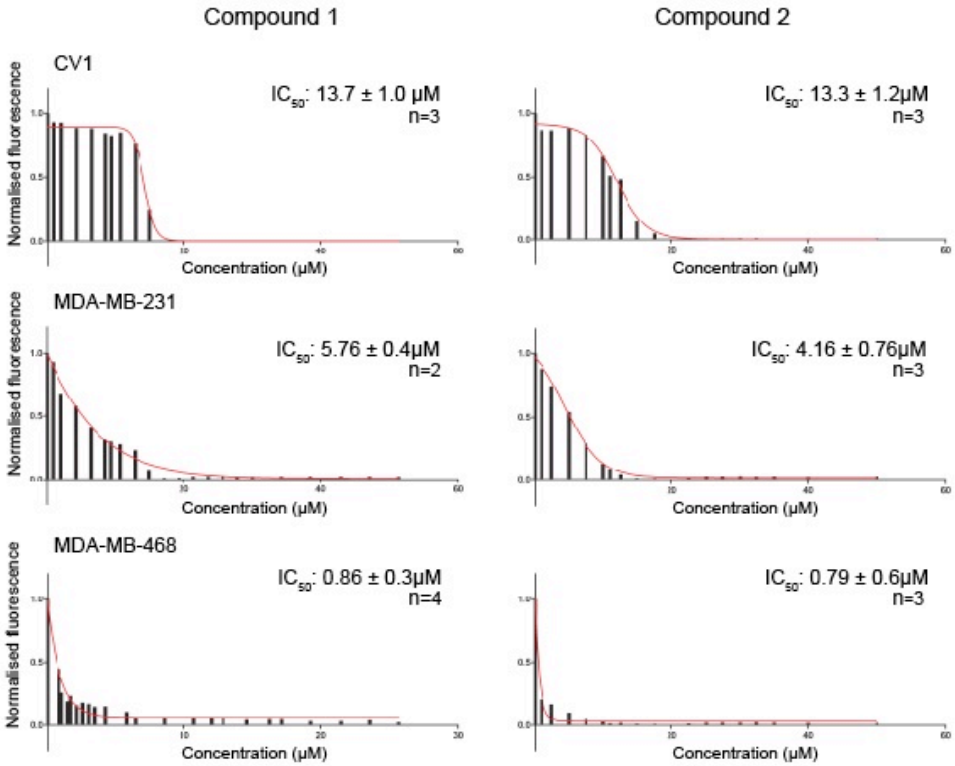
Supplementary figures



Supplemental Figure 1 - IC_{50} estimation for compounds 1 and 2. Representative response curves for CV-1 control cells and the two cancer cells lines are shown. The IC_{50} values were estimated from curve-fitting using GraphPad. S.E. represents the standard error of the mean, calculated from n independent experiments.

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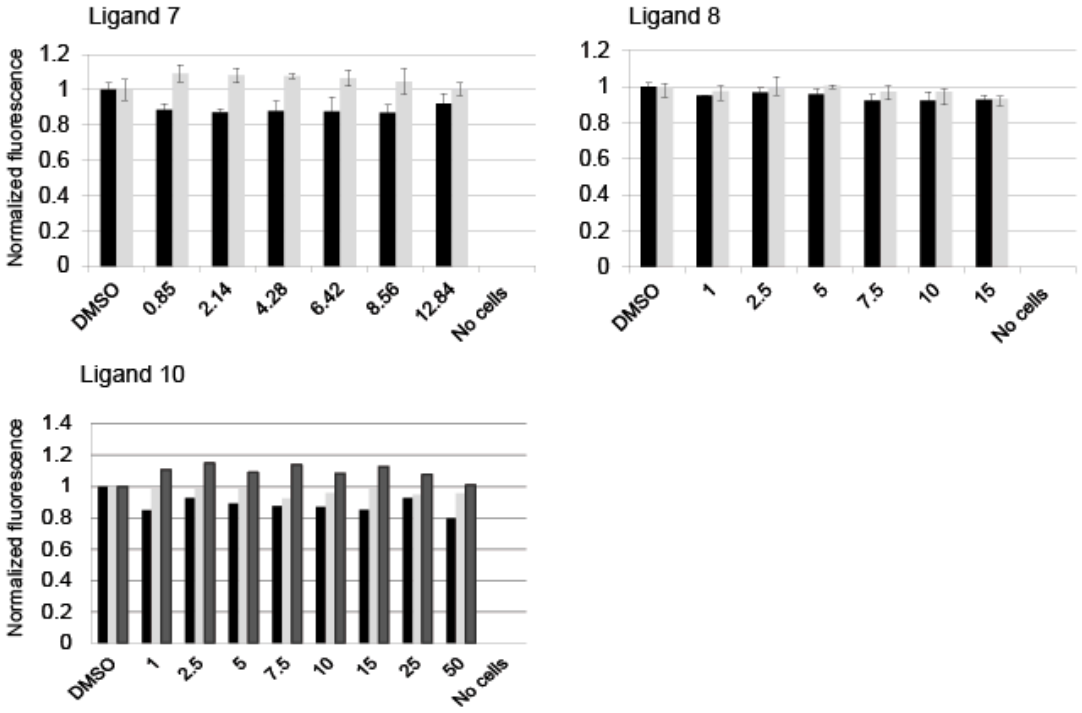

Supplemental Figure 2 – Cell viability assays for the ligands of compounds 1 and 2 using the resazurin reductase activity assay on breast cancer cell line MDA-MB-231 and control epithelial cell line (CV-1). Cell viability was determined by measuring the fluorescence of DMSO-treated ('0 μM'), and ligand treated cells. The 'No cells' control was used for background subtraction. The normalized fluorescence was calculated as the background-subtracted fluorescence reading, divided by the background-subtracted fluorescence reading of the DMSO-treated control. The error bars correspond to the standard deviation of the mean of three replicates.