

Supporting Information

Ligand-Enabled Hydrohydrazidation of Alkynes Catalyzed by Unsymmetrical Gold(I)–Thiazol-2-ylidenes

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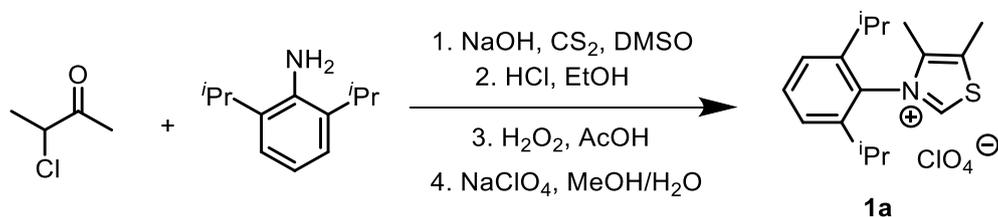
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1. General Information

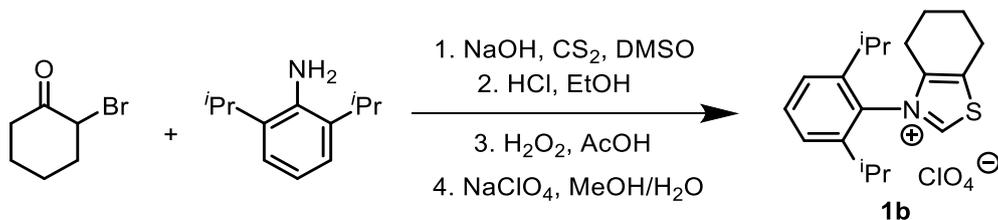
All starting materials reported in the manuscript have been previously described in literature or prepared by the method reported previously unless stated otherwise. All experiments were performed using standard Schlenk techniques under air unless stated otherwise. All solvents were purchased at the highest commercial grade and used as received or after purification by passing through activated alumina columns or distillation from sodium/benzophenone under nitrogen. All other chemicals were purchased at the highest commercial grade and used as received. All products were identified using ^1H NMR and ^{13}C NMR analysis and comparison with authentic samples. Reaction glassware was oven-dried at 140 °C for at least 24 h or flame-dried prior to use, allowed to cool under vacuum and purged with argon (three cycles). All yields refer to yields determined by ^1H NMR using an internal standard (optimization) unless stated otherwise. ^1H NMR and ^{13}C NMR spectra were recorded in CDCl_3 or $\text{DMSO-}d_6$ on a Bruker Ascend spectrometers at 400 (^1H NMR) and 101 MHz (^{13}C NMR) or 600 (^1H NMR) and 151 MHz (^{13}C NMR). All shifts are reported in parts per million (ppm) relative to residual CHCl_3 peak (7.26 and 77.16 ppm, ^1H NMR and ^{13}C NMR, respectively), $\text{DMSO-}d_6$ peak (2.50 and 39.52 ppm, ^1H NMR and ^{13}C NMR, respectively). All coupling constants (J) are reported in hertz (Hz). Abbreviations are: s = singlet, brs = broad singlet, d = doublet, t = triplet, q = quartet. Dibromomethane was used as an internal standard to determine NMR yields. High resolution mass spectra were acquired on a Q-Exactive Focus Hybrid Quadrupole-Orbitrap Mass Spectrometer (Thermo Fisher). Powder diffraction data were recorded on a Rigaku Smart Lab diffractometer with Cu-K radiation and D/teX Ultra detector covering 3-60° (2 θ). All flash chromatography was performed using silica gel, 60 Å, 300 mesh. TLC analysis was carried out on glass plates coated with silica gel 60 F254, 0.2 mm thickness. The plates were visualized using a 254 nm ultraviolet lamp. ^1H NMR, ^{13}C NMR and HRMS data are given for all new compounds in the Supporting Experimental for characterization purposes.

2 . Experimental Procedures and Characterization Data

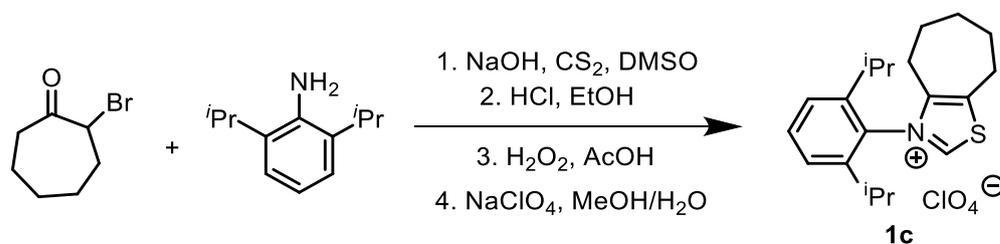
2.1 General Procedure for the Synthesis of Thiazolium Salts.



3-(2,6-Diisopropylphenyl)-4,5-dimethylthiazol-3-ium perchlorate (1a). An oven-dried 250 mL round-bottomed flask equipped with a stir bar was charged with 2,6-Diisopropylaniline (7.09 g, 40 mmol, 1.0 eq.), 20 N aq. NaOH solution (2 mL, 40 mmol, 1.0 eq.) and DMSO (20 mL). The mixture was cooled to 0 °C and the CS₂ (3.05 g, 40 mmol, 1.0 eq) was added dropwise and stirred for 1 h at room temperature. Then the 3-chlorobutan-2-one (4.26 g, 40 mmol, 1.0 eq.) was added at 0 °C and the mixture was stirred for 12 h at room temperature. H₂O (40 mL) was added, the mixture was stirred for 10 min at 0 °C and the supernatant solution was decanted. The resulting slurry was suspended in EtOH (40 mL), concd. HCl (2 mL) was added and the mixture was heated to reflux for 1 h. After cooling to room temperature, the mixture was placed in the fridge, where crystals precipitated. The solid was collected by suction filtration and was washed with a small amount of H₂O. Continue to add the solid washed in the previous step to the bottle and glacial acetic acid (82.4 mL). The mixture was cooled to 0 °C and the H₂O₂ (7.48 g, 66 mmol, 3.3 eq.) was added dropwise and stirred for 1 h at 0 °C. Then the volatile components were removed under reduced pressure and the residue was dissolved in MeOH (13.8 mL). At 0 °C a mixture of sodium perchlorate monohydrate (11.57 g, 82.4 mmol, 4.12 eq) in a mixture of MeOH/H₂O = 2/1 (69 mL) was added. After stirring for 30 min, the solid was collected by suction filtration and was washed with H₂O (100 mL). The following recrystallisation with MeOH afforded the product **1a** as a white solid (6.87 g, 83%). ¹H NMR (600 MHz, CDCl₃) δ 9.78 (s, 1H), 7.59 (t, *J* = 7.9 Hz, 1H), 7.36 (d, *J* = 7.9 Hz, 2H), 2.69 (s, 3H), 2.11 (s, 3H), 2.10 – 1.93 (m, 2H), 1.17 (d, *J* = 6.8 Hz, 6H), 1.12 (d, *J* = 6.8 Hz, 6H). ¹³C NMR (151 MHz, CDCl₃) δ 156.5, 144.7, 142.7, 135.5, 132.6, 132.2, 125.4, 28.8, 25.0, 23.1, 13.1, 11.8. The compound showed identical spectroscopic properties to those reported previously¹.



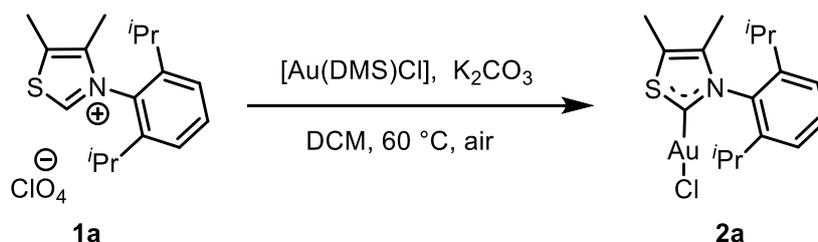
3-(2,6-Diisopropylphenyl)-4,5,6,7-tetrahydrobenzo[*d*]thiazol-3-ium perchlorate (1b). An oven-dried 250 mL round-bottomed flask equipped with a stir bar was charged with 2,6-Diisopropylaniline (7.09 g, 40 mmol, 1.0 eq.), 20 N aq. NaOH solution (2 mL, 40 mmol, 1.0 eq.) and DMSO (20 mL). The mixture was cooled to 0 °C and the CS₂ (3.05 g, 40 mmol, 1.0 eq) was added dropwise and stirred for 1 h at room temperature. Then the 2-bromocyclohexanone (7.08 g, 40 mmol, 1.0 eq.) was added at 0 °C and the mixture was stirred for 12 h at room temperature. H₂O (40 mL) was added, the mixture was stirred for 10 min at 0 °C and the supernatant solution was decanted. The resulting slurry was suspended in EtOH (40 mL), concd. HCl (2 mL) was added and the mixture was heated to reflux for 1 h. After cooling to room temperature, the solid was collected by suction filtration and was recrystallized from EtOH. Continue to add the solid washed in the previous step to the bottle and glacial acetic acid (82.4 mL). The mixture was cooled to 0 °C and the H₂O₂ (7.48 g, 66 mmol, 3.3 eq.) was added dropwise and stirred for 1 h at 0 °C. Then the volatile components were removed under reduced pressure and the residue was dissolved in MeOH (13.8 mL). At 0 °C a mixture of sodium perchlorate monohydrate (11.57 g, 82.4 mmol, 4.12 eq) in a mixture of MeOH/H₂O = 2/1 (69 mL) was added. After stirring for 30 min, the solid was collected by suction filtration and was washed with H₂O (50 mL). The following recrystallisation with MeOH afforded the product **1b** as a white solid (4.81 g, 80%). ¹H NMR (600 MHz, CDCl₃) δ 9.84 (s, 1H), 7.58 (t, *J* = 7.8 Hz, 1H), 7.35 (d, *J* = 7.9 Hz, 2H), 3.10 (t, *J* = 6.2 Hz, 2H), 2.26 (t, *J* = 6.3 Hz, 2H), 2.06 (p, *J* = 6.8 Hz, 2H), 2.00 – 1.95 (m, 2H), 1.91 – 1.86 (m, 3H), 1.17 (d, *J* = 6.8 Hz, 6H), 1.13 (d, *J* = 6.8 Hz, 6H). ¹³C NMR (151 MHz, CDCl₃) δ 157.3, 144.9, 144.7, 138.0, 132.8, 131.5, 125.6, 29.1, 25.3, 24.1, 23.8, 23.3, 21.9, 21.0. The compound showed identical spectroscopic properties to those reported previously¹.



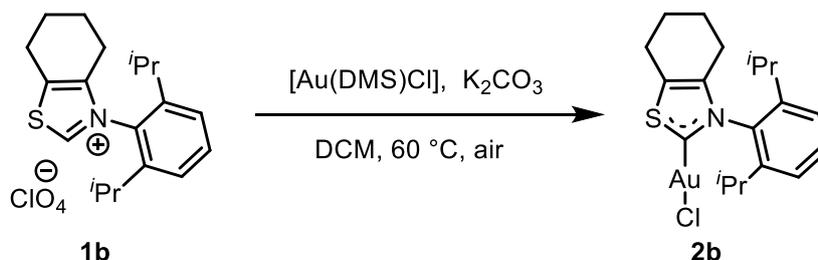
3-(2,6-Diisopropylphenyl)-5,6,7,8-tetrahydro-4H-cyclohepta[*d*]thiazol-3-ium perchlorate (1c). An oven-dried 250 mL round-bottomed flask equipped with a stir bar was charged with 2,6-Diisopropylaniline (7.09 g, 40 mmol, 1.0 eq.), 20 N aq. NaOH solution (2 mL, 40 mmol, 1.0 eq.) and DMSO (20 mL). The mixture was cooled to 0 °C and the CS₂ (3.05 g, 40 mmol, 1.0 eq) was added dropwise and stirred for 1 h at room temperature. Then the 2-bromocycloheptanone (7.64 g, 40 mmol, 1.0 eq.) was added at 0 °C and the mixture was stirred for 12 h at room temperature. H₂O (40 mL) was added, the mixture was stirred for 10 min at 0 °C and the supernatant solution was decanted. The resulting slurry was suspended in EtOH (40 mL), concd. HCl (2 mL) was added and the mixture was heated to reflux for 1 h. After cooling to room temperature, the resulting precipitate was collected by suction filtration and was washed with cold EtOH

(20 mL). Continue to add the solid washed in the previous step to the bottle and glacial acetic acid (82.4 mL). The mixture was cooled to 0 °C and the H₂O₂ (7.48 g, 66 mmol, 3.3 eq.) was added dropwise and stirred for 1 h at 0 °C. Then the volatile components were removed under reduced pressure and the residue was dissolved in MeOH (13.8 mL). At 0 °C a mixture of sodium perchlorate monohydrate (11.57 g, 82.4 mmol, 4.12 eq) in a mixture of MeOH/H₂O = 2/1 (69 mL) was added. After stirring for 30 min, the solid was collected by suction filtration and was washed with H₂O (50 mL). The following recrystallisation with MeOH afforded the product **1c** as a white solid (7.14 g, 81%). ¹H NMR (600 MHz, CDCl₃) δ 9.65 (s, 1H), 7.59 (t, *J* = 7.8 Hz, 1H), 7.35 (d, *J* = 7.9 Hz, 2H), 3.20 – 3.15 (m, 2H), 2.57 – 2.53 (m, 2H), 2.05 (p, *J* = 6.8 Hz, 2H), 1.98 – 1.92 (m, 2H), 1.89 (td, *J* = 6.9, 3.5 Hz, 2H), 1.62 (dd, *J* = 7.1, 4.1 Hz, 2H), 1.16 (d, *J* = 6.8 Hz, 12H). ¹³C NMR (151 MHz, CDCl₃) δ 155.3, 148.6, 144.8, 141.0, 132.4, 132.0, 125.1, 30.7, 28.7, 28.1, 27.2, 26.5, 25.4, 24.7, 23.1. The compound showed identical spectroscopic properties to those reported previously¹.

2.2. General Procedure for the Synthesis of gold(I)–thiazol-2-ylidenes.

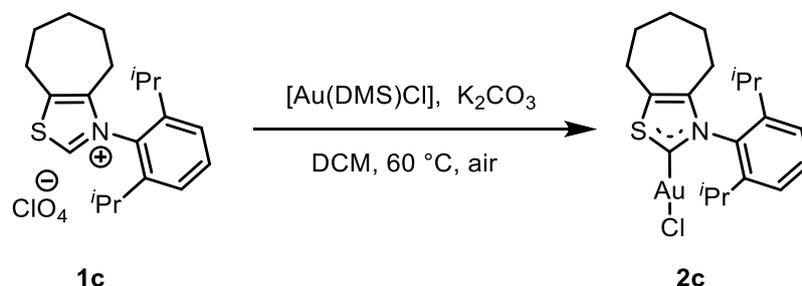


(3-(2,6-Diisopropylphenyl)-4,5-dimethyl-2,3-dihydrothiazol-2-yl) gold (I) chloride (2a). An oven-dried vial equipped with a stir bar was charged with 3-(2,6-Diisopropylphenyl)-4,5-dimethylthiazol-3-ium perchlorate (**1a**) (74.8 mg, 0.2 mmol, 1.0 eq.), [Au(DMS)Cl] (64.8 mg, 0.22 mmol, 1.1 eq.), K₂CO₃ (30.4 mg, 0.22 mmol, 1.1 eq.), DCM (5 mL, 0.04 M) was added and the reaction mixture was stirred overnight at 60 °C. The reaction mixture was filtered through Celite with DCM as eluent and concentrated under reduced pressure, and dried under high vacuum to afford Gold(I) complex **2a** as a white solid (92.1 mg, 91%). M.p. = 235–237 °C. ¹H NMR (600 MHz, CDCl₃) δ 7.51 (t, *J* = 7.8 Hz, 1H), 7.29 (d, *J* = 7.8 Hz, 2H), 2.42 (s, 3H), 2.12 (p, *J* = 6.8 Hz, 2H), 1.94 (s, 3H), 1.32 (d, *J* = 6.8 Hz, 6H), 1.14 (d, *J* = 6.9 Hz, 6H). ¹³C NMR (151 MHz, CDCl₃) δ 194.2, 144.4, 141.0, 137.0, 130.9, 129.9, 124.8, 28.4, 24.9, 23.3, 12.5. HRMS calcd for C₁₇H₂₃AuNS⁺[M-Cl]⁺ 470.1211, found 470.1236.

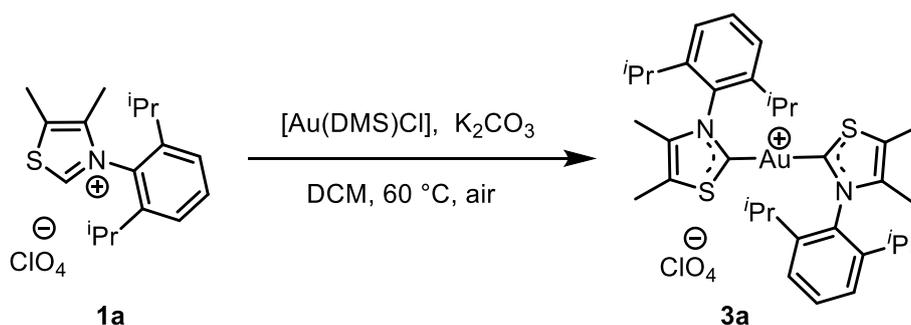


(3-(2,6-Diisopropylphenyl)-2,3,4,5,6,7-hexahydrobenzo[d]thiazol-2-yl) gold(I) 3-

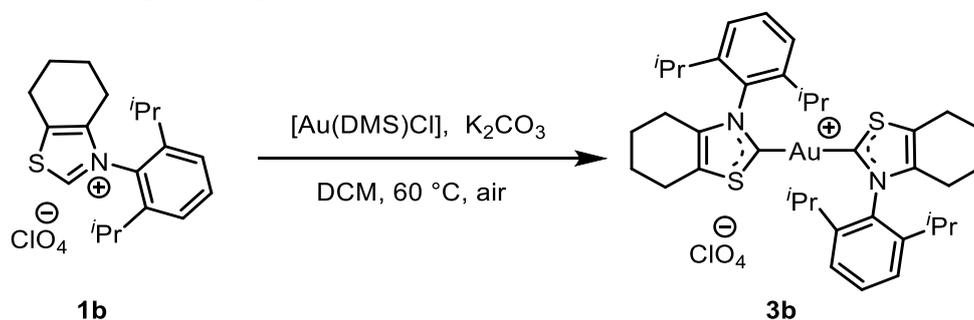
(2,6-diisopropylphenyl)-4,5,6,7-tetrahydrobenzo[d]thiazol-3-iumbis(3-(2,6-diisopropylphenyl)-2,3,4,5,6,7-hexahydrobenzo[d]thiazol-2-yl) gold(I) chloride diperchlorate (2b). An oven-dried vial equipped with a stir bar was charged with 3-(2,6-Diisopropylphenyl)-4,5,6,7-tetrahydrobenzo[d]thiazol-3-ium perchlorate (**1b**) (80.1 mg, 0.2 mmol, 1.0 eq.), [Au(DMS)Cl] (64.8 mg, 0.22 mmol, 1.1 eq.), K₂CO₃ (30.4 mg, 0.22 mmol, 1.1 eq.), DCM (5 mL, 0.04 M) was added and the reaction mixture was stirred overnight at 60 °C. The reaction mixture was filtered through Celite with DCM as eluent and concentrated under reduced pressure, and dried under high vacuum to afford Gold(I) complex **2b** as a white solid (93.6 mg, 88%). M.p.= 220-222 °C. ¹H NMR (600 MHz, CDCl₃) δ 7.51 (t, *J* = 7.8 Hz, 1H), 7.28 (d, *J* = 7.8 Hz, 2H), 2.80 (t, *J* = 6.0 Hz, 2H), 2.18 – 2.09 (m, 4H), 1.92 – 1.86 (m, 2H), 1.82 – 1.77 (m, 2H), 1.32 (d, *J* = 6.8 Hz, 6H), 1.14 (d, *J* = 6.9 Hz, 6H). ¹³C NMR (151 MHz, CDCl₃) δ 194.3, 144.4, 143.4, 135.9, 132.3, 130.9, 124.8, 28.4, 25.0, 24.4, 23.6, 23.3, 22.0, 21.4. HRMS calcd for C₁₉H₂₅AuNS⁺[M-Cl]⁺ 496.1368, found 496.1340.



(3-(2,6-Diisopropylphenyl)-3,4,5,6,7,8-hexahydro-2H-cyclohepta[d]thiazol-2-yl) gold(I) chloride (2c). An oven-dried vial equipped with a stir bar was charged with 3-(2,6-Diisopropylphenyl)-5,6,7,8-tetrahydro-4H-cyclohepta[d]thiazol-3-ium perchlorate (**1c**) (82.8 mg, 0.2 mmol, 1.0 eq.), [Au(DMS)Cl] (64.8 mg, 0.22 mmol, 1.1 eq.), K₂CO₃ (30.4 mg, 0.22 mmol, 1.1 eq.), DCM (5 mL, 0.04 M) was added and the reaction mixture was stirred overnight at 60 °C. The reaction mixture was filtered through Celite with DCM as eluent and concentrated under reduced pressure, and dried under high vacuum to afford Gold(I) complex **2c** as a white solid (92.8 mg, 85%). M.p.= 183-185 °C. ¹H NMR (600 MHz, CDCl₃) δ 7.51 (t, *J* = 7.8 Hz, 1H), 7.28 (d, *J* = 7.9 Hz, 2H), 2.91 – 2.84 (m, 2H), 2.44 – 2.37 (m, 2H), 2.14 (p, *J* = 6.9 Hz, 2H), 1.84 (d, *J* = 38.3 Hz, 4H), 1.57 (s, 2H), 1.32 (d, *J* = 6.8 Hz, 6H), 1.12 (d, *J* = 6.9 Hz, 6H). ¹³C NMR (151 MHz, CDCl₃) δ 192.9, 147.8, 144.7, 137.2, 136.0, 130.8, 124.7, 31.0, 28.4, 28.2, 27.8, 26.9, 25.9, 24.7, 23.4. HRMS calcd for C₂₀H₂₇AuClNS⁺[M-Cl]⁺ 510.1524, found 510.1607.



(3-(2,6-Diisopropylphenyl)-4,5-dimethyl-2,3-dihydrothiazol-2-yl) gold(I) 3-(2,6-diisopropylphenyl)-4,5-dimethylthiazol-3-ium bis(3-(2,6-diisopropylphenyl)-4,5-dimethyl-2,3-dihydrothiazol-2-yl) gold(I) chloride diperchlorate (3a). An oven-dried vial equipped with a stir bar was charged with 3-(2,6-Diisopropylphenyl)-4,5-dimethylthiazol-3-ium perchlorate (**1a**) (74.8 mg, 0.2 mmol, 1.0 eq.), [Au(DMS)Cl] (29.5 mg, 0.1 mmol, 0.5 eq.), K₂CO₃ (30.4 mg, 0.22 mmol, 1.1 eq.), DCM (5 mL, 0.04 M) was added and the reaction mixture was stirred overnight at 60 °C. The reaction mixture was filtered through Celite with DCM as eluent and concentrated under reduced pressure, and dried under high vacuum to afford Gold(I) complex **3a** as a white solid (67.6 mg, 80%). M.p.= 217-219 °C. ¹H NMR (600 MHz, CDCl₃) δ 7.46 (t, *J* = 7.8 Hz, 2H), 7.21 (d, *J* = 7.8 Hz, 4H), 2.49 (s, 6H), 1.92 (d, *J* = 3.7 Hz, 10H), 1.09 (d, *J* = 6.8 Hz, 12H), 0.90 (d, *J* = 6.8 Hz, 12H). ¹³C NMR (151 MHz, CDCl₃) δ 204.5, 144.3, 142.5, 136.5, 132.3, 131.0, 124.8, 28.2, 25.0, 23.1, 12.6, 12.3. HRMS calcd for C₃₄H₄₆AuN₂S₂⁺[M-ClO₄]⁺ 743.2762, found 743.2753.



bis(3-(2,6-Diisopropylphenyl)-4,5,6,7-tetrahydrobenzo[d]thiazol-2(3H)-ylidene) gold(I) (3b). An oven-dried vial equipped with a stir bar was charged with 3-(2,6-Diisopropylphenyl)-4,5,6,7-tetrahydrobenzo[d]thiazol-3-ium perchlorate (**1b**) (80.1 mg, 0.2 mmol, 1.0 eq.), [Au(DMS)Cl] (29.5 mg, 0.1 mmol, 0.5 eq.), K₂CO₃ (30.4 mg, 0.22 mmol, 1.1 eq.), DCM (5 mL, 0.04 M) was added and the reaction mixture was stirred overnight at 60 °C. The reaction mixture was filtered through Celite with DCM as eluent and concentrated under reduced pressure, and dried under high vacuum to afford Gold(I) complex **3b** as a white solid (73.6 mg, 82%). M.p.= 240-242 °C. ¹H NMR (600 MHz, CDCl₃) δ 7.46 (t, *J* = 7.8 Hz, 2H), 7.20 (d, *J* = 7.8 Hz, 4H), 2.87 (t, *J* = 6.3 Hz, 4H), 2.08 (t, *J* = 6.3 Hz, 4H), 1.93 (p, *J* = 6.9 Hz, 4H), 1.89 – 1.84 (m, 4H), 1.80 – 1.75 (m, 4H), 1.09 (d, *J* = 6.9 Hz, 12H), 0.89 (d, *J* = 6.8 Hz, 12H). ¹³C NMR (151 MHz, CDCl₃) δ 205.1, 144.8, 144.4, 135.5, 134.6, 131.1, 124.8, 28.3, 25.1, 24.3, 23.8, 23.1, 21.9, 21.3. HRMS calcd for C₃₈H₅₀AuN₂S₂⁺[M-ClO₄]⁺ 795.3075, found

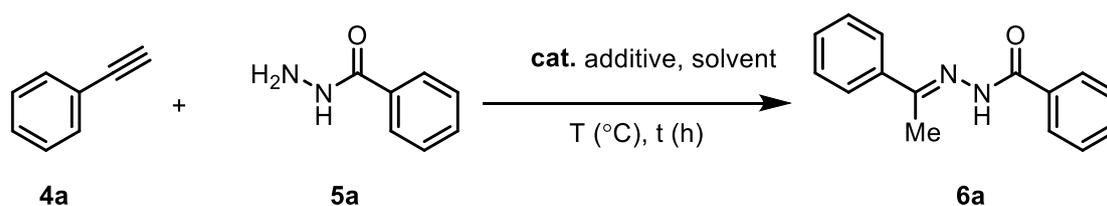
Table S1. Summary of % buried volume of NHC-Au Complexes.^a

Au(I)-NHC	SW	NW	NE	SE	%V _{bur}
2a	45.1	48.0	23.1	23.2	34.8
3a	38.1	51.1	23.3	23.5	34.0
2b	41.0	49.9	23.2	23.2	34.3
3b	46.9	39.7	24.3	22.4	33.3
2c	46.7	40.9	23.6	23.6	33.7
3c	45.4	45.5	23.0	22.5	34.1

^aX-ray crystallographic data

2.4 Optimization of Conditions for Gold catalyzed Hydrazine Reaction

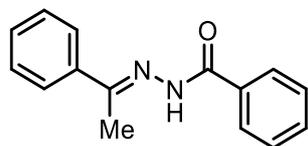
An oven-dried seal tube equipped with a stir bar was charged with the Au-NHC catalyst, additive, **4a** (2.0 eq, 0.4 mmol, 40.8 mg), **5a** (1.0 eq, 0.2 mmol, 27.2 mg) and solvent (2.0 mL, 0.1 M). The reaction mixture was stirred at 60 °C (oil bath) for 6 h. Upon completion of the reaction, as indicated by the specified time, the mixture was allowed to cool to room temperature. It was then diluted with CH₂Cl₂, filtered through a plug of silica gel to remove any insoluble materials, and concentrated in vacuo. The crude product was purified by column chromatography on silica gel, using an appropriate eluent system to afford the desired product.

**Table S2** Optimization of Reaction Conditions.

entry	Cat. (mol%)	additive	solvent	T (°C)	yield (%)
1	2a (2.0)	NaBAr ^F ₄	CHCl ₃	80	91
2	3a (2.0)	NaBAr ^F ₄	CHCl ₃	80	trace
3	2b (2.0)	NaBAr ^F ₄	CHCl ₃	80	88
4	3b (2.0)	NaBAr ^F ₄	CHCl ₃	80	trace
5	2c (2.0)	NaBAr ^F ₄	CHCl ₃	80	86
6	3c (2.0)	NaBAr ^F ₄	CHCl ₃	80	trace
7 ^b	IPrAuCl	NaBAr ^F ₄	CHCl ₃	80	55

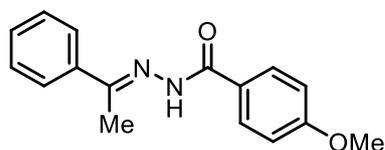
2.6 Characterization Data of Products

(E)-N'-(1-Phenylethylidene) benzohydrazide (6a).



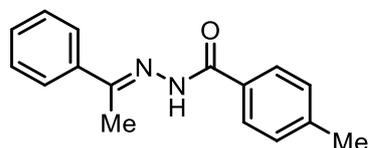
Purification by flash chromatography (DCM/EtOAc = 10:1): pale white solid (43.3 mg, 91%). ¹H NMR (600 MHz, DMSO) δ 10.77 (s, 1H), 7.88 (br, 4H), 7.58 (br, 1H), 7.57-7.50 (m, 2H), 7.43 (s, 3H), 2.37 (s, 3H). ¹³C NMR (151 MHz, DMSO) δ 163.9, 155.6, 138.1, 134.1, 131.5, 129.5, 128.4, 127.9, 126.4, 14.6. The compound showed identical spectroscopic properties to those reported previously².

(E)-4-Methoxy-N'-(1-phenylethylidene)benzohydrazide (6b)



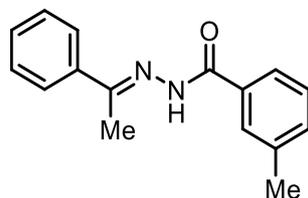
Purification by flash chromatography (DCM/EtOAc = 10:1): pale yellow solid (42.9 mg, 90%). ¹H NMR (600 MHz, DMSO) δ 10.61 (s, 1H), 7.92 – 7.78 (m, 4H), 7.42 (s, 3H), 7.04 (d, J = 8.8 Hz, 2H), 3.83 (s, 3H), 2.36 (s, 3H). ¹³C NMR (151 MHz, DMSO) δ 161.8, 138.2, 129.7, 129.3, 128.4, 126.3, 126.1, 113.5, 55.4, 14.4. The compound showed identical spectroscopic properties to those reported previously².

(E)-4-Methyl-N'-(1-phenylethylidene)benzohydrazide (6c)



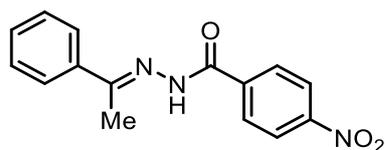
Purification by flash chromatography (DCM/EtOAc = 10:1): pale yellow solid (44.9 mg, 89%). ¹H NMR (600 MHz, DMSO) δ 10.68 (s, 1H), 7.97 – 7.80 (m, 4H), 7.43 (s, 3H), 7.32 (d, J = 8.1 Hz, 2H), 2.38 (s, 3H), 2.36 (s, 3H). ¹³C NMR (151 MHz, DMSO) δ 138.2, 131.2, 129.7, 129.4, 128.9, 128.4, 128.0, 126.4, 21.1, 14.6. The compound showed identical spectroscopic properties to those reported previously².

(E)-3-Methyl-N'-(1-phenylethylidene)benzohydrazide (6d)



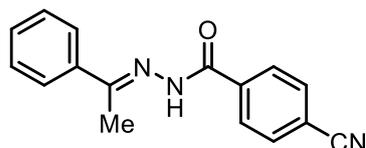
Purification by flash chromatography (DCM/EtOAc = 10:1): pale yellow solid (42.4 mg, 84%). ¹H NMR (600 MHz, DMSO) δ 10.74 (s, 1H), 7.89 (s, 2H), 7.71 – 7.48 (m, 5H), 7.28 (br, 2H), 2.36 (s, 6H). ¹³C NMR (151 MHz, DMSO) δ 163.9, 155.7, 138.1, 137.4, 134.1, 131.5, 130.1, 128.2, 126.9, 123.7, 21.1, 14.6. HRMS calcd for C₁₆H₁₇N₂O⁺ [M+H]⁺ 253.1335, found 253.1373.

(E)-4-Nitro-N'-(1-phenylethylidene)benzohydrazide (6e)



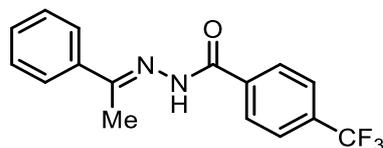
Purification by flash chromatography (DCM/EtOAc = 10:1): pale yellow solid (40.8 mg, 72%). ¹H NMR (600 MHz, DMSO) δ 11.09 (s, 1H), 8.35 (d, J = 8.6 Hz, 2H), 8.13 (d, J = 8.3 Hz, 2H), 7.87 (s, 2H), 7.45 (s, 3H), 2.39 (s, 3H). ¹³C NMR (151 MHz, DMSO) δ 162.4, 156.9, 149.1, 139.9, 137.9, 129.7, 129.4, 128.4, 126.6, 123.5, 14.9. The compound showed identical spectroscopic properties to those reported previously³.

(E)-4-Cyano-N'-(1-phenylethylidene)benzohydrazide (6f)



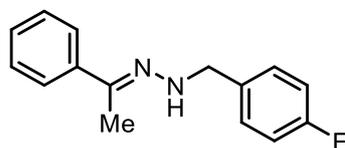
Purification by flash chromatography (DCM/EtOAc = 10:1): pale yellow solid (41.4 mg, 78%). ¹H NMR (600 MHz, DMSO) δ 11.01 (s, 1H), 8.07 – 7.99 (m, 4H), 7.87 (s, 2H), 7.45 (s, 3H), 2.38 (s, 3H). ¹³C NMR (151 MHz, DMSO) δ 162.7, 156.7, 137.9, 132.4, 129.7, 128.8, 128.4, 126.5, 118.4, 113.8, 14.8. HRMS calcd for C₁₆H₁₄N₃O⁺ [M+H]⁺ 264.1131, found 264.1146.

(E)-N'-(1-Phenylethylidene)-4-(trifluoromethyl)benzohydrazide (6g)



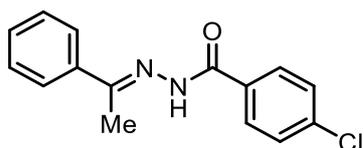
Purification by flash chromatography (DCM/EtOAc = 10:1): pale yellow solid (50.2 mg, 82%). ¹H NMR (600 MHz, DMSO) δ 10.99 (s, 1H), 8.09 (d, J = 8.2 Hz, 2H), 7.90 – 7.87 (m, 4H), 7.44 (s, 3H), 2.39 (s, 3H). ¹³C NMR (151 MHz, DMSO) δ 162.9, 156.4, 138.0, 129.7, 128.8, 128.4, 126.5, 125.3, 123.1 (q, J = 241.6 Hz), 14.8. ¹⁹F NMR (565 MHz, DMSO) δ -61.38. The compound showed identical spectroscopic properties to those reported previously⁴.

(E)-1-(4-Fluorobenzyl)-2-(1-phenylethylidene)hydrazine (6h)



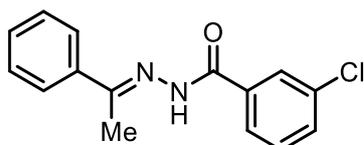
Purification by flash chromatography (DCM/EtOAc = 10:1): pale yellow solid (41.7 mg, 86%). ¹H NMR (600 MHz, DMSO) δ 10.80 (s, 1H), 7.91 (br, 4H), 7.43 (br, 3H), 7.34 (br, 2H), 2.37 (s, 3H). ¹³C NMR (151 MHz, DMSO) δ 164.9 (d, J = 256.7 Hz), 162.9, 155.7, 138.1, 130.6, 129.5, 128.4, 126.4, 115.3 (d, J = 15.1 Hz), 14.7. ¹⁹F NMR (565 MHz, DMSO) δ -108.8. The compound showed identical spectroscopic properties to those reported previously⁵.

(E)-4-Chloro-N'-(1-phenylethylidene)benzohydrazide (6i)



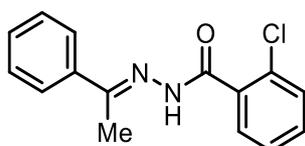
Purification by flash chromatography (DCM/EtOAc = 10:1): pale yellow solid (46.4 mg, 85%). ^1H NMR (600 MHz, DMSO) δ 10.84 (s, 1H), 7.89 (br, 4H), 7.58 (br, 2H), 7.44 (br, 3H), 2.37 (s, 3H). ^{13}C NMR (151 MHz, DMSO) δ 162.88, 155.95, 138.03, 136.31, 132.77, 129.84, 129.55, 128.38, 126.47, 14.69. The compound showed identical spectroscopic properties to those reported previously².

(E)-3-Chloro-N'-(1-phenylethylidene)benzohydrazide (6j)



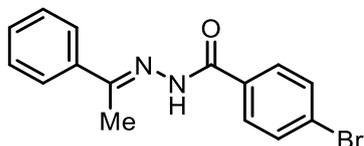
Purification by flash chromatography (DCM/EtOAc = 10:1): pale yellow solid (49.1 mg, 90%). ^1H NMR (600 MHz, DMSO) δ 10.89 (s, 1H), 7.88 (br, 4H), 7.67–7.63 (m, 1H), 7.57–7.52 (m, 1H), 7.44 (s, 3H), 2.38 (s, 3H). ^{13}C NMR (151 MHz, DMSO) δ 162.6, 156.2, 138.0, 136.1, 133.1, 131.3, 130.3, 129.6, 128.4, 127.6, 126.7, 126.5, 14.8. HRMS calcd for $\text{C}_{15}\text{H}_{14}\text{ClN}_2\text{O}^+$ $[\text{M}+\text{H}]^+$ 273.0789, found 273.0814.

(E/Z)-2-Chloro-N'-(1-phenylethylidene)benzohydrazide (6k)



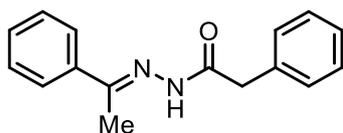
Purification by flash chromatography (DCM/EtOAc = 10:1): pale yellow solid (46.9 mg, 86%), $Z/E = 2:3$; ^1H NMR (600 MHz, DMSO) δ 11.24 (s, 1H), 11.00 (s, 1H), 7.87–7.84 (m, 1H), 7.59–7.49 (m, 2H), 7.47–7.41 (m, 4H), 7.34–7.10 (m, 2H), 2.31 (s, 1H), 2.28 (s, 1H). ^{13}C NMR (151 MHz, DMSO) δ 169.7, 163.0, 154.6, 148.5, 138.0, 138.0, 136.7, 135.7, 131.1, 130.5, 130.3, 129.7, 129.6, 129.6, 129.5, 129.0, 128.8, 128.5, 128.4, 128.2, 127.1, 126.8, 126.5, 125.8, 14.7, 13.8. HRMS calcd for $\text{C}_{15}\text{H}_{14}\text{ClN}_2\text{O}^+$ $[\text{M}+\text{H}]^+$ 273.0789, found 273.0814.

(E)-4-Bromo-N'-(1-phenylethylidene)benzohydrazide (6l)



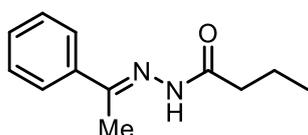
Purification by flash chromatography (DCM/EtOAc = 10:1): pale yellow solid (59.6 mg, 94%). ^1H NMR (600 MHz, DMSO) δ 10.82 (s, 1H), 7.84 (br, 3H), 7.72 (br, 3H), 7.43 (s, 3H), 2.36 (s, 3H). ^{13}C NMR (151 MHz, DMSO) δ 163.0, 156.0, 138.0, 133.1, 131.3, 130.0, 129.5, 128.3, 126.4, 14.7. The compound showed identical spectroscopic properties to those reported previously⁶.

(E/Z)-2l-Pheny N'-(1-phenylethylidene)acetohydrazide (6m)



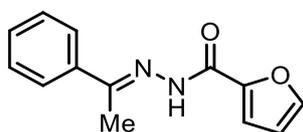
Purification by flash chromatography (DCM/EtOAc = 10:1): colorless solid (45.4 mg, 90%), *Z/E* = 2:3; ^1H NMR (600 MHz, DMSO) δ 10.58 (s, 0.6H), 10.56 (s, 0.4H), 7.81–7.76 (m, 2H), 7.43 – 7.38 (m, 3H), 7.35 – 7.28 (m, 4H), 7.25 – 7.20 (m, 1H), 4.03 (s, 1.2H), 3.68 (s, 0.8H), 2.30 (s, 1.2H), 2.25 (s, 0.8H). ^{13}C NMR (151 MHz, DMSO) δ 173.2, 167.1, 151.7, 147.3, 138.2, 136.1, 135.9, 129.4, 129.2, 129.1, 129.0, 128.4, 128.3, 128.2, 126.5, 126.3, 126.0, 14.2, 13.6. The compound showed identical spectroscopic properties to those reported previously³.

(*E/Z*)-*N'*-(1-Phenylethylidene)butyrohydrazide (6n)



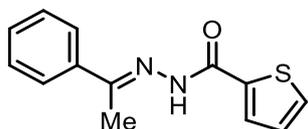
Purification by flash chromatography (DCM/EtOAc = 10:1): colorless solid (27.4 mg, 67%), *Z/E* = 2:3; ^1H NMR (600 MHz, DMSO) δ 10.40 (s, 0.6H), 10.29 (s, 0.4H), 7.78 – 7.75 (m, 2H), 7.38 (br, 3H), 2.64 (br, 1.2H), 2.30 (br, 0.8H), 2.29 (s, 1.1H), 2.23 (s, 1.9H), 1.63 (s, 2H), 0.92 (s, 3H). ^{13}C NMR (151 MHz, DMSO) δ 175.0, 169.1, 150.7, 146.6, 138.3, 129.0, 128.8, 128.3 (d, J = 15.1 Hz), 126.2, 125.9, 36.0, 34.4, 18.7, 17.7, 14.0, 13.9, 13.7, 13.4. The compound showed identical spectroscopic properties to those reported previously³.

(*E*)-*N'*-(1-Phenylethylidene)furan-2-carbohydrazide (6o)



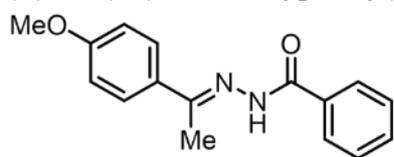
Purification by flash chromatography (DCM/EtOAc = 10:1): colorless solid (33.8 mg, 74%). ^1H NMR (600 MHz, DMSO) δ 10.59 (s, 1H), 7.94 (s, 1H), 7.82 (s, 2H), 7.44 (br, 3H), 7.37 (s, 1H), 6.70 (s, 1H), 2.35 (s, 3H). ^{13}C NMR (151 MHz, DMSO) δ 145.9, 138.1, 129.5, 128.4, 126.4, 112.0, 14.3. The compound showed identical spectroscopic properties to those reported previously³.

(*E*)-*N'*-(1-Phenylethylidene)thiophene-2-carbohydrazide (6p)



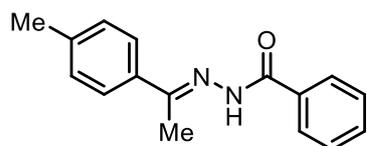
Purification by flash chromatography (DCM/EtOAc = 10:1): colorless solid (39.1 mg, 80%). ^1H NMR (600 MHz, DMSO) δ 10.92 (s, 1H), 8.04 (s, 1H), 7.95 – 7.85 (m, 3H), 7.45 (br, 3H), 7.22 – 7.20 (m, 1H), 2.36 (s, 3H). ^{13}C NMR (151 MHz, DMSO) δ 162.1, 149.7, 138.0, 135.1, 134.9, 133.1, 129.3, 128.5, 126.7, 14.2. The compound showed identical spectroscopic properties to those reported previously⁷.

(E)-N'-(1-(4-Methoxyphenyl)ethylidene)benzohydrazide (6aa)



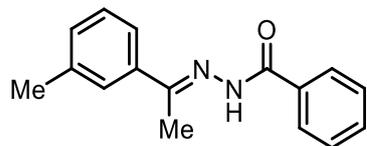
Purification by flash chromatography (DCM/EtOAc = 10:1): colorless solid (46.2 mg, 86%). ¹H NMR (600 MHz, DMSO) δ 10.70 (s, 1H), 7.85 (br, 4H), 7.59 – 7.50 (m, 3H), 7.00 (s, 2H), 3.80 (s, 3H), 2.33 (s, 3H). ¹³C NMR (151 MHz, DMSO) δ 163.7, 160.4, 155.9, 134.2, 131.4, 130.5, 128.3, 128.0, 127.8, 113.7, 55.3, 14.5. The compound showed identical spectroscopic properties to those reported previously².

(E)-N'-(1-(P-tolyl)ethylidene)benzohydrazide (6ab)



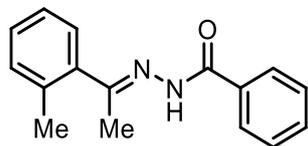
Purification by flash chromatography (DCM/EtOAc = 10:1): pale yellow solid (41.9 mg, 83%). ¹H NMR (600 MHz, DMSO) δ 10.73 (s, 1H), 7.83 (br, 4H), 7.54 (br, 3H), 7.24 (s, 2H), 2.34 (s, 6H). ¹³C NMR (151 MHz, DMSO) δ 163.8, 155.7, 139.1, 135.3, 134.1, 131.5, 129.0, 128.3, 127.8, 126.4, 20.9, 14.5. The compound showed identical spectroscopic properties to those reported previously².

(E)-N'-(1-(m-Tolyl)ethylidene)benzohydrazide (6ac)



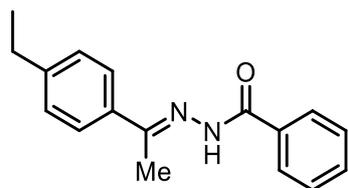
Purification by flash chromatography (DCM/EtOAc = 10:1): pale yellow solid (40.4 mg, 80%). ¹H NMR (600 MHz, DMSO) δ 10.74 (s, 1H), 7.89 (s, 2H), 7.66 (br, 2H), 7.57 (br, 1H), 7.56-7.50 (m, 2H), 7.28 (br, 2H), 2.36 (s, 6H). ¹³C NMR (151 MHz, DMSO) δ 163.9, 155.7, 138.1, 137.4, 134.1, 131.5, 130.1, 128.2, 127.8, 126.9, 123.7, 21.1, 14.6. The compound showed identical spectroscopic properties to those reported previously⁸.

(E)-N'-(1-(o-Tolyl)ethylidene)benzohydrazide (6ad)



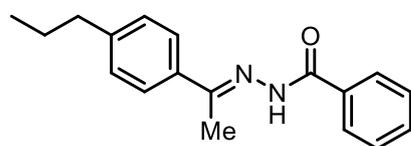
Purification by flash chromatography (DCM/EtOAc = 10:1): pale yellow solid (37.8 mg, 75%), Z/E = 1:2; ¹H NMR (600 MHz, DMSO) δ 10.99 (s, 0.3H), 10.77 (s, 0.6H), 7.85 (br, 1H), 7.48 – 7.41 (m, 3H), 7.39 (br, 1H), 7.29 (br, 4H), 2.40 (s, 2H), 2.30 (d, *J* = 15.3 Hz, 3H), 2.25 (s, 1H). ¹³C NMR (151 MHz, DMSO) δ 172.4, 165.8, 154.0, 148.0, 138.2, 138.0, 136.8, 135.9, 135.7, 134.3, 130.4, 129.7, 129.6, 129.4, 128.9, 128.8, 128.3, 128.3, 127.7, 127.1, 126.4, 125.8, 125.5, 19.4, 19.3, 14.6, 13.6. HRMS calcd for C₁₆H₁₇N₂O⁺ [M+H]⁺ 253.1335, found 253.1345.

(E)-N'-(1-(4-Ethylphenyl)ethylidene)benzohydrazide (6ae)



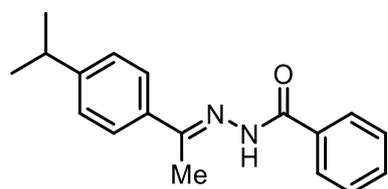
Purification by flash chromatography (DCM/EtOAc = 10:1): pale yellow solid (31.9 mg, 60%). ^1H NMR (600 MHz, DMSO) δ 10.72 (s, 1H), 7.83 (br, 4H), 7.58 – 7.50 (m, 3H), 7.27 (br, 2H), 2.64 (d, J = 7.9 Hz, 2H), 2.35 (s, 3H), 1.19 (br, 3H). ^{13}C NMR (151 MHz, DMSO) δ 163.8, 155.7, 145.4, 135.6, 134.1, 131.4, 128.3, 127.7, 126.5, 27.9, 15.4. The compound showed identical spectroscopic properties to those reported previously¹⁰.

(E)-N'-(1-(4-Propylphenyl)ethylidene)benzohydrazide (6af)



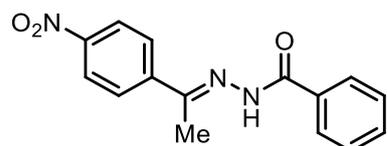
Purification by flash chromatography (DCM/EtOAc = 10:1): pale yellow solid (51.6 mg, 92%). ^1H NMR (400 MHz, DMSO) δ 10.74 (s, 1H), 7.83 (br, 4H), 7.61 – 7.45 (m, 3H), 7.25 (br, 2H), 2.58 (s, 2H), 2.35 (s, 3H), 1.60 (q, J = 7.2 Hz, 2H), 0.89 (t, J = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, DMSO) δ 163.8, 143.8, 135.6, 134.2, 131.4, 128.3, 127.8, 37.0, 23.9, 14.5, 13.6. HRMS calcd for $\text{C}_{18}\text{H}_{21}\text{N}_2\text{O}^+$ $[\text{M}+\text{H}]^+$ 281.1648, found 281.1668.

(E)-N'-(1-(4-Isopropylphenyl)ethylidene)benzohydrazide (6ag)



Purification by flash chromatography (DCM/EtOAc = 10:1): pale yellow solid (51.6 mg, 92%). ^1H NMR (600 MHz, DMSO) δ 10.71 (s, 1H), 7.83 (br, 3H), 7.59 – 7.48 (m, 3H), 7.29 (br, 2H), 2.97 – 2.86 (m, 1H), 2.34 (s, 3H), 1.22 (d, J = 7.0 Hz, 6H). ^{13}C NMR (151 MHz, DMSO) δ 163.7, 155.9, 149.9, 135.8, 134.1, 131.4, 128.4, 128.3, 127.8, 126.6, 126.5, 126.2, 33.2, 23.7, 14.6. HRMS calcd for $\text{C}_{18}\text{H}_{21}\text{N}_2\text{O}^+$ $[\text{M}+\text{H}]^+$ 281.1648, found 281.1674.

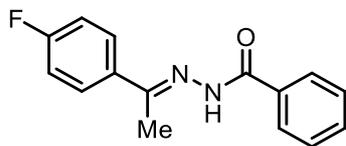
(E)-N'-(1-(4-Nitrophenyl)ethylidene)benzohydrazide (6ah)



Purification by flash chromatography (DCM/EtOAc = 10:1): pale yellow solid (37.2 mg, 80%). ^1H NMR (600 MHz, DMSO) δ 10.97 (s, 1H), 8.27 (s, 2H), 8.10 (s, 2H), 7.88 (s, 2H), 7.60 (br, 1H), 7.52 (br, 2H), 2.42 (s, 3H). ^{13}C NMR (151 MHz, DMSO) δ 147.7,

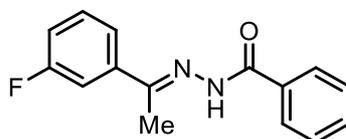
144.4, 133.9, 131.8, 129.8, 128.4, 127.6, 123.7, 14.5. The compound showed identical spectroscopic properties to those reported previously⁹.

(E)-N'-(1-(4-Fluorophenyl)ethylidene)benzohydrazide (6ai)



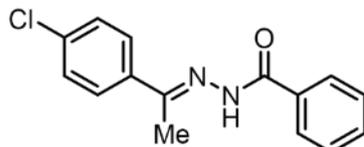
Purification by flash chromatography (DCM/EtOAc = 10:1): pale yellow solid (40.4 mg, 75%); ¹H NMR (600 MHz, DMSO) δ 10.78 (s, 1H), 7.90 (s, 4H), 7.57 (br, 1H), 7.51 (br, 2H), 7.26 (s, 2H), 2.36 (s, 3H). ¹³C NMR (151 MHz, DMSO) δ 163.9 (d, J = 271.8 Hz), 154.5, 134.6 (d, J = 3.0 Hz), 134.1, 131.5, 128.7, 128.3, 127.9, 115.3, 115.2, 14.6. ¹⁹F NMR (565 MHz, DMSO) δ -112.14. The compound showed identical spectroscopic properties to those reported previously².

(E)-N'-(1-(3-Fluorophenyl)ethylidene)benzohydrazide (6aj)



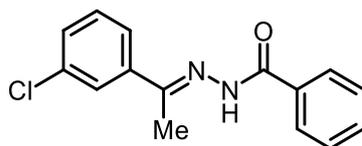
Purification by flash chromatography (DCM/EtOAc = 10:1): pale yellow solid (41.5 mg, 81%); ¹H NMR (600 MHz, DMSO) δ 10.87 (s, 1H), 8.04 – 7.54 (m, 5H), 7.50 (br, 3H), 7.26 (s, 1H), 2.39 (s, 3H). ¹³C NMR (151 MHz, DMSO) δ 164.1, 163.1, 161.5, 153.7, 140.7, 140.7, 134.0, 131.6, 130.4, 130.3, 128.3, 128.0, 122.6, 116.2, 116.1, 113.0, 112.8, 14.5. ¹⁹F NMR (565 MHz, DMSO) δ -113.12. The compound showed identical spectroscopic properties to those reported previously¹⁰.

(E)-N'-(1-(4-Chlorophenyl)ethylidene)benzohydrazide (6ak)



Purification by flash chromatography (DCM/EtOAc = 10:1): pale yellow solid (43.1 mg, 79%); ¹H NMR (600 MHz, DMSO) δ 10.81 (s, 1H), 7.88 (s, 4H), 7.58 (br, 1H), 7.51 (br, 4H), 2.36 (s, 3H). ¹³C NMR (151 MHz, DMSO) δ 164.0, 154.0, 137.0, 134.2, 131.5, 128.4, 128.2, 14.4. The compound showed identical spectroscopic properties to those reported previously¹⁰.

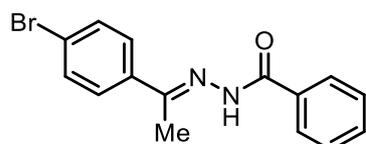
(E)-N'-(1-(3-Chlorophenyl)ethylidene)benzohydrazide (6al)



Purification by flash chromatography (DCM/EtOAc = 10:1): pale yellow solid (40.4 mg, 73%). ¹H NMR (600 MHz, DMSO) δ 10.85 (s, 1H), 7.84 (br, 4H), 7.60-7.55 (m, 1H), 7.54 – 7.45 (m, 4H), 2.37 (s, 3H). ¹³C NMR (151 MHz, DMSO) δ 164.2, 153.5, 140.3, 133.9, 133.3, 131.6, 130.3, 129.2, 128.3, 128.0, 126.0, 125.2, 14.5. The

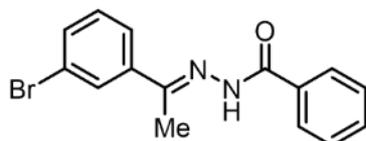
compound showed identical spectroscopic properties to those reported previously¹⁰.

(E)-N'-(1-(4-Bromophenyl)ethylidene)benzohydrazide (6am)



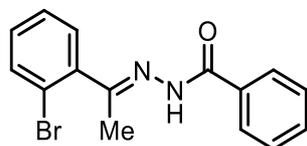
Purification by flash chromatography (DCM/EtOAc = 10:1): pale yellow solid (46.3 mg, 73%). ¹H NMR (600 MHz, DMSO) δ 10.80 (s, 1H), 7.84 (br, 4H), 7.61 (br, 3H), 7.51 (br, 2H), 2.35 (s, 3H). ¹³C NMR (151 MHz, DMSO) δ 164.0, 154.0, 137.3, 134.0, 131.3, 128.4, 127.9, 122.9, 14.3. The compound showed identical spectroscopic properties to those reported previously⁸.

(E)-N'-(1-(3-Bromophenyl)ethylidene)benzohydrazide (6an)



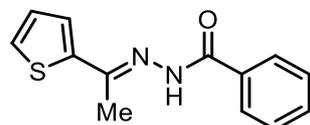
Purification by flash chromatography (DCM/EtOAc = 10:1): pale yellow solid (44.4 mg, 70%). ¹H NMR (600 MHz, DMSO) δ 10.84 (s, 1H), 8.08 – 7.76 (m, 4H), 7.63 – 7.49 (m, 4H), 7.41 (s, 1H), 2.36 (s, 3H). ¹³C NMR (151 MHz, DMSO) δ 153.4, 140.5, 132.0, 131.6, 130.6, 128.8, 128.3, 128.0, 121.9, 14.5. The compound showed identical spectroscopic properties to those reported previously¹⁰.

(E)-N'-(1-(2-Bromophenyl)ethylidene)benzohydrazide (6ao)



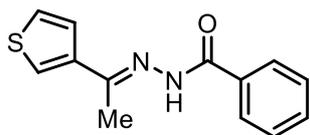
Purification by flash chromatography (DCM/EtOAc = 10:1): pale yellow solid (39.9 mg, 63%). ¹H NMR (600 MHz, DMSO) δ 10.80 (s, 1H), 7.88 (br, 2H), 7.74-7.37 (m, 1H), 7.52 – 7.33 (m, 6H), 2.35 (s, 3H). ¹³C NMR (151 MHz, DMSO) δ 164.2, 157.0, 141.2, 133.0, 132.8, 131.1, 130.4, 130.3, 129.4, 128.3, 128.0, 127.8, 120.5, 18.8. HRMS calcd for C₁₆H₁₃BrN₂O⁺ [M+H]⁺ 317.0284, found 317.0293.

(E)-N'-(1-(Thiophen-2-yl)ethylidene)benzohydrazide (6ap)



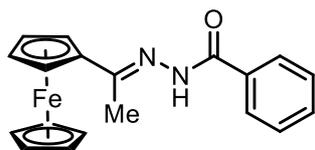
Purification by flash chromatography (DCM/EtOAc = 10:1): pale yellow solid (39.1 mg, 80%). ¹H NMR (600 MHz, DMSO) δ 10.76 (s, 1H), 7.86 (br, 2H), 7.63 (br, 2H), 7.56 (br, 3H), 7.11 (s, 1H), 2.38 (s, 3H). ¹³C NMR (151 MHz, DMSO) δ 163.5, 152.7, 143.2, 134.0, 131.5, 129.0, 128.3, 127.8, 127.6, 14.9. The compound showed identical spectroscopic properties to those reported previously².

(E)-N'-(1-(Thiophen-3-yl)ethylidene)benzohydrazide (6aq)



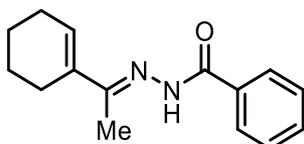
Purification by flash chromatography (DCM/EtOAc = 10:1): pale yellow solid (37.6 mg, 77%). ^1H NMR (600 MHz, DMSO) δ 10.70 (s, 1H), 7.93 (br, 3H), 7.58 (br, 2H), 7.51 (br, 3H), 2.36 (s, 3H). ^{13}C NMR (151 MHz, DMSO) δ 163.6, 152.8, 141.2, 134.1, 131.4, 128.3, 127.8, 126.7, 126.1, 125.7, 15.2. The compound showed identical spectroscopic properties to those reported previously².

(E)-N'-(1-Ferrocene)benzohydrazide (6ar)



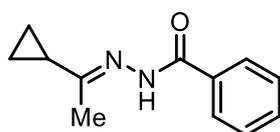
Purification by flash chromatography (DCM/EtOAc = 10:1): pale red solid (43.6 mg, 63%). ^1H NMR (600 MHz, DMSO) δ 10.59 (s, 1H), 7.88 (br, 2H), 7.61 – 7.45 (m, 3H), 4.71 (s, 2H), 4.41 (s, 2H), 4.23 (s, 5H), 2.24 (s, 3H). ^{13}C NMR (151 MHz, DMSO) δ 162.8, 134.2, 131.3, 128.3, 127.6, 82.8, 72.1, 70.0, 69.2, 67.3, 15.9. HRMS calcd for $\text{C}_{19}\text{H}_{19}\text{FeN}_2\text{O}^+$ $[\text{M}+\text{H}]^+$ 347.0841, found 347.0893.

(E)-N'-(1-(Cyclohex-1-en-1-yl)ethylidene)benzohydrazide (6as)



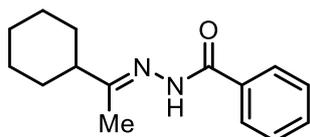
Purification by flash chromatography (DCM/EtOAc = 10:1): pale yellow solid (42.6 mg, 88%). ^1H NMR (600 MHz, DMSO) δ 10.50 (s, 1H), 7.83 (s, 2H), 7.58 – 7.40 (m, 3H), 6.37 (s, 1H), 2.43 – 2.14 (m, 4H), 2.05 (s, 3H), 1.58 (br, 4H). ^{13}C NMR (151 MHz, DMSO) δ 163.6, 158.1, 136.9, 134.3, 131.4, 128.4, 127.8, 25.7, 24.4, 22.2, 21.8, 12.8. The compound showed identical spectroscopic properties to those reported previously¹¹.

(E)-N'-(1-Cyclopropylethylidene)benzohydrazide (6at)

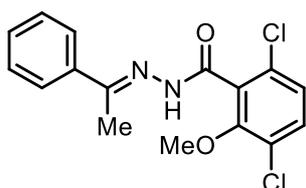


Purification by flash chromatography (DCM/EtOAc = 10:1): pale yellow solid (33.2 mg, 82%). ^1H NMR (600 MHz, DMSO) δ 10.38 (s, 1H), 7.81 (br, 2H), 7.53 (br, 1H), 7.46 (br, 2H), 1.76 (s, 3H), 0.78 (br, 4H). ^{13}C NMR (151 MHz, DMSO) δ 164.2, 162.9, 134.2, 128.3, 127.5, 14.1, 5.8. The compound showed identical spectroscopic properties to those reported previously¹⁴.

(E)-N'-(1-Cyclohexylethylidene)benzohydrazide (6au)

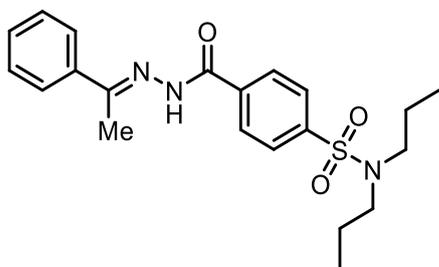


Purification by flash chromatography (DCM/EtOAc = 10:1): pale yellow solid (39.6 mg, 81%). $^1\text{H NMR}$ (600 MHz, DMSO) δ 10.36 (s, 1H), 7.82 (s, 2H), 7.54 (s, 1H), 7.47 (s, 2H), 2.24 (s, 1H), 1.91 (s, 3H), 1.75 (br, 4H), 1.40 – 1.12 (m, 6H). $^{13}\text{C NMR}$ (151 MHz, DMSO) δ 165.9, 163.2, 134.3, 134.1, 131.2, 128.3, 127.6, 46.6, 29.7, 25.6, 14.9. The compound showed identical spectroscopic properties to those reported previously².
(Z/E)-3,6-Dichloro-2-methoxy-N'-(1-phenylethylidene)benzohydrazide (6av)



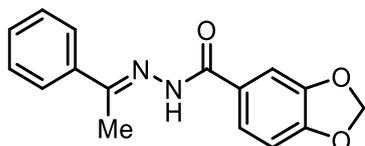
Purification by flash chromatography (DCM/EtOAc = 10:1): colorless solid (60.6 mg, 90%), $Z/E = 1:2$; $^1\text{H NMR}$ (600 MHz, DMSO) δ 11.40 (s, 0.6H), 11.10 (s, 0.4H), 7.93 (br, 0.25H), 7.85 (br, 0.65H), 7.61 (br, 0.4H), 7.58 (br, 0.6H), 7.46 – 7.42 (m, 1H), 7.41 – 7.38 (m, 1H), 7.34 (br, 1H), 7.31 – 7.26 (m, 2H), 3.86 (s, 1H), 3.78 (s, 2H), 2.29 (s, 2.7H), 2.27 (s, 0.3H). $^{13}\text{C NMR}$ (151 MHz, DMSO) δ 166.6, 159.8, 154.6, 153.7, 152.3, 149.1, 137.8, 137.7, 133.4, 132.6, 131.4, 130.8, 129.8, 129.6, 129.1, 128.6, 128.3, 128.3, 126.5, 126.0, 125.8, 125.7, 125.6, 125.4, 62.1, 61.4, 14.6, 13.8. HRMS calcd for $\text{C}_{16}\text{H}_{15}\text{Cl}_2\text{N}_2\text{O}_2^+$ $[\text{M}+\text{H}]^+$ 337.0505, found 337.0498.

(E)-4-(2-(1-Phenylethylidene)hydrazine-1-carbonyl)-N,N-dipropylbenzenesulfonamide (6aw)



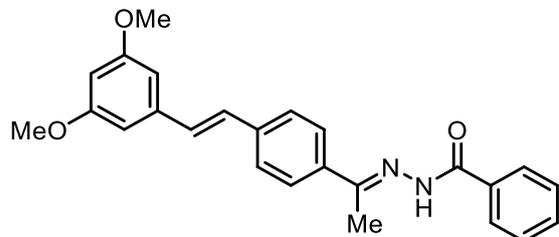
Purification by flash chromatography (DCM/EtOAc = 10:1): colorless solid (72.3 mg, 90%). $^1\text{H NMR}$ (600 MHz, DMSO) δ 10.99 (s, 1H), 8.07 (br, 2H), 7.96 – 7.79 (m, 4H), 7.44 (s, 3H), 3.07 (t, $J = 7.6$ Hz, 4H), 2.38 (s, 3H), 1.49 (q, $J = 7.5$ Hz, 4H), 0.82 (t, $J = 7.4$ Hz, 6H). $^{13}\text{C NMR}$ (151 MHz, DMSO) δ 162.9, 156.4, 141.9, 137.9, 137.7, 129.7, 128.9, 128.4, 126.8, 126.5, 49.8, 21.7, 14.8, 11.0. HRMS calcd for $\text{C}_{21}\text{H}_{28}\text{N}_3\text{O}_3\text{S}^+$ $[\text{M}+\text{H}]^+$ 402.1846, found 402.1834.

(E)-N'-(1-Phenylethylidene)benzo[d][1,3]dioxole-5-carbohydrazide (6ax)



Purification by flash chromatography (DCM/EtOAc = 10:1): colorless solid (50.8 mg, 91%). ¹H NMR (600 MHz, DMSO) δ 10.59 (s, 1H), 7.83 (s, 2H), 7.43 (br, 1H), 7.42 (br, 4H), 7.04 (br, 1H), 6.12 (s, 2H), 2.35 (s, 3H). ¹³C NMR (151 MHz, DMSO) δ 147.2, 138.2, 129.4, 129.4, 128.4, 127.8, 126.4, 107.9, 101.7, 14.5. HRMS calcd for C₁₆H₁₅N₂O₃⁺ [M+H]⁺ 283.1077, found 283.1048.

***N'*-((*E*)-1-(4-((*E*)-3,5-Dimethoxystyryl)phenyl)ethylidene)benzohydrazide (6ay)**



Purification by flash chromatography (DCM/EtOAc = 10:1): colorless solid (50.8 mg, 91%). ¹H NMR (600 MHz, DMSO) δ 10.78 (s, 1H), 7.89 (s, 3H), 7.70 – 7.48 (m, 6H), 7.35-7.26 (m, 2H), 6.82 (s, 2H), 6.43 (s, 1H), 3.79 (s, 6H), 2.38 (s, 3H). ¹³C NMR (151 MHz, DMSO) δ 160.7, 139.0, 137.2, 129.4, 128.3, 127.9, 126.8, 126.5, 104.6, 100.2, 55.2, 14.4. HRMS calcd for C₂₅H₂₅N₂O₃⁺ [M+H]⁺ 401.1860, found 401.1842.

3. Crystallographic Studies

Crystal structure of 2a.

Single crystal of complex **2a** were grown by slow evaporation in a mixture of DCM and n-hexane (DCM: n-hexane = 1:3) at low temperature.

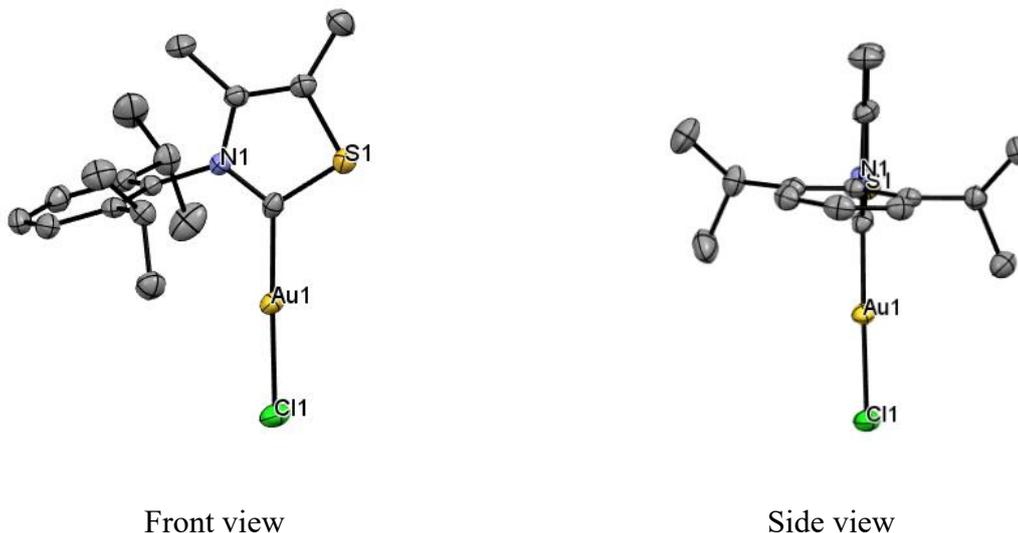


Chart S1. Crystal structure of **3a** (50% ellipsoids). Two views: front (left); side (right). Hydrogen atoms have been omitted for clarity. (Crystallographic data has been deposited with the Cambridge Crystallographic Data Center as supplementary publication no. 2503055).

Table S3. Crystal Data and Structure Refinement Summary for **2a**.

Crystal data

$C_{17}H_{23}AuClNS$	$F(000) = 976$
$M_r = 505.84$	$D_x = 1.860 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$a = 8.7118 (2) \text{ \AA}$	Cell parameters from 9907 reflections
$b = 12.4990 (4) \text{ \AA}$	$\theta = 2.4\text{--}27.5^\circ$
$c = 16.8567 (5) \text{ \AA}$	$\mu = 8.40 \text{ mm}^{-1}$
$\beta = 100.279 (1)^\circ$	$T = 170 \text{ K}$
$V = 1806.05 (9) \text{ \AA}^3$	Block, colourless
$Z = 4$	$0.2 \times 0.06 \times 0.05 \text{ mm}$

Data collection

Bruker D8 Venture diffractometer	3715 reflections with $I > 2\sigma(I)$
ω and ϕ scans	$R_{\text{int}} = 0.036$
Absorption correction: multi-scan <i>SADABS2016/2</i> (Bruker,2016/2) was used for absorption correction. $wR2(\text{int})$ was 0.0992 before and 0.0515 after correction. The Ratio of minimum to maximum transmission is 0.5841. The $\lambda/2$ correction factor is Not present.	$\theta_{\text{max}} = 27.5^\circ$, $\theta_{\text{min}} = 2.0^\circ$
$T_{\text{min}} = 0.436$, $T_{\text{max}} = 0.746$	$h = -11 \rightarrow 11$
21019 measured reflections	$k = -16 \rightarrow 14$
4134 independent reflections	$l = -21 \rightarrow 21$

Refinement

Refinement on F^2	Primary atom site location: dual
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.022$	H-atom parameters constrained
$wR(F^2) = 0.040$	$w = 1/[\sigma^2(F_o^2) + (0.0066P)^2 + 2.4051P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.10$	$(\Delta/\sigma)_{\text{max}} = 0.001$
4134 reflections	$\Delta_{\text{max}} = 0.66 \text{ e } \text{\AA}^{-3}$
196 parameters	$\Delta_{\text{min}} = -0.83 \text{ e } \text{\AA}^{-3}$
0 restraints	

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2) for (mo_231008_230925156118_gb_0m)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Au1	0.39652 (2)	0.23232 (2)	0.31812 (2)	0.02399 (4)
Cl1	0.24864 (9)	0.25722 (7)	0.19360 (5)	0.03277 (18)
S1	0.44453 (9)	0.14863 (7)	0.50202 (5)	0.02985 (18)
N1	0.6632 (3)	0.24477 (19)	0.45797 (15)	0.0213 (5)
C1	0.5176 (3)	0.2110 (2)	0.42784 (19)	0.0240 (7)

C2	0.6112 (4)	0.1677 (3)	0.57375 (19)	0.0283 (7)
C3	0.7172 (3)	0.2213 (3)	0.53997 (18)	0.0241 (6)
C4	0.6235 (4)	0.1260 (3)	0.6574 (2)	0.0406 (9)
H4A	0.527795	0.143176	0.677746	0.061*
H4B	0.712942	0.159227	0.692176	0.061*
H4C	0.637728	0.048259	0.657312	0.061*
C5	0.8771 (4)	0.2585 (3)	0.5801 (2)	0.0379 (9)
H5A	0.955880	0.228094	0.551769	0.057*
H5B	0.897342	0.234710	0.636387	0.057*
H5C	0.881796	0.336747	0.578152	0.057*
C6	0.7635 (3)	0.2956 (2)	0.40834 (18)	0.0221 (6)
C7	0.8631 (3)	0.2293 (3)	0.37398 (18)	0.0251 (6)
C8	0.9624 (4)	0.2792 (3)	0.3292 (2)	0.0309 (7)
H8	1.032380	0.236978	0.305200	0.037*
C9	0.9614 (4)	0.3884 (3)	0.3191 (2)	0.0327 (8)
H9	1.030477	0.420578	0.288483	0.039*
C10	0.8602 (4)	0.4516 (3)	0.3533 (2)	0.0297 (7)
H10	0.859370	0.526769	0.344891	0.036*
C11	0.7594 (3)	0.4069 (3)	0.39999 (18)	0.0241 (6)
C12	0.8606 (4)	0.1080 (3)	0.3799 (2)	0.0336 (8)
H12	0.804314	0.088469	0.424563	0.040*
C13	0.7682 (5)	0.0630 (3)	0.3015 (3)	0.0505 (11)
H13A	0.661971	0.092004	0.292590	0.076*
H13B	0.763916	-0.015176	0.305105	0.076*
H13C	0.819279	0.083223	0.256386	0.076*
C14	1.0237 (4)	0.0590 (3)	0.3988 (3)	0.0502 (11)
H14A	1.080135	0.075156	0.354844	0.075*
H14B	1.015099	-0.018682	0.404326	0.075*
H14C	1.080469	0.089176	0.449241	0.075*
C15	0.6509 (4)	0.4775 (3)	0.4374 (2)	0.0273 (7)
H15	0.598682	0.432190	0.473603	0.033*

C16	0.7425 (4)	0.5660 (3)	0.4888 (2)	0.0388 (9)
H16A	0.827249	0.533767	0.527442	0.058*
H16B	0.672333	0.604919	0.518028	0.058*
H16C	0.786164	0.615609	0.453696	0.058*
C17	0.5247 (4)	0.5243 (3)	0.3720 (2)	0.0354 (8)
H17A	0.456368	0.571048	0.396823	0.053*
H17B	0.462966	0.466003	0.343255	0.053*
H17C	0.573644	0.565674	0.333877	0.053*

Atomic displacement parameters (\AA^2) for (mo_231008_230925156118_gb_0m)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Au1	0.01802 (6)	0.02745 (7)	0.02526 (7)	-0.00044 (5)	0.00047 (4)	-0.00214 (5)
Cl1	0.0272 (4)	0.0414 (5)	0.0269 (4)	0.0038 (3)	-0.0029 (3)	-0.0035 (4)
S1	0.0227 (4)	0.0336 (5)	0.0329 (5)	-0.0034 (3)	0.0040 (3)	0.0050 (4)
N1	0.0174 (12)	0.0227 (14)	0.0231 (13)	-0.0007 (10)	0.0019 (10)	-0.0006 (10)
C1	0.0174 (14)	0.0234 (16)	0.0311 (17)	0.0006 (12)	0.0045 (12)	-0.0001 (13)
C2	0.0252 (16)	0.0304 (18)	0.0283 (17)	0.0027 (13)	0.0020 (13)	0.0031 (14)
C3	0.0206 (15)	0.0285 (17)	0.0224 (15)	0.0035 (13)	0.0015 (12)	0.0014 (13)
C4	0.038 (2)	0.054 (2)	0.032 (2)	0.0037 (17)	0.0104 (16)	0.0131 (18)
C5	0.0318 (18)	0.051 (2)	0.0274 (18)	-0.0053 (17)	-0.0042 (15)	0.0030 (17)
C6	0.0191 (14)	0.0266 (16)	0.0198 (15)	-0.0015 (12)	0.0015 (12)	-0.0005 (12)
C7	0.0195 (14)	0.0297 (16)	0.0250 (15)	-0.0019 (13)	0.0009 (12)	-0.0007 (14)
C8	0.0231 (16)	0.041 (2)	0.0294 (17)	0.0009 (14)	0.0071 (13)	-0.0035 (15)
C9	0.0277 (17)	0.044 (2)	0.0272 (18)	-0.0085 (15)	0.0071 (14)	0.0031 (15)
C10	0.0299 (18)	0.0296 (18)	0.0283 (18)	-0.0052 (14)	0.0019 (14)	0.0027 (14)
C11	0.0232 (15)	0.0289 (17)	0.0188 (15)	-0.0015 (13)	-0.0001 (12)	-0.0004 (13)
C12	0.0305 (18)	0.0291 (18)	0.044 (2)	0.0050 (14)	0.0134 (16)	0.0004 (16)
C13	0.044 (2)	0.038 (2)	0.067 (3)	0.0008 (18)	0.003 (2)	-0.021 (2)
C14	0.039 (2)	0.044 (2)	0.068 (3)	0.0156 (18)	0.011 (2)	0.010 (2)
C15	0.0305 (17)	0.0244 (16)	0.0276 (17)	0.0015 (13)	0.0065 (14)	0.0001 (13)
C16	0.043 (2)	0.034 (2)	0.038 (2)	0.0046 (16)	0.0039 (17)	-0.0088 (16)

C17	0.0311 (19)	0.033 (2)	0.041 (2)	0.0030 (15)	0.0030 (16)	0.0030 (16)
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Geometric parameters (Å, °) for (mo_231008_230925156118_gb_0m)

Au1—C11	2.2796 (8)	C9—C10	1.384 (5)
Au1—C1	1.977 (3)	C10—H10	0.9500
S1—C1	1.692 (3)	C10—C11	1.396 (4)
S1—C2	1.732 (3)	C11—C15	1.511 (4)
N1—C1	1.347 (4)	C12—H12	1.0000
N1—C3	1.409 (4)	C12—C13	1.527 (5)
N1—C6	1.459 (4)	C12—C14	1.528 (5)
C2—C3	1.347 (4)	C13—H13A	0.9800
C2—C4	1.489 (4)	C13—H13B	0.9800
C3—C5	1.508 (4)	C13—H13C	0.9800
C4—H4A	0.9800	C14—H14A	0.9800
C4—H4B	0.9800	C14—H14B	0.9800
C4—H4C	0.9800	C14—H14C	0.9800
C5—H5A	0.9800	C15—H15	1.0000
C5—H5B	0.9800	C15—C16	1.537 (5)
C5—H5C	0.9800	C15—C17	1.527 (4)
C6—C7	1.398 (4)	C16—H16A	0.9800
C6—C11	1.398 (4)	C16—H16B	0.9800
C7—C8	1.393 (4)	C16—H16C	0.9800
C7—C12	1.519 (5)	C17—H17A	0.9800
C8—H8	0.9500	C17—H17B	0.9800
C8—C9	1.375 (5)	C17—H17C	0.9800
C9—H9	0.9500		
C1—Au1—C11	177.87 (9)	C11—C10—H10	119.4
C1—S1—C2	94.19 (15)	C6—C11—C15	123.1 (3)
C1—N1—C3	115.6 (3)	C10—C11—C6	116.6 (3)
C1—N1—C6	122.7 (3)	C10—C11—C15	120.3 (3)

C3—N1—C6	121.6 (2)	C7—C12—H12	107.9
S1—C1—Au1	123.04 (16)	C7—C12—C13	108.8 (3)
N1—C1—Au1	128.3 (2)	C7—C12—C14	113.0 (3)
N1—C1—S1	108.6 (2)	C13—C12—H12	107.9
C3—C2—S1	109.0 (2)	C13—C12—C14	111.1 (3)
C3—C2—C4	129.5 (3)	C14—C12—H12	107.9
C4—C2—S1	121.5 (3)	C12—C13—H13A	109.5
N1—C3—C5	119.7 (3)	C12—C13—H13B	109.5
C2—C3—N1	112.6 (3)	C12—C13—H13C	109.5
C2—C3—C5	127.7 (3)	H13A—C13—H13B	109.5
C2—C4—H4A	109.5	H13A—C13—H13C	109.5
C2—C4—H4B	109.5	H13B—C13—H13C	109.5
C2—C4—H4C	109.5	C12—C14—H14A	109.5
H4A—C4—H4B	109.5	C12—C14—H14B	109.5
H4A—C4—H4C	109.5	C12—C14—H14C	109.5
H4B—C4—H4C	109.5	H14A—C14—H14B	109.5
C3—C5—H5A	109.5	H14A—C14—H14C	109.5
C3—C5—H5B	109.5	H14B—C14—H14C	109.5
C3—C5—H5C	109.5	C11—C15—H15	108.1
H5A—C5—H5B	109.5	C11—C15—C16	110.8 (3)
H5A—C5—H5C	109.5	C11—C15—C17	110.2 (3)
H5B—C5—H5C	109.5	C16—C15—H15	108.1
C7—C6—N1	117.3 (3)	C17—C15—H15	108.1
C7—C6—C11	123.7 (3)	C17—C15—C16	111.5 (3)
C11—C6—N1	119.0 (3)	C15—C16—H16A	109.5
C6—C7—C12	123.2 (3)	C15—C16—H16B	109.5
C8—C7—C6	116.7 (3)	C15—C16—H16C	109.5
C8—C7—C12	120.0 (3)	H16A—C16—H16B	109.5
C7—C8—H8	119.3	H16A—C16—H16C	109.5
C9—C8—C7	121.4 (3)	H16B—C16—H16C	109.5
C9—C8—H8	119.3	C15—C17—H17A	109.5

C8—C9—H9	119.8	C15—C17—H17B	109.5
C8—C9—C10	120.4 (3)	C15—C17—H17C	109.5
C10—C9—H9	119.8	H17A—C17—H17B	109.5
C9—C10—H10	119.4	H17A—C17—H17C	109.5
C9—C10—C11	121.2 (3)	H17B—C17—H17C	109.5
S1—C2—C3—N1	-0.5 (3)	C6—N1—C1—S1	175.8 (2)
S1—C2—C3—C5	178.0 (3)	C6—N1—C3—C2	-175.5 (3)
N1—C6—C7—C8	-177.7 (3)	C6—N1—C3—C5	5.9 (4)
N1—C6—C7—C12	5.6 (4)	C6—C7—C8—C9	-0.4 (5)
N1—C6—C11—C10	178.6 (3)	C6—C7—C12—C13	99.4 (4)
N1—C6—C11—C15	-2.5 (4)	C6—C7—C12—C14	-136.7 (3)
C1—S1—C2—C3	0.4 (3)	C6—C11—C15—C16	126.3 (3)
C1—S1—C2—C4	-178.5 (3)	C6—C11—C15—C17	-109.8 (3)
C1—N1—C3—C2	0.4 (4)	C7—C6—C11—C10	1.0 (5)
C1—N1—C3—C5	-178.2 (3)	C7—C6—C11—C15	179.9 (3)
C1—N1—C6—C7	-91.7 (3)	C7—C8—C9—C10	-0.2 (5)
C1—N1—C6—C11	90.5 (4)	C8—C7—C12—C13	-77.2 (4)
C2—S1—C1—Au1	-177.9 (2)	C8—C7—C12—C14	46.7 (4)
C2—S1—C1—N1	-0.2 (2)	C8—C9—C10—C11	1.3 (5)
C3—N1—C1—Au1	177.5 (2)	C9—C10—C11—C6	-1.6 (5)
C3—N1—C1—S1	0.0 (3)	C9—C10—C11—C15	179.5 (3)
C3—N1—C6—C7	83.9 (4)	C10—C11—C15— C16	-54.9 (4)
C3—N1—C6—C11	-93.9 (3)	C10—C11—C15— C17	69.0 (4)
C4—C2—C3—N1	178.3 (3)	C11—C6—C7—C8	0.0 (5)
C4—C2—C3—C5	-3.2 (6)	C11—C6—C7—C12	-176.8 (3)
C6—N1—C1—Au1	-6.7 (4)	C12—C7—C8—C9	176.4 (3)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated

using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Crystal structure of **3a**.

Single crystal of complex **3a** were grown by slow evaporation in a mixture of DCM and n-hexane (DCM: n-hexane = 1:3) at low temperature.

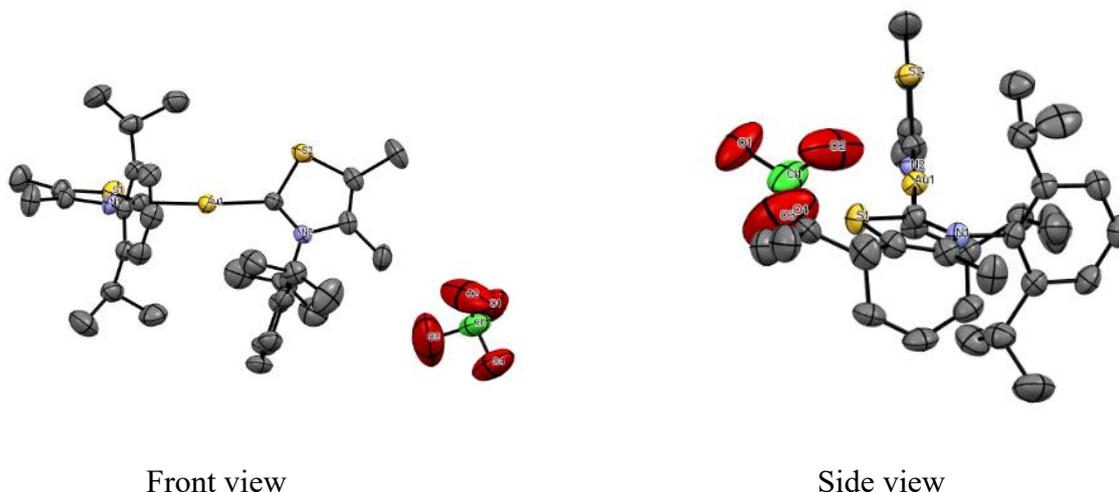


Chart S2. Crystal structure of **3a** (50% ellipsoids). Two views: front (left); side (right). Hydrogen atoms have been omitted for clarity. (Crystallographic data has been deposited with the Cambridge Crystallographic Data Center as supplementary publication no. 2503058).

Table S4. Crystal Data and Structure Refinement Summary for **3a**.

Crystal data

$C_{34}H_{46}AuN_2S_2 \cdot ClO_4$	$F(000) = 1696$
$M_r = 843.26$	$D_x = 1.534 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$a = 9.3961 (3) \text{ \AA}$	Cell parameters from 9602 reflections
$b = 19.0591 (5) \text{ \AA}$	$\theta = 2.4\text{--}27.3^\circ$
$c = 20.4987 (5) \text{ \AA}$	$\mu = 4.25 \text{ mm}^{-1}$
$\beta = 95.856 (1)^\circ$	$T = 273 \text{ K}$
$V = 3651.77 (18) \text{ \AA}^3$	Block, colourless
$Z = 4$	

Data collection

Bruker APEX-II CCD diffractometer	7574 reflections with $I > 2\sigma(I)$
ϕ and ω scans	$R_{\text{int}} = 0.036$
Absorption correction: multi-scan <i>SADABS2016/2</i> (Bruker,2016/2) was used for absorption correction. $wR2(\text{int})$ was 0.0824 before and 0.0478 after correction. The Ratio of minimum to maximum transmission is 0.8260. The $\lambda/2$ correction factor is Not present.	$\theta_{\text{max}} = 27.5^\circ$, $\theta_{\text{min}} = 2.2^\circ$
$T_{\text{min}} = 0.616$, $T_{\text{max}} = 0.746$	$h = -12 \rightarrow 12$
111808 measured reflections	$k = -24 \rightarrow 24$
8408 independent reflections	$l = -26 \rightarrow 26$

Refinement

Refinement on F^2	Primary atom site location: dual
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.026$	H-atom parameters constrained
$wR(F^2) = 0.064$	$w = 1/[\sigma^2(F_o^2) + (0.0257P)^2 + 4.5427P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.10$	$(\Delta/\sigma)_{\text{max}} = 0.005$
8408 reflections	$\Delta_{\text{max}} = 1.06 \text{ e } \text{\AA}^{-3}$
409 parameters	$\Delta_{\text{min}} = -0.98 \text{ e } \text{\AA}^{-3}$
0 restraints	

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2) for (sust_3488_0m)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Au1	0.38412 (2)	0.78295 (2)	0.52069 (2)	0.03561 (4)
S1	0.72252 (9)	0.82230 (5)	0.51708 (4)	0.04582 (19)
S2	0.13966 (10)	0.81886 (4)	0.61763 (4)	0.04567 (19)
N1	0.5632 (2)	0.83127 (13)	0.41422 (12)	0.0350 (5)

N2	0.1449 (3)	0.69899 (13)	0.57246 (12)	0.0339 (5)
C1	0.3921 (4)	0.95783 (18)	0.40949 (19)	0.0502 (8)
H1	0.483079	0.947614	0.435512	0.060*
C2	0.3687 (6)	0.5433 (3)	0.6758 (2)	0.0829 (14)
H2A	0.271857	0.527549	0.676408	0.124*
H2B	0.407996	0.554843	0.719532	0.124*
H2C	0.424727	0.506743	0.658748	0.124*
C3	-0.0526 (4)	0.6321 (2)	0.6174 (2)	0.0613 (10)
H3A	-0.102287	0.620609	0.575502	0.092*
H3B	-0.120639	0.638780	0.648760	0.092*
H3C	0.011206	0.594541	0.631633	0.092*
C4	0.2612 (5)	0.52524 (19)	0.4659 (2)	0.0604 (10)
H4	0.289570	0.487524	0.441492	0.072*
C5	0.2145 (3)	0.75950 (16)	0.56950 (14)	0.0345 (6)
C6	0.0308 (3)	0.69773 (18)	0.61168 (15)	0.0405 (7)
C7	0.5222 (6)	0.6842 (3)	0.2612 (3)	0.0885 (16)
H7A	0.591784	0.647126	0.265075	0.133*
H7B	0.555500	0.721542	0.235312	0.133*
H7C	0.433208	0.666473	0.240436	0.133*
C8	0.1510 (4)	0.56717 (19)	0.44042 (18)	0.0541 (9)
H8	0.103359	0.556639	0.399592	0.065*
C9	0.3307 (4)	0.53813 (19)	0.52717 (19)	0.0547 (9)
H9	0.403626	0.508231	0.543956	0.066*
C10	0.2813 (4)	0.9727 (2)	0.4570 (2)	0.0644 (11)
H10A	0.191652	0.984433	0.432692	0.097*
H10B	0.312989	1.011173	0.484944	0.097*
H10C	0.269366	0.931751	0.483163	0.097*
C11	-0.0097 (4)	0.6723 (2)	0.44503 (17)	0.0501 (8)
H11	-0.031602	0.705928	0.478730	0.060*
C12	0.5573 (3)	0.81143 (16)	0.47656 (14)	0.0355 (6)
C13	-0.1460 (5)	0.6319 (3)	0.4235 (3)	0.0956 (18)

H13A	-0.219491	0.664058	0.406835	0.143*
H13B	-0.176623	0.606930	0.460272	0.143*
H13C	-0.127965	0.599085	0.389725	0.143*
C14	0.3517 (3)	0.89391 (16)	0.36711 (15)	0.0394 (7)
C15	0.0386 (5)	0.7135 (2)	0.3880 (2)	0.0691 (12)
H15A	0.061625	0.681626	0.354336	0.104*
H15B	0.121657	0.740680	0.402801	0.104*
H15C	-0.036901	0.744260	0.370680	0.104*
C16	0.4348 (3)	0.83383 (16)	0.36803 (14)	0.0353 (6)
C17	0.5001 (4)	0.71174 (18)	0.3293 (2)	0.0518 (9)
H17	0.593935	0.725454	0.350773	0.062*
C18	0.1846 (3)	0.63776 (15)	0.53608 (15)	0.0357 (6)
C19	0.1914 (4)	0.8376 (2)	0.28445 (16)	0.0489 (8)
H19	0.107029	0.838494	0.256464	0.059*
C20	0.6962 (3)	0.85570 (17)	0.39761 (16)	0.0418 (7)
C21	0.7126 (4)	0.8775 (3)	0.32912 (19)	0.0648 (11)
H21A	0.682072	0.840006	0.299659	0.097*
H21B	0.811166	0.888176	0.325130	0.097*
H21C	0.655104	0.918300	0.318356	0.097*
C22	0.1095 (3)	0.62512 (18)	0.47469 (15)	0.0426 (7)
C23	0.4422 (5)	0.6540 (2)	0.3704 (2)	0.0692 (11)
H23A	0.425198	0.672500	0.412460	0.104*
H23B	0.510649	0.616557	0.376144	0.104*
H23C	0.354143	0.636471	0.348501	0.104*
C24	0.2268 (4)	0.89423 (19)	0.32410 (17)	0.0483 (8)
H24	0.166875	0.933190	0.322280	0.058*
C25	-0.0971 (4)	0.7798 (2)	0.6854 (2)	0.0660 (12)
H25A	-0.051803	0.783874	0.729336	0.099*
H25B	-0.169694	0.744245	0.683806	0.099*
H25C	-0.139861	0.823896	0.671816	0.099*
C26	0.7960 (3)	0.85562 (18)	0.44938 (17)	0.0435 (7)

C27	0.2939 (3)	0.59482 (17)	0.56424 (16)	0.0424 (7)
C28	0.0129 (3)	0.76009 (19)	0.64000 (15)	0.0427 (7)
C29	0.4144 (6)	1.0223 (2)	0.3675 (3)	0.0875 (16)
H29A	0.326981	1.033075	0.340963	0.131*
H29B	0.488405	1.012857	0.339716	0.131*
H29C	0.441763	1.061456	0.395454	0.131*
C30	0.4042 (3)	0.77596 (16)	0.32730 (16)	0.0399 (7)
C31	0.3714 (4)	0.6080 (2)	0.63234 (17)	0.0514 (8)
H31	0.319696	0.645370	0.652811	0.062*
C32	0.2782 (4)	0.77936 (19)	0.28524 (17)	0.0486 (8)
H32	0.252510	0.741908	0.257410	0.058*
C33	0.5248 (5)	0.6339 (3)	0.6280 (2)	0.0801 (14)
H33A	0.582012	0.596113	0.614083	0.120*
H33B	0.564573	0.650186	0.670345	0.120*
H33C	0.523768	0.671686	0.597002	0.120*
C34	0.9460 (4)	0.8822 (2)	0.4536 (2)	0.0623 (10)
H34A	0.962282	0.913839	0.490090	0.093*
H34B	0.960945	0.906493	0.413858	0.093*
H34C	1.011274	0.843476	0.459675	0.093*
Cl1	-0.08209 (17)	0.46484 (6)	0.75911 (6)	0.0844 (4)
O1	-0.0445 (6)	0.4747 (2)	0.82538 (19)	0.1264 (17)
O2	-0.1386 (11)	0.5211 (3)	0.7286 (3)	0.237 (4)
O3	0.0517 (8)	0.4598 (5)	0.7261 (4)	0.239 (4)
O4	-0.1350 (6)	0.4003 (2)	0.7447 (2)	0.1315 (18)

Atomic displacement parameters (\AA^2) for (sust_3488_0m)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Au1	0.03804 (7)	0.03514 (7)	0.03407 (6)	-0.00465 (5)	0.00567 (4)	-0.00084 (5)
S1	0.0379 (4)	0.0544 (5)	0.0432 (4)	-0.0041 (4)	-0.0060 (3)	0.0015 (4)
S2	0.0571 (5)	0.0403 (4)	0.0410 (4)	0.0059 (4)	0.0116 (4)	-0.0066 (3)
N1	0.0286 (12)	0.0379 (13)	0.0382 (13)	-0.0063 (10)	0.0020 (10)	0.0023 (10)

N2	0.0323 (12)	0.0345 (13)	0.0358 (12)	0.0020 (10)	0.0076 (10)	-0.0008 (10)
C1	0.0412 (18)	0.0414 (18)	0.066 (2)	-0.0044 (14)	-0.0033 (16)	-0.0098 (16)
C2	0.104 (4)	0.080 (3)	0.065 (3)	0.015 (3)	0.008 (3)	0.015 (2)
C3	0.054 (2)	0.071 (3)	0.061 (2)	-0.0195 (19)	0.0202 (18)	-0.001 (2)
C4	0.078 (3)	0.0396 (19)	0.065 (2)	0.0013 (18)	0.015 (2)	-0.0169 (17)
C5	0.0378 (15)	0.0325 (14)	0.0334 (14)	0.0002 (12)	0.0049 (12)	-0.0032 (12)
C6	0.0341 (15)	0.0525 (19)	0.0355 (15)	0.0008 (13)	0.0064 (12)	0.0043 (13)
C7	0.095 (4)	0.087 (4)	0.088 (4)	0.018 (3)	0.030 (3)	-0.021 (3)
C8	0.066 (2)	0.048 (2)	0.0488 (19)	-0.0082 (18)	0.0049 (17)	-0.0106 (16)
C9	0.059 (2)	0.0400 (19)	0.066 (2)	0.0117 (16)	0.0135 (18)	-0.0051 (17)
C10	0.064 (2)	0.056 (2)	0.073 (3)	-0.0050 (19)	0.006 (2)	-0.017 (2)
C11	0.0480 (19)	0.057 (2)	0.0442 (18)	0.0009 (16)	0.0007 (15)	-0.0001 (16)
C12	0.0342 (15)	0.0339 (15)	0.0378 (15)	-0.0029 (12)	0.0004 (12)	-0.0008 (12)
C13	0.058 (3)	0.109 (4)	0.112 (4)	-0.018 (3)	-0.028 (3)	0.023 (3)
C14	0.0378 (16)	0.0360 (16)	0.0439 (16)	-0.0059 (13)	0.0020 (13)	0.0006 (13)
C15	0.088 (3)	0.064 (3)	0.056 (2)	0.016 (2)	0.012 (2)	0.0096 (19)
C16	0.0290 (14)	0.0439 (17)	0.0326 (14)	-0.0075 (12)	0.0008 (11)	0.0019 (12)
C17	0.0441 (19)	0.047 (2)	0.065 (2)	-0.0026 (15)	0.0050 (16)	-0.0118 (17)
C18	0.0366 (15)	0.0325 (15)	0.0392 (15)	-0.0041 (12)	0.0107 (12)	-0.0033 (12)
C19	0.0409 (17)	0.060 (2)	0.0426 (17)	-0.0052 (16)	-0.0096 (14)	0.0031 (15)
C20	0.0326 (15)	0.0441 (18)	0.0490 (17)	-0.0077 (13)	0.0060 (13)	0.0017 (14)
C21	0.048 (2)	0.090 (3)	0.057 (2)	-0.016 (2)	0.0094 (17)	0.018 (2)
C22	0.0429 (17)	0.0421 (17)	0.0433 (17)	-0.0066 (14)	0.0067 (14)	-0.0012 (14)
C23	0.075 (3)	0.044 (2)	0.089 (3)	0.006 (2)	0.007 (2)	0.004 (2)
C24	0.0433 (18)	0.0480 (19)	0.0516 (19)	0.0015 (15)	-0.0048 (15)	0.0064 (15)
C25	0.055 (2)	0.096 (3)	0.050 (2)	0.018 (2)	0.0216 (18)	-0.004 (2)
C26	0.0326 (15)	0.0433 (18)	0.0540 (19)	-0.0059 (13)	0.0020 (13)	-0.0016 (15)
C27	0.0424 (17)	0.0393 (17)	0.0469 (17)	0.0016 (14)	0.0108 (14)	-0.0016 (14)
C28	0.0383 (16)	0.057 (2)	0.0337 (15)	0.0092 (14)	0.0066 (13)	0.0003 (14)
C29	0.115 (4)	0.048 (2)	0.104 (4)	-0.029 (3)	0.032 (3)	-0.009 (2)
C30	0.0388 (16)	0.0410 (17)	0.0403 (16)	-0.0040 (13)	0.0053 (13)	-0.0001 (13)

C31	0.052 (2)	0.053 (2)	0.0484 (19)	0.0174 (16)	-0.0001 (15)	-0.0021 (16)
C32	0.0482 (19)	0.055 (2)	0.0409 (17)	-0.0105 (16)	-0.0043 (14)	-0.0078 (15)
C33	0.061 (3)	0.093 (4)	0.082 (3)	0.000 (2)	-0.014 (2)	-0.008 (3)
C34	0.0331 (17)	0.072 (3)	0.080 (3)	-0.0148 (17)	-0.0003 (17)	-0.002 (2)
Cl1	0.1311 (11)	0.0490 (6)	0.0736 (7)	-0.0175 (6)	0.0121 (7)	-0.0090 (5)
O1	0.188 (5)	0.116 (3)	0.075 (2)	-0.071 (3)	0.014 (3)	-0.018 (2)
O2	0.484 (14)	0.111 (4)	0.135 (5)	0.108 (6)	0.127 (7)	0.054 (4)
O3	0.193 (7)	0.333 (11)	0.210 (7)	-0.099 (7)	0.113 (6)	-0.083 (7)
O4	0.201 (5)	0.086 (3)	0.101 (3)	-0.052 (3)	-0.016 (3)	-0.006 (2)

Geometric parameters (Å, °) for (sust_3488_0m)

Au1—C5	2.016 (3)	C14—C16	1.385 (4)
Au1—C12	2.015 (3)	C14—C24	1.395 (4)
S1—C12	1.697 (3)	C15—H15A	0.9600
S1—C26	1.732 (4)	C15—H15B	0.9600
S2—C5	1.700 (3)	C15—H15C	0.9600
S2—C28	1.731 (4)	C16—C30	1.395 (4)
N1—C12	1.339 (4)	C17—H17	0.9800
N1—C16	1.456 (4)	C17—C23	1.519 (6)
N1—C20	1.408 (4)	C17—C30	1.518 (5)
N2—C5	1.330 (4)	C18—C22	1.399 (4)
N2—C6	1.405 (4)	C18—C27	1.392 (4)
N2—C18	1.454 (4)	C19—H19	0.9300
C1—H1	0.9800	C19—C24	1.372 (5)
C1—C10	1.522 (5)	C19—C32	1.376 (5)
C1—C14	1.522 (4)	C20—C21	1.487 (5)
C1—C29	1.526 (6)	C20—C26	1.342 (4)
C2—H2A	0.9600	C21—H21A	0.9600
C2—H2B	0.9600	C21—H21B	0.9600
C2—H2C	0.9600	C21—H21C	0.9600
C2—C31	1.522 (6)	C23—H23A	0.9600

C3—H3A	0.9600	C23—H23B	0.9600
C3—H3B	0.9600	C23—H23C	0.9600
C3—H3C	0.9600	C24—H24	0.9300
C3—C6	1.487 (5)	C25—H25A	0.9600
C4—H4	0.9300	C25—H25B	0.9600
C4—C8	1.369 (6)	C25—H25C	0.9600
C4—C9	1.377 (5)	C25—C28	1.507 (5)
C6—C28	1.341 (5)	C26—C34	1.492 (4)
C7—H7A	0.9600	C27—C31	1.528 (5)
C7—H7B	0.9600	C29—H29A	0.9600
C7—H7C	0.9600	C29—H29B	0.9600
C7—C17	1.526 (6)	C29—H29C	0.9600
C8—H8	0.9300	C30—C32	1.393 (5)
C8—C22	1.386 (5)	C31—H31	0.9800
C9—H9	0.9300	C31—C33	1.535 (6)
C9—C27	1.385 (5)	C32—H32	0.9300
C10—H10A	0.9600	C33—H33A	0.9600
C10—H10B	0.9600	C33—H33B	0.9600
C10—H10C	0.9600	C33—H33C	0.9600
C11—H11	0.9800	C34—H34A	0.9600
C11—C13	1.521 (6)	C34—H34B	0.9600
C11—C15	1.516 (5)	C34—H34C	0.9600
C11—C22	1.514 (5)	C11—O1	1.381 (4)
C13—H13A	0.9600	C11—O2	1.325 (6)
C13—H13B	0.9600	C11—O3	1.491 (7)
C13—H13C	0.9600	C11—O4	1.349 (4)
C12—Au1—C5	176.10 (12)	C23—C17—H17	107.6
C12—S1—C26	94.13 (15)	C30—C17—C7	112.9 (4)
C5—S2—C28	93.42 (16)	C30—C17—H17	107.6
C12—N1—C16	121.2 (2)	C30—C17—C23	110.8 (3)

C12—N1—C20	116.6 (3)	C22—C18—N2	117.9 (3)
C20—N1—C16	121.9 (2)	C27—C18—N2	118.4 (3)
C5—N2—C6	116.6 (3)	C27—C18—C22	123.7 (3)
C5—N2—C18	121.3 (2)	C24—C19—H19	119.3
C6—N2—C18	122.0 (3)	C24—C19—C32	121.3 (3)
C10—C1—H1	107.7	C32—C19—H19	119.3
C10—C1—C29	110.7 (3)	N1—C20—C21	120.0 (3)
C14—C1—H1	107.7	C26—C20—N1	112.0 (3)
C14—C1—C10	111.5 (3)	C26—C20—C21	128.0 (3)
C14—C1—C29	111.3 (3)	C20—C21—H21A	109.5
C29—C1—H1	107.7	C20—C21—H21B	109.5
H2A—C2—H2B	109.5	C20—C21—H21C	109.5
H2A—C2—H2C	109.5	H21A—C21—H21B	109.5
H2B—C2—H2C	109.5	H21A—C21—H21C	109.5
C31—C2—H2A	109.5	H21B—C21—H21C	109.5
C31—C2—H2B	109.5	C8—C22—C11	120.3 (3)
C31—C2—H2C	109.5	C8—C22—C18	116.8 (3)
H3A—C3—H3B	109.5	C18—C22—C11	122.9 (3)
H3A—C3—H3C	109.5	C17—C23—H23A	109.5
H3B—C3—H3C	109.5	C17—C23—H23B	109.5
C6—C3—H3A	109.5	C17—C23—H23C	109.5
C6—C3—H3B	109.5	H23A—C23—H23B	109.5
C6—C3—H3C	109.5	H23A—C23—H23C	109.5
C8—C4—H4	119.6	H23B—C23—H23C	109.5
C8—C4—C9	120.9 (3)	C14—C24—H24	119.7
C9—C4—H4	119.6	C19—C24—C14	120.6 (3)
S2—C5—Au1	122.35 (17)	C19—C24—H24	119.7
N2—C5—Au1	129.2 (2)	H25A—C25—H25B	109.5
N2—C5—S2	108.4 (2)	H25A—C25—H25C	109.5
N2—C6—C3	119.9 (3)	H25B—C25—H25C	109.5
C28—C6—N2	111.7 (3)	C28—C25—H25A	109.5

C28—C6—C3	128.4 (3)	C28—C25—H25B	109.5
H7A—C7—H7B	109.5	C28—C25—H25C	109.5
H7A—C7—H7C	109.5	C20—C26—S1	109.3 (2)
H7B—C7—H7C	109.5	C20—C26—C34	128.7 (3)
C17—C7—H7A	109.5	C34—C26—S1	121.9 (3)
C17—C7—H7B	109.5	C9—C27—C18	116.5 (3)
C17—C7—H7C	109.5	C9—C27—C31	120.5 (3)
C4—C8—H8	119.6	C18—C27—C31	123.0 (3)
C4—C8—C22	120.9 (3)	C6—C28—S2	109.8 (2)
C22—C8—H8	119.6	C6—C28—C25	127.8 (3)
C4—C9—H9	119.4	C25—C28—S2	122.4 (3)
C4—C9—C27	121.2 (4)	C1—C29—H29A	109.5
C27—C9—H9	119.4	C1—C29—H29B	109.5
C1—C10—H10A	109.5	C1—C29—H29C	109.5
C1—C10—H10B	109.5	H29A—C29—H29B	109.5
C1—C10—H10C	109.5	H29A—C29—H29C	109.5
H10A—C10—H10B	109.5	H29B—C29—H29C	109.5
H10A—C10—H10C	109.5	C16—C30—C17	122.4 (3)
H10B—C10—H10C	109.5	C32—C30—C16	116.4 (3)
C13—C11—H11	107.8	C32—C30—C17	121.3 (3)
C15—C11—H11	107.8	C2—C31—C27	111.5 (3)
C15—C11—C13	110.4 (4)	C2—C31—H31	107.5
C22—C11—H11	107.8	C2—C31—C33	111.4 (4)
C22—C11—C13	112.5 (3)	C27—C31—H31	107.5
C22—C11—C15	110.5 (3)	C27—C31—C33	111.3 (3)
S1—C12—Au1	123.60 (16)	C33—C31—H31	107.5
N1—C12—Au1	128.2 (2)	C19—C32—C30	120.7 (3)
N1—C12—S1	107.9 (2)	C19—C32—H32	119.7
C11—C13—H13A	109.5	C30—C32—H32	119.7
C11—C13—H13B	109.5	C31—C33—H33A	109.5
C11—C13—H13C	109.5	C31—C33—H33B	109.5

H13A—C13—H13B	109.5	C31—C33—H33C	109.5
H13A—C13—H13C	109.5	H33A—C33—H33B	109.5
H13B—C13—H13C	109.5	H33A—C33—H33C	109.5
C16—C14—C1	123.1 (3)	H33B—C33—H33C	109.5
C16—C14—C24	116.7 (3)	C26—C34—H34A	109.5
C24—C14—C1	120.1 (3)	C26—C34—H34B	109.5
C11—C15—H15A	109.5	C26—C34—H34C	109.5
C11—C15—H15B	109.5	H34A—C34—H34B	109.5
C11—C15—H15C	109.5	H34A—C34—H34C	109.5
H15A—C15—H15B	109.5	H34B—C34—H34C	109.5
H15A—C15—H15C	109.5	O1—C11—O3	108.2 (4)
H15B—C15—H15C	109.5	O2—C11—O1	113.8 (4)
C14—C16—N1	117.7 (3)	O2—C11—O3	98.8 (5)
C14—C16—C30	124.3 (3)	O2—C11—O4	120.9 (5)
C30—C16—N1	118.0 (3)	O4—C11—O1	113.1 (3)
C7—C17—H17	107.6	O4—C11—O3	98.7 (4)
C23—C17—C7	110.3 (4)		
N1—C16—C30—C17	-0.6 (4)	C12—N1—C20—C26	-0.9 (4)
N1—C16—C30—C32	178.0 (3)	C13—C11—C22—C8	53.8 (5)
N1—C20—C26—S1	1.9 (4)	C13—C11—C22— C18	-127.5 (4)
N1—C20—C26—C34	-175.1 (3)	C14—C16—C30— C17	178.9 (3)
N2—C6—C28—S2	-0.4 (3)	C14—C16—C30— C32	-2.5 (5)
N2—C6—C28—C25	-179.9 (3)	C15—C11—C22—C8	-70.1 (4)
N2—C18—C22—C8	178.8 (3)	C15—C11—C22— C18	108.6 (4)
N2—C18—C22—C11	0.1 (4)	C16—N1—C12—Au1	-0.7 (4)
N2—C18—C27—C9	-178.4 (3)	C16—N1—C12—S1	-174.7 (2)
N2—C18—C27—C31	1.7 (5)	C16—N1—C20—C21	-7.1 (5)

C1—C14—C16—N1	2.9 (4)	C16—N1—C20—C26	173.1 (3)
C1—C14—C16—C30	-176.5 (3)	C16—C14—C24— C19	-0.9 (5)
C1—C14—C24—C19	178.3 (3)	C16—C30—C32— C19	0.6 (5)
C3—C6—C28—S2	179.6 (3)	C17—C30—C32— C19	179.2 (3)
C3—C6—C28—C25	0.1 (6)	C18—N2—C5—Au1	-1.8 (4)
C4—C8—C22—C11	178.2 (3)	C18—N2—C5—S2	179.9 (2)
C4—C8—C22—C18	-0.6 (5)	C18—N2—C6—C3	0.6 (5)
C4—C9—C27—C18	-0.4 (5)	C18—N2—C6—C28	-179.4 (3)
C4—C9—C27—C31	179.5 (4)	C18—C27—C31—C2	126.5 (4)
C5—S2—C28—C6	0.7 (3)	C18—C27—C31— C33	-108.4 (4)
C5—S2—C28—C25	-179.8 (3)	C20—N1—C12—Au1	173.5 (2)
C5—N2—C6—C3	179.8 (3)	C20—N1—C12—S1	-0.5 (3)
C5—N2—C6—C28	-0.2 (4)	C20—N1—C16—C14	-89.3 (4)
C5—N2—C18—C22	-95.3 (3)	C20—N1—C16—C30	90.2 (4)
C5—N2—C18—C27	85.1 (4)	C21—C20—C26—S1	-177.9 (3)
C6—N2—C5—Au1	179.0 (2)	C21—C20—C26— C34	5.2 (7)
C6—N2—C5—S2	0.7 (3)	C22—C18—C27—C9	2.1 (5)
C6—N2—C18—C22	83.8 (4)	C22—C18—C27— C31	-177.9 (3)
C6—N2—C18—C27	-95.7 (3)	C23—C17—C30— C16	98.4 (4)
C7—C17—C30—C16	-137.4 (4)	C23—C17—C30— C32	-80.1 (4)
C7—C17—C30—C32	44.1 (5)	C24—C14—C16—N1	-177.8 (3)
C8—C4—C9—C27	-1.7 (6)	C24—C14—C16— C30	2.7 (5)
C9—C4—C8—C22	2.2 (6)	C24—C19—C32— C30	0.9 (6)
C9—C27—C31—C2	-53.5 (5)	C26—S1—C12—Au1	-172.9 (2)

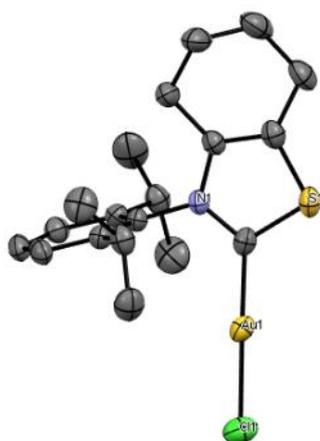
C9—C27—C31—C33	71.6 (5)	C26—S1—C12—N1	1.4 (2)
C10—C1—C14—C16	-118.0 (4)	C27—C18—C22—C8	-1.6 (5)
C10—C1—C14—C24	62.8 (4)	C27—C18—C22— C11	179.6 (3)
C12—S1—C26—C20	-1.9 (3)	C28—S2—C5—Au1	-179.19 (19)
C12—S1—C26—C34	175.3 (3)	C28—S2—C5—N2	-0.8 (2)
C12—N1—C16—C14	84.5 (4)	C29—C1—C14—C16	117.9 (4)
C12—N1—C16—C30	-96.0 (4)	C29—C1—C14—C24	-61.3 (5)
C12—N1—C20—C21	178.9 (3)	C32—C19—C24— C14	-0.8 (6)

Special details

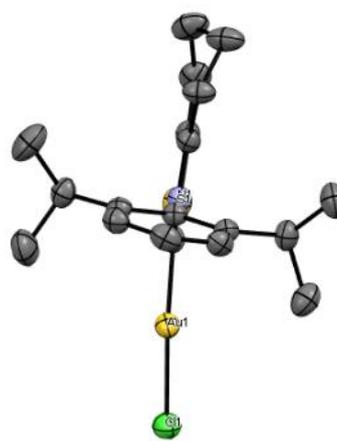
Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Crystal structure of 2b.

Single crystal of complex **2b** were grown by slow evaporation in a mixture of DCM and n-hexane (DCM: n-hexane = 1:3) at low temperature.



Front view



Side view

Chart S3. Crystal structure of **2b** (50% ellipsoids). Two views: front (left); side (right). Hydrogen atoms have been omitted for clarity. (Crystallographic data has been deposited with the Cambridge Crystallographic Data Center as supplementary

publication no. 2503056).

Table S5. Crystal Data and Structure Refinement Summary for **2b**.

Crystal data

C ₁₉ H ₂₅ AuCINS	$F(000) = 1032$
$M_r = 531.88$	$D_x = 1.811 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$a = 8.8055 (3) \text{ \AA}$	Cell parameters from 9872 reflections
$b = 18.4450 (5) \text{ \AA}$	$\theta = 2.7\text{--}27.5^\circ$
$c = 12.1333 (4) \text{ \AA}$	$\mu = 7.79 \text{ mm}^{-1}$
$\beta = 98.215 (1)^\circ$	$T = 223 \text{ K}$
$V = 1950.44 (11) \text{ \AA}^3$	Block
$Z = 4$	$0.16 \times 0.15 \times 0.12 \text{ mm}$

Data collection

Bruker D8 VENTURE diffractometer	3980 reflections with $I > 2\sigma(I)$
ϕ and ω scans	$R_{\text{int}} = 0.045$
Absorption correction: multi-scan <i>SADABS2016/2</i> (Bruker,2016/2) was used for absorption correction. $wR2(\text{int})$ was 0.1475 before and 0.0601 after correction. The Ratio of minimum to maximum transmission is 0.4289. The $\lambda/2$ correction factor is Not present.	$\theta_{\text{max}} = 27.5^\circ$, $\theta_{\text{min}} = 2.0^\circ$
$T_{\text{min}} = 0.112$, $T_{\text{max}} = 0.262$	$h = -10 \rightarrow 11$
21554 measured reflections	$k = -20 \rightarrow 23$
4425 independent reflections	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	Primary atom site location: dual
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites

$R[F^2 > 2\sigma(F^2)] = 0.022$	H-atom parameters constrained
$wR(F^2) = 0.051$	$w = 1/[\sigma^2(F_o^2) + (0.018P)^2 + 0.2987P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.09$	$(\Delta/\sigma)_{\max} = 0.003$
4425 reflections	$\Delta)_{\max} = 0.37 \text{ e } \text{Å}^{-3}$
212 parameters	$\Delta)_{\min} = -1.24 \text{ e } \text{Å}^{-3}$
0 restraints	

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2) for (mo_20241113_zzh_241106105317_0)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Au1	0.56507 (2)	0.67177 (2)	0.77409 (2)	0.03332 (5)
C1	0.4827 (3)	0.57449 (15)	0.7951 (2)	0.0321 (5)
C2	0.3227 (3)	0.47322 (14)	0.7724 (2)	0.0309 (5)
C3	0.4446 (3)	0.44294 (15)	0.8355 (2)	0.0355 (6)
C4	0.4526 (4)	0.36497 (17)	0.8723 (3)	0.0480 (8)
H4A	0.490381	0.362095	0.952219	0.058*
H4B	0.523698	0.338181	0.832173	0.058*
C5	0.2918 (4)	0.33159 (17)	0.8482 (4)	0.0568 (10)
H5A	0.299848	0.278684	0.853634	0.068*
H5B	0.229942	0.348297	0.904289	0.068*
C6	0.2128 (4)	0.35214 (17)	0.7337 (3)	0.0523 (9)
H6A	0.116000	0.325426	0.717483	0.063*
H6B	0.277905	0.338437	0.678008	0.063*
C7	0.1803 (3)	0.43382 (15)	0.7258 (3)	0.0408 (7)
H7A	0.149284	0.447755	0.647855	0.049*
H7B	0.096806	0.446154	0.767846	0.049*
C8	0.2237 (3)	0.59039 (13)	0.6918 (2)	0.0283 (5)
C9	0.2162 (3)	0.59737 (14)	0.5764 (2)	0.0302 (5)
C10	0.0946 (3)	0.63795 (15)	0.5213 (2)	0.0356 (6)
H10	0.087225	0.645115	0.443965	0.043*

C11	-0.0150 (3)	0.66777 (14)	0.5786 (3)	0.0388 (7)
H11	-0.097088	0.694128	0.539805	0.047*
C12	-0.0049 (3)	0.65916 (14)	0.6923 (3)	0.0365 (6)
H12	-0.080376	0.679889	0.730036	0.044*
C13	0.1144 (3)	0.62049 (14)	0.7519 (2)	0.0311 (5)
C14	0.1280 (3)	0.61493 (16)	0.8777 (2)	0.0394 (6)
H14	0.208447	0.578693	0.902991	0.047*
C15	0.1793 (5)	0.6877 (2)	0.9304 (3)	0.0620 (10)
H15A	0.275824	0.701915	0.906935	0.093*
H15B	0.192530	0.683317	1.010834	0.093*
H15C	0.102063	0.724188	0.906793	0.093*
C16	-0.0220 (4)	0.5890 (2)	0.9142 (3)	0.0674 (11)
H16A	-0.100887	0.625421	0.895195	0.101*
H16B	-0.006708	0.581152	0.994058	0.101*
H16C	-0.053716	0.543955	0.876464	0.101*
C17	0.3322 (3)	0.56321 (16)	0.5114 (2)	0.0386 (6)
H17	0.396860	0.529795	0.561878	0.046*
C18	0.4367 (4)	0.6204 (2)	0.4712 (3)	0.0521 (8)
H18A	0.375533	0.654334	0.422440	0.078*
H18B	0.510712	0.597045	0.430921	0.078*
H18C	0.490337	0.646244	0.534805	0.078*
C19	0.2524 (4)	0.5188 (2)	0.4131 (3)	0.0554 (8)
H19A	0.182027	0.484626	0.439608	0.083*
H19B	0.328668	0.492583	0.378639	0.083*
H19C	0.195841	0.551071	0.358930	0.083*
Cl1	0.67098 (9)	0.78118 (4)	0.74257 (7)	0.04792 (18)
N1	0.3453 (2)	0.54669 (11)	0.75208 (18)	0.0281 (4)
S1	0.58706 (8)	0.50670 (4)	0.86621 (6)	0.03948 (16)

Atomic displacement parameters (\AA^2) for (mo_20241113_zzh_241106105317_0)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
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Au1	0.02608 (7)	0.03848 (7)	0.03517 (7)	-0.00136 (4)	0.00364 (4)	-0.00508 (4)
C1	0.0270 (12)	0.0413 (14)	0.0276 (13)	0.0019 (10)	0.0025 (10)	-0.0026 (11)
C2	0.0305 (13)	0.0307 (13)	0.0316 (14)	0.0048 (10)	0.0046 (10)	0.0028 (10)
C3	0.0344 (14)	0.0400 (15)	0.0322 (14)	0.0070 (11)	0.0054 (11)	0.0023 (11)
C4	0.0494 (18)	0.0419 (17)	0.053 (2)	0.0171 (14)	0.0078 (15)	0.0139 (14)
C5	0.054 (2)	0.0411 (18)	0.079 (3)	0.0098 (14)	0.0204 (19)	0.0228 (16)
C6	0.0411 (17)	0.0328 (15)	0.082 (3)	-0.0031 (13)	0.0049 (16)	0.0086 (16)
C7	0.0327 (14)	0.0328 (14)	0.0547 (19)	0.0001 (11)	-0.0008 (13)	0.0069 (13)
C8	0.0227 (11)	0.0288 (12)	0.0321 (14)	0.0007 (9)	0.0001 (10)	0.0023 (10)
C9	0.0282 (12)	0.0306 (13)	0.0313 (14)	-0.0001 (10)	0.0026 (10)	0.0014 (10)
C10	0.0398 (15)	0.0345 (14)	0.0301 (14)	0.0029 (11)	-0.0029 (11)	0.0048 (11)
C11	0.0327 (15)	0.0330 (14)	0.0474 (18)	0.0066 (11)	-0.0058 (12)	0.0019 (12)
C12	0.0320 (14)	0.0322 (14)	0.0454 (17)	0.0052 (10)	0.0062 (12)	-0.0002 (12)
C13	0.0275 (12)	0.0303 (13)	0.0353 (15)	-0.0007 (10)	0.0038 (10)	0.0018 (10)
C14	0.0369 (15)	0.0454 (16)	0.0369 (16)	0.0099 (12)	0.0089 (12)	0.0048 (12)
C15	0.080 (3)	0.064 (2)	0.041 (2)	0.002 (2)	0.0070 (19)	-0.0129 (17)
C16	0.055 (2)	0.092 (3)	0.060 (2)	0.003 (2)	0.0257 (18)	0.022 (2)
C17	0.0396 (15)	0.0454 (16)	0.0310 (15)	0.0087 (12)	0.0058 (12)	0.0010 (12)
C18	0.0413 (17)	0.070 (2)	0.0461 (19)	0.0003 (15)	0.0116 (14)	0.0058 (16)
C19	0.058 (2)	0.062 (2)	0.0476 (19)	0.0062 (16)	0.0108 (16)	-0.0147 (16)
Cl1	0.0455 (4)	0.0428 (4)	0.0583 (5)	-0.0086 (3)	0.0168 (3)	-0.0079 (3)
N1	0.0244 (10)	0.0301 (11)	0.0292 (11)	0.0035 (8)	0.0019 (8)	0.0014 (9)
S1	0.0286 (3)	0.0500 (4)	0.0374 (4)	0.0070 (3)	-0.0036 (3)	0.0038 (3)

Geometric parameters (Å, °) for (mo_20241113_zzh_241106105317_0)

Au1—C1	1.966 (3)	C10—H10	0.9400
Au1—Cl1	2.2783 (7)	C10—C11	1.382 (4)
C1—N1	1.349 (3)	C11—H11	0.9400
C1—S1	1.710 (3)	C11—C12	1.379 (5)
C2—C3	1.347 (4)	C12—H12	0.9400
C2—C7	1.489 (4)	C12—C13	1.385 (4)

C2—N1	1.397 (3)	C13—C14	1.517 (4)
C3—C4	1.505 (4)	C14—H14	0.9900
C3—S1	1.721 (3)	C14—C15	1.527 (5)
C4—H4A	0.9800	C14—C16	1.529 (4)
C4—H4B	0.9800	C15—H15A	0.9700
C4—C5	1.534 (5)	C15—H15B	0.9700
C5—H5A	0.9800	C15—H15C	0.9700
C5—H5B	0.9800	C16—H16A	0.9700
C5—C6	1.510 (6)	C16—H16B	0.9700
C6—H6A	0.9800	C16—H16C	0.9700
C6—H6B	0.9800	C17—H17	0.9900
C6—C7	1.534 (4)	C17—C18	1.525 (4)
C7—H7A	0.9800	C17—C19	1.532 (4)
C7—H7B	0.9800	C18—H18A	0.9700
C8—C9	1.398 (4)	C18—H18B	0.9700
C8—C13	1.403 (4)	C18—H18C	0.9700
C8—N1	1.452 (3)	C19—H19A	0.9700
C9—C10	1.396 (4)	C19—H19B	0.9700
C9—C17	1.513 (4)	C19—H19C	0.9700
C1—Au1—C11	176.26 (8)	C11—C12—H12	119.4
N1—C1—Au1	128.61 (19)	C11—C12—C13	121.1 (3)
N1—C1—S1	107.75 (19)	C13—C12—H12	119.4
S1—C1—Au1	123.46 (14)	C8—C13—C14	122.3 (2)
C3—C2—C7	124.9 (2)	C12—C13—C8	117.3 (3)
C3—C2—N1	112.3 (2)	C12—C13—C14	120.4 (2)
N1—C2—C7	122.7 (2)	C13—C14—H14	108.0
C2—C3—C4	124.4 (3)	C13—C14—C15	109.7 (3)
C2—C3—S1	109.7 (2)	C13—C14—C16	111.4 (3)
C4—C3—S1	125.9 (2)	C15—C14—H14	108.0
C3—C4—H4A	109.9	C15—C14—C16	111.7 (3)

C3—C4—H4B	109.9	C16—C14—H14	108.0
C3—C4—C5	108.9 (2)	C14—C15—H15A	109.5
H4A—C4—H4B	108.3	C14—C15—H15B	109.5
C5—C4—H4A	109.9	C14—C15—H15C	109.5
C5—C4—H4B	109.9	H15A—C15—H15B	109.5
C4—C5—H5A	109.3	H15A—C15—H15C	109.5
C4—C5—H5B	109.3	H15B—C15—H15C	109.5
H5A—C5—H5B	108.0	C14—C16—H16A	109.5
C6—C5—C4	111.5 (3)	C14—C16—H16B	109.5
C6—C5—H5A	109.3	C14—C16—H16C	109.5
C6—C5—H5B	109.3	H16A—C16—H16B	109.5
C5—C6—H6A	109.4	H16A—C16—H16C	109.5
C5—C6—H6B	109.4	H16B—C16—H16C	109.5
C5—C6—C7	111.2 (3)	C9—C17—H17	107.9
H6A—C6—H6B	108.0	C9—C17—C18	111.2 (2)
C7—C6—H6A	109.4	C9—C17—C19	111.1 (2)
C7—C6—H6B	109.4	C18—C17—H17	107.9
C2—C7—C6	108.4 (2)	C18—C17—C19	110.6 (3)
C2—C7—H7A	110.0	C19—C17—H17	107.9
C2—C7—H7B	110.0	C17—C18—H18A	109.5
C6—C7—H7A	110.0	C17—C18—H18B	109.5
C6—C7—H7B	110.0	C17—C18—H18C	109.5
H7A—C7—H7B	108.4	H18A—C18—H18B	109.5
C9—C8—C13	123.2 (2)	H18A—C18—H18C	109.5
C9—C8—N1	118.8 (2)	H18B—C18—H18C	109.5
C13—C8—N1	118.0 (2)	C17—C19—H19A	109.5
C8—C9—C17	123.0 (2)	C17—C19—H19B	109.5
C10—C9—C8	116.9 (2)	C17—C19—H19C	109.5
C10—C9—C17	120.1 (2)	H19A—C19—H19B	109.5
C9—C10—H10	119.5	H19A—C19—H19C	109.5
C11—C10—C9	121.0 (3)	H19B—C19—H19C	109.5

C11—C10—H10	119.5	C1—N1—C2	116.3 (2)
C10—C11—H11	119.7	C1—N1—C8	122.7 (2)
C12—C11—C10	120.6 (3)	C2—N1—C8	120.9 (2)
C12—C11—H11	119.7	C1—S1—C3	93.89 (13)
Au1—C1—N1—C2	173.99 (19)	C9—C10—C11—C12	1.2 (4)
Au1—C1—N1—C8	-8.5 (4)	C10—C9—C17—C18	72.0 (3)
Au1—C1—S1—C3	-175.03 (17)	C10—C9—C17—C19	-51.6 (4)
C2—C3—C4—C5	-11.8 (4)	C10—C11—C12— C13	-0.1 (4)
C2—C3—S1—C1	0.4 (2)	C11—C12—C13—C8	-0.2 (4)
C3—C2—C7—C6	-15.3 (4)	C11—C12—C13— C14	176.8 (3)
C3—C2—N1—C1	1.5 (3)	C12—C13—C14— C15	-72.2 (3)
C3—C2—N1—C8	-176.0 (2)	C12—C13—C14— C16	52.0 (4)
C3—C4—C5—C6	44.5 (4)	C13—C8—C9—C10	1.5 (4)
C4—C3—S1—C1	-179.8 (3)	C13—C8—C9—C17	-178.4 (2)
C4—C5—C6—C7	-65.8 (4)	C13—C8—N1—C1	-93.0 (3)
C5—C6—C7—C2	47.9 (4)	C13—C8—N1—C2	84.3 (3)
C7—C2—C3—C4	-2.6 (5)	C17—C9—C10—C11	178.0 (3)
C7—C2—C3—S1	177.3 (2)	N1—C1—S1—C3	0.4 (2)
C7—C2—N1—C1	-176.9 (3)	N1—C2—C3—C4	179.1 (3)
C7—C2—N1—C8	5.6 (4)	N1—C2—C3—S1	-1.1 (3)
C8—C9—C10—C11	-1.8 (4)	N1—C2—C7—C6	162.9 (3)
C8—C9—C17—C18	-108.1 (3)	N1—C8—C9—C10	178.0 (2)
C8—C9—C17—C19	128.3 (3)	N1—C8—C9—C17	-1.9 (4)
C8—C13—C14—C15	104.7 (3)	N1—C8—C13—C12	-177.0 (2)
C8—C13—C14—C16	-131.1 (3)	N1—C8—C13—C14	6.0 (4)
C9—C8—C13—C12	-0.5 (4)	S1—C1—N1—C2	-1.2 (3)
C9—C8—C13—C14	-177.4 (2)	S1—C1—N1—C8	176.29 (18)

C9—C8—N1—C1	90.3 (3)	S1—C3—C4—C5	168.3 (2)
C9—C8—N1—C2	-92.4 (3)		

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Crystal structure of 3b

Single crystal of complex **3b** were grown by slow evaporation in a mixture of DCM and n-hexane (DCM: n-hexane = 1:3) at low temperature.

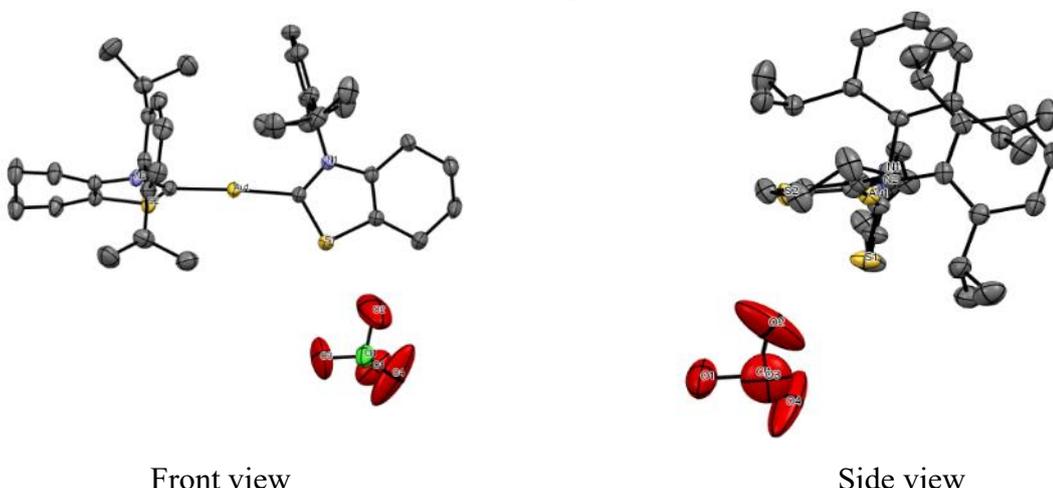


Chart S4. Crystal structure of **3b** (50% ellipsoids). Two views: front (left); side (right). Hydrogen atoms have been omitted for clarity. (Crystallographic data has been deposited with the Cambridge Crystallographic Data Center as supplementary publication no. 2503059).

Table S6. Crystal Data and Structure Refinement Summary for **3b**.

Crystal data

$C_{38}H_{50}AuN_2S_2 \cdot ClO_4 \cdot CH_2Cl_2$	$F(000) = 1976$
$M_r = 980.26$	$D_x = 1.540 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$a = 15.8785 (6) \text{ \AA}$	Cell parameters from 9873 reflections
$b = 15.8206 (5) \text{ \AA}$	$\theta = 2.7\text{--}28.3^\circ$
$c = 17.8935 (7) \text{ \AA}$	$\mu = 3.81 \text{ mm}^{-1}$

$\beta = 109.890 (1)^\circ$	$T = 200 \text{ K}$
$V = 4226.8 (3) \text{ \AA}^3$	Block, colourless
$Z = 4$	$0.35 \times 0.12 \times 0.07 \text{ mm}$

Data collection

Bruker diffractometer	$R_{\text{int}} = 0.051$
Absorption correction: multi-scan <i>SADABS2016/2</i> (Bruker,2016/2) was used for absorption correction. $wR2(\text{int})$ was 0.1172 before and 0.0607 after correction. The Ratio of minimum to maximum transmission is 0.7794. The $\lambda/2$ correction factor is Not present.	$\theta_{\text{max}} = 28.3^\circ$, $\theta_{\text{min}} = 1.9^\circ$
$T_{\text{min}} = 0.581$, $T_{\text{max}} = 0.746$	$h = -21 \rightarrow 21$
99514 measured reflections	$k = -21 \rightarrow 21$
10487 independent reflections	$l = -23 \rightarrow 23$
9069 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Primary atom site location: dual
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.034$	H-atom parameters constrained
$wR(F^2) = 0.070$	$w = 1/[\sigma^2(F_o^2) + (0.0134P)^2 + 13.6525P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.09$	$(\Delta/\sigma)_{\text{max}} = 0.002$
10487 reflections	$\Delta_{\text{max}} = 1.26 \text{ e \AA}^{-3}$
468 parameters	$\Delta_{\text{min}} = -1.04 \text{ e \AA}^{-3}$
0 restraints	

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2) for (mo_240422160078)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
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Au1	0.39339 (2)	0.65386 (2)	0.65014 (2)	0.02388 (4)
S1	0.61194 (6)	0.63868 (7)	0.70855 (6)	0.0354 (2)
S2	0.26019 (6)	0.79819 (6)	0.54695 (6)	0.02809 (19)
N1	0.53588 (19)	0.60488 (18)	0.80502 (17)	0.0230 (6)
N2	0.20414 (19)	0.65083 (18)	0.52778 (17)	0.0240 (6)
C1	0.5154 (2)	0.6258 (2)	0.7284 (2)	0.0258 (7)
C2	0.6787 (2)	0.6146 (3)	0.8043 (2)	0.0307 (8)
C3	0.6266 (2)	0.5970 (2)	0.8484 (2)	0.0261 (7)
C4	0.6612 (3)	0.5733 (3)	0.9348 (2)	0.0321 (8)
H4A	0.627238	0.524229	0.943995	0.039*
H4B	0.652887	0.621126	0.967239	0.039*
C5	0.7605 (3)	0.5510 (3)	0.9592 (2)	0.0368 (9)
H5A	0.786803	0.549640	1.017938	0.044*
H5B	0.766954	0.493940	0.939071	0.044*
C6	0.8112 (3)	0.6145 (3)	0.9270 (3)	0.0392 (10)
H6A	0.875959	0.601241	0.948151	0.047*
H6B	0.802663	0.671845	0.945321	0.047*
C7	0.7791 (3)	0.6132 (3)	0.8359 (3)	0.0442 (11)
H7A	0.802858	0.663073	0.816186	0.053*
H7B	0.801290	0.561666	0.817357	0.053*
C8	0.4674 (2)	0.5940 (2)	0.8411 (2)	0.0239 (7)
C9	0.4383 (2)	0.6661 (2)	0.8708 (2)	0.0273 (7)
C10	0.3735 (3)	0.6539 (3)	0.9061 (2)	0.0335 (8)
H10	0.352020	0.701055	0.927141	0.040*
C11	0.3400 (3)	0.5744 (3)	0.9109 (2)	0.0351 (9)
H11	0.295528	0.567706	0.935018	0.042*
C12	0.3701 (3)	0.5047 (3)	0.8813 (2)	0.0326 (8)
H12	0.346308	0.450475	0.885433	0.039*
C13	0.4351 (2)	0.5128 (2)	0.8453 (2)	0.0269 (7)
C14	0.4651 (3)	0.4367 (2)	0.8095 (3)	0.0348 (9)
H14	0.520076	0.452776	0.797558	0.042*

C15	0.3923 (3)	0.4126 (3)	0.7315 (3)	0.0504 (12)
H15A	0.337692	0.396804	0.741978	0.076*
H15B	0.412811	0.364709	0.707522	0.076*
H15C	0.379772	0.460897	0.695062	0.076*
C16	0.4882 (3)	0.3617 (3)	0.8668 (3)	0.0524 (12)
H16A	0.531350	0.379656	0.917916	0.079*
H16B	0.514458	0.316410	0.844455	0.079*
H16C	0.433677	0.341024	0.874669	0.079*
C17	0.4733 (3)	0.7544 (2)	0.8654 (3)	0.0364 (9)
H17	0.519341	0.749706	0.839001	0.044*
C18	0.3988 (3)	0.8115 (3)	0.8144 (3)	0.0472 (11)
H18A	0.353136	0.818052	0.839526	0.071*
H18B	0.371672	0.786234	0.761647	0.071*
H18C	0.423691	0.866986	0.809244	0.071*
C19	0.5188 (4)	0.7925 (3)	0.9480 (3)	0.0590 (14)
H19A	0.542843	0.848366	0.942634	0.089*
H19B	0.567662	0.755523	0.978965	0.089*
H19C	0.474905	0.798164	0.975179	0.089*
C20	0.2771 (2)	0.6938 (2)	0.5715 (2)	0.0252 (7)
C21	0.1560 (2)	0.7814 (2)	0.4767 (2)	0.0265 (7)
C22	0.0964 (3)	0.8478 (3)	0.4256 (2)	0.0355 (9)
H22A	0.131928	0.885622	0.403755	0.043*
H22B	0.069692	0.882315	0.457983	0.043*
C23	0.0225 (3)	0.8058 (3)	0.3580 (3)	0.0478 (11)
H23A	-0.025051	0.847745	0.333294	0.057*
H23B	0.047388	0.786978	0.316992	0.057*
C24	-0.0178 (3)	0.7311 (3)	0.3853 (3)	0.0523 (13)
H24A	-0.067648	0.708468	0.339785	0.063*
H24B	-0.043054	0.750049	0.426097	0.063*
C25	0.0507 (3)	0.6601 (3)	0.4204 (3)	0.0366 (9)
H25A	0.026678	0.620077	0.450656	0.044*

H25B	0.062071	0.628641	0.377003	0.044*
C26	0.1359 (2)	0.6982 (2)	0.4741 (2)	0.0261 (7)
C27	0.1966 (2)	0.5601 (2)	0.5388 (2)	0.0263 (7)
C28	0.1590 (2)	0.5339 (2)	0.5952 (2)	0.0284 (8)
C29	0.1575 (3)	0.4475 (2)	0.6084 (2)	0.0339 (9)
H29	0.134435	0.427236	0.647534	0.041*
C30	0.1888 (3)	0.3904 (3)	0.5655 (3)	0.0395 (10)
H30	0.186766	0.331603	0.575354	0.047*
C31	0.2231 (3)	0.4183 (2)	0.5086 (3)	0.0366 (9)
H31	0.243082	0.378237	0.478729	0.044*
C32	0.2289 (3)	0.5044 (2)	0.4941 (2)	0.0309 (8)
C33	0.2696 (3)	0.5338 (3)	0.4333 (2)	0.0394 (10)
H33	0.263886	0.596705	0.428914	0.047*
C34	0.3689 (3)	0.5115 (3)	0.4602 (3)	0.0474 (11)
H34A	0.399821	0.537403	0.512040	0.071*
H34B	0.394669	0.532750	0.421246	0.071*
H34C	0.375949	0.449951	0.464540	0.071*
C35	0.2206 (4)	0.4959 (4)	0.3514 (3)	0.0568 (13)
H35A	0.227113	0.434265	0.354045	0.085*
H35B	0.246381	0.518415	0.312907	0.085*
H35C	0.156978	0.510725	0.334773	0.085*
C36	0.1236 (3)	0.5955 (3)	0.6424 (2)	0.0339 (8)
H36	0.123888	0.653310	0.619905	0.041*
C37	0.1851 (3)	0.5967 (3)	0.7294 (3)	0.0495 (11)
H37A	0.185250	0.540723	0.752900	0.074*
H37B	0.163416	0.638767	0.758660	0.074*
H37C	0.246125	0.611279	0.732202	0.074*
C38	0.0274 (3)	0.5747 (4)	0.6366 (3)	0.0566 (13)
H38A	-0.010288	0.569914	0.580579	0.085*
H38B	0.004264	0.619848	0.661799	0.085*
H38C	0.026550	0.521053	0.663727	0.085*

Cl1	0.80257 (8)	0.79170 (8)	0.65554 (8)	0.0512 (3)
O1	0.8347 (3)	0.8747 (3)	0.6725 (4)	0.1064 (18)
O2	0.7753 (5)	0.7722 (6)	0.7200 (4)	0.206 (5)
O3	0.7253 (4)	0.7872 (4)	0.5906 (3)	0.133 (2)
O4	0.8689 (4)	0.7396 (4)	0.6582 (6)	0.214 (5)
Cl2	1.13883 (14)	0.82571 (12)	0.70528 (14)	0.1011 (6)
Cl3	1.02859 (15)	0.95185 (13)	0.60283 (13)	0.1069 (7)
C39	1.0324 (5)	0.8640 (5)	0.6603 (6)	0.112 (3)
H39A	1.006420	0.878407	0.701800	0.134*
H39B	0.994847	0.819084	0.626584	0.134*

Atomic displacement parameters (\AA^2) for (mo_240422160078)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Au1	0.01963 (7)	0.02657 (7)	0.02309 (7)	0.00039 (5)	0.00422 (5)	0.00223 (6)
S1	0.0235 (5)	0.0576 (7)	0.0259 (4)	0.0058 (4)	0.0092 (4)	0.0096 (4)
S2	0.0252 (5)	0.0236 (4)	0.0314 (5)	-0.0034 (3)	0.0042 (4)	0.0021 (4)
N1	0.0204 (14)	0.0254 (15)	0.0238 (14)	0.0017 (11)	0.0081 (12)	0.0019 (12)
N2	0.0213 (14)	0.0218 (14)	0.0263 (14)	0.0017 (12)	0.0046 (12)	0.0023 (12)
C1	0.0207 (17)	0.0297 (18)	0.0260 (17)	0.0022 (14)	0.0065 (14)	0.0034 (14)
C2	0.0243 (19)	0.041 (2)	0.0269 (18)	0.0023 (16)	0.0084 (15)	0.0055 (16)
C3	0.0221 (18)	0.0278 (18)	0.0252 (17)	-0.0010 (14)	0.0039 (14)	0.0005 (14)
C4	0.028 (2)	0.040 (2)	0.0248 (18)	-0.0019 (16)	0.0051 (16)	0.0041 (16)
C5	0.031 (2)	0.040 (2)	0.032 (2)	0.0001 (17)	0.0005 (17)	0.0083 (17)
C6	0.0206 (19)	0.046 (2)	0.042 (2)	-0.0046 (17)	-0.0008 (17)	0.0064 (19)
C7	0.024 (2)	0.068 (3)	0.039 (2)	0.002 (2)	0.0089 (18)	0.013 (2)
C8	0.0210 (17)	0.0270 (17)	0.0239 (16)	0.0006 (13)	0.0079 (14)	0.0019 (14)
C9	0.0271 (18)	0.0272 (18)	0.0274 (17)	-0.0001 (14)	0.0090 (15)	-0.0004 (14)
C10	0.035 (2)	0.038 (2)	0.0316 (19)	0.0022 (17)	0.0166 (17)	-0.0025 (17)
C11	0.032 (2)	0.045 (2)	0.032 (2)	0.0004 (17)	0.0166 (17)	0.0043 (17)
C12	0.029 (2)	0.034 (2)	0.035 (2)	-0.0032 (16)	0.0115 (17)	0.0061 (16)
C13	0.0233 (18)	0.0261 (18)	0.0287 (18)	0.0009 (14)	0.0055 (15)	0.0005 (14)

C14	0.028 (2)	0.0268 (19)	0.047 (2)	-0.0007 (15)	0.0095 (18)	-0.0039 (17)
C15	0.053 (3)	0.045 (3)	0.045 (3)	0.008 (2)	0.007 (2)	-0.014 (2)
C16	0.050 (3)	0.031 (2)	0.067 (3)	0.009 (2)	0.008 (2)	0.003 (2)
C17	0.041 (2)	0.0255 (19)	0.048 (2)	-0.0048 (17)	0.022 (2)	-0.0056 (17)
C18	0.064 (3)	0.030 (2)	0.049 (3)	0.004 (2)	0.021 (2)	0.0003 (19)
C19	0.060 (3)	0.040 (3)	0.065 (3)	-0.007 (2)	0.004 (3)	-0.015 (2)
C20	0.0207 (17)	0.0280 (18)	0.0252 (17)	-0.0020 (14)	0.0055 (14)	0.0026 (14)
C21	0.0196 (17)	0.0276 (18)	0.0286 (18)	0.0003 (14)	0.0035 (14)	0.0023 (14)
C22	0.0273 (19)	0.0303 (19)	0.043 (2)	0.0059 (16)	0.0042 (17)	0.0124 (18)
C23	0.034 (2)	0.044 (3)	0.052 (3)	0.0031 (19)	-0.002 (2)	0.017 (2)
C24	0.030 (2)	0.045 (3)	0.063 (3)	-0.0040 (19)	-0.009 (2)	0.015 (2)
C25	0.0267 (19)	0.031 (2)	0.041 (2)	-0.0055 (16)	-0.0019 (17)	0.0003 (18)
C26	0.0212 (17)	0.0279 (18)	0.0265 (17)	0.0004 (14)	0.0047 (14)	0.0033 (14)
C27	0.0227 (18)	0.0207 (17)	0.0289 (18)	0.0000 (13)	0.0003 (14)	0.0009 (14)
C28	0.0244 (18)	0.0277 (18)	0.0293 (18)	-0.0017 (14)	0.0042 (15)	0.0024 (15)
C29	0.028 (2)	0.030 (2)	0.041 (2)	-0.0034 (16)	0.0091 (17)	0.0051 (17)
C30	0.040 (2)	0.0227 (19)	0.053 (3)	-0.0039 (17)	0.011 (2)	0.0019 (18)
C31	0.039 (2)	0.0249 (19)	0.044 (2)	0.0022 (16)	0.0118 (19)	-0.0048 (17)
C32	0.030 (2)	0.0285 (19)	0.0323 (19)	0.0032 (15)	0.0081 (16)	0.0008 (15)
C33	0.051 (3)	0.032 (2)	0.040 (2)	0.0087 (19)	0.021 (2)	0.0026 (18)
C34	0.046 (3)	0.051 (3)	0.051 (3)	0.002 (2)	0.024 (2)	0.004 (2)
C35	0.063 (3)	0.068 (3)	0.039 (3)	0.011 (3)	0.018 (2)	0.000 (2)
C36	0.035 (2)	0.032 (2)	0.035 (2)	-0.0015 (16)	0.0134 (18)	-0.0006 (16)
C37	0.050 (3)	0.059 (3)	0.037 (2)	0.004 (2)	0.012 (2)	-0.003 (2)
C38	0.037 (3)	0.066 (3)	0.072 (4)	0.000 (2)	0.026 (3)	-0.014 (3)
Cl1	0.0377 (6)	0.0514 (7)	0.0582 (7)	0.0028 (5)	0.0082 (5)	0.0166 (6)
O1	0.094 (4)	0.063 (3)	0.170 (6)	-0.009 (3)	0.056 (4)	-0.025 (3)
O2	0.154 (6)	0.319 (11)	0.117 (5)	-0.098 (7)	0.009 (5)	0.105 (6)
O3	0.098 (4)	0.166 (6)	0.085 (4)	0.005 (4)	-0.032 (3)	0.009 (4)
O4	0.069 (4)	0.107 (5)	0.441 (14)	0.008 (3)	0.055 (6)	-0.132 (7)
Cl2	0.0872 (13)	0.0713 (11)	0.1349 (18)	0.0189 (9)	0.0251 (12)	-0.0066 (11)

Cl3	0.1039 (15)	0.0787 (12)	0.1099 (15)	-0.0136 (11)	-0.0004 (12)	0.0244 (11)
C39	0.062 (4)	0.109 (6)	0.160 (8)	-0.007 (4)	0.031 (5)	0.057 (6)

Geometric parameters (Å, °) for (mo_240422160078)

Au1—C1	2.016 (4)	C19—H19B	0.9800
Au1—C20	2.006 (3)	C19—H19C	0.9800
S1—C1	1.699 (4)	C21—C22	1.499 (5)
S1—C2	1.724 (4)	C21—C26	1.351 (5)
S2—C20	1.706 (4)	C22—H22A	0.9900
S2—C21	1.724 (4)	C22—H22B	0.9900
N1—C1	1.339 (4)	C22—C23	1.522 (6)
N1—C3	1.390 (4)	C23—H23A	0.9900
N1—C8	1.451 (4)	C23—H23B	0.9900
N2—C20	1.341 (4)	C23—C24	1.503 (6)
N2—C26	1.396 (4)	C24—H24A	0.9900
N2—C27	1.459 (4)	C24—H24B	0.9900
C2—C3	1.352 (5)	C24—C25	1.541 (6)
C2—C7	1.500 (5)	C25—H25A	0.9900
C3—C4	1.501 (5)	C25—H25B	0.9900
C4—H4A	0.9900	C25—C26	1.494 (5)
C4—H4B	0.9900	C27—C28	1.398 (5)
C4—C5	1.528 (5)	C27—C32	1.399 (5)
C5—H5A	0.9900	C28—C29	1.390 (5)
C5—H5B	0.9900	C28—C36	1.517 (5)
C5—C6	1.518 (6)	C29—H29	0.9500
C6—H6A	0.9900	C29—C30	1.381 (6)
C6—H6B	0.9900	C30—H30	0.9500
C6—C7	1.533 (6)	C30—C31	1.382 (6)
C7—H7A	0.9900	C31—H31	0.9500
C7—H7B	0.9900	C31—C32	1.395 (5)
C8—C9	1.401 (5)	C32—C33	1.516 (5)

C8—C13	1.395 (5)	C33—H33	1.0000
C9—C10	1.391 (5)	C33—C34	1.524 (6)
C9—C17	1.518 (5)	C33—C35	1.528 (6)
C10—H10	0.9500	C34—H34A	0.9800
C10—C11	1.379 (6)	C34—H34B	0.9800
C11—H11	0.9500	C34—H34C	0.9800
C11—C12	1.378 (6)	C35—H35A	0.9800
C12—H12	0.9500	C35—H35B	0.9800
C12—C13	1.396 (5)	C35—H35C	0.9800
C13—C14	1.514 (5)	C36—H36	1.0000
C14—H14	1.0000	C36—C37	1.530 (6)
C14—C15	1.526 (6)	C36—C38	1.532 (6)
C14—C16	1.529 (6)	C37—H37A	0.9800
C15—H15A	0.9800	C37—H37B	0.9800
C15—H15B	0.9800	C37—H37C	0.9800
C15—H15C	0.9800	C38—H38A	0.9800
C16—H16A	0.9800	C38—H38B	0.9800
C16—H16B	0.9800	C38—H38C	0.9800
C16—H16C	0.9800	C11—O1	1.404 (5)
C17—H17	1.0000	C11—O2	1.397 (7)
C17—C18	1.521 (6)	C11—O3	1.375 (5)
C17—C19	1.530 (6)	C11—O4	1.325 (5)
C18—H18A	0.9800	C12—C39	1.717 (7)
C18—H18B	0.9800	C13—C39	1.718 (7)
C18—H18C	0.9800	C39—H39A	0.9900
C19—H19A	0.9800	C39—H39B	0.9900
C20—Au1—C1	174.01 (14)	N2—C20—S2	108.2 (3)
C1—S1—C2	93.37 (17)	C22—C21—S2	125.9 (3)
C20—S2—C21	93.77 (17)	C26—C21—S2	109.4 (3)
C1—N1—C3	116.0 (3)	C26—C21—C22	124.7 (3)

C1—N1—C8	121.8 (3)	C21—C22—H22A	109.8
C3—N1—C8	122.1 (3)	C21—C22—H22B	109.8
C20—N2—C26	116.3 (3)	C21—C22—C23	109.5 (3)
C20—N2—C27	121.0 (3)	H22A—C22—H22B	108.2
C26—N2—C27	122.7 (3)	C23—C22—H22A	109.8
S1—C1—Au1	123.41 (19)	C23—C22—H22B	109.8
N1—C1—Au1	127.4 (3)	C22—C23—H23A	109.1
N1—C1—S1	108.8 (3)	C22—C23—H23B	109.1
C3—C2—S1	109.5 (3)	H23A—C23—H23B	107.8
C3—C2—C7	124.1 (3)	C24—C23—C22	112.5 (4)
C7—C2—S1	126.4 (3)	C24—C23—H23A	109.1
N1—C3—C4	123.0 (3)	C24—C23—H23B	109.1
C2—C3—N1	112.3 (3)	C23—C24—H24A	109.1
C2—C3—C4	124.7 (3)	C23—C24—H24B	109.1
C3—C4—H4A	109.8	C23—C24—C25	112.6 (4)
C3—C4—H4B	109.8	H24A—C24—H24B	107.8
C3—C4—C5	109.5 (3)	C25—C24—H24A	109.1
H4A—C4—H4B	108.2	C25—C24—H24B	109.1
C5—C4—H4A	109.8	C24—C25—H25A	109.9
C5—C4—H4B	109.8	C24—C25—H25B	109.9
C4—C5—H5A	109.3	H25A—C25—H25B	108.3
C4—C5—H5B	109.3	C26—C25—C24	109.1 (3)
H5A—C5—H5B	108.0	C26—C25—H25A	109.9
C6—C5—C4	111.6 (3)	C26—C25—H25B	109.9
C6—C5—H5A	109.3	N2—C26—C25	123.2 (3)
C6—C5—H5B	109.3	C21—C26—N2	112.3 (3)
C5—C6—H6A	109.3	C21—C26—C25	124.5 (3)
C5—C6—H6B	109.3	C28—C27—N2	117.6 (3)
C5—C6—C7	111.6 (3)	C28—C27—C32	123.7 (3)
H6A—C6—H6B	108.0	C32—C27—N2	118.7 (3)
C7—C6—H6A	109.3	C27—C28—C36	122.8 (3)

C7—C6—H6B	109.3	C29—C28—C27	116.8 (4)
C2—C7—C6	109.1 (3)	C29—C28—C36	120.4 (3)
C2—C7—H7A	109.9	C28—C29—H29	119.4
C2—C7—H7B	109.9	C30—C29—C28	121.2 (4)
C6—C7—H7A	109.9	C30—C29—H29	119.4
C6—C7—H7B	109.9	C29—C30—H30	119.7
H7A—C7—H7B	108.3	C29—C30—C31	120.5 (4)
C9—C8—N1	117.8 (3)	C31—C30—H30	119.7
C13—C8—N1	118.6 (3)	C30—C31—H31	119.5
C13—C8—C9	123.6 (3)	C30—C31—C32	121.1 (4)
C8—C9—C17	123.3 (3)	C32—C31—H31	119.5
C10—C9—C8	116.7 (3)	C27—C32—C33	123.1 (3)
C10—C9—C17	119.9 (3)	C31—C32—C27	116.7 (4)
C9—C10—H10	119.5	C31—C32—C33	120.3 (4)
C11—C10—C9	121.0 (4)	C32—C33—H33	108.2
C11—C10—H10	119.5	C32—C33—C34	110.5 (3)
C10—C11—H11	119.5	C32—C33—C35	111.4 (4)
C12—C11—C10	120.9 (4)	C34—C33—H33	108.2
C12—C11—H11	119.5	C34—C33—C35	110.2 (4)
C11—C12—H12	119.6	C35—C33—H33	108.2
C11—C12—C13	120.7 (4)	C33—C34—H34A	109.5
C13—C12—H12	119.6	C33—C34—H34B	109.5
C8—C13—C12	116.9 (3)	C33—C34—H34C	109.5
C8—C13—C14	122.3 (3)	H34A—C34—H34B	109.5
C12—C13—C14	120.7 (3)	H34A—C34—H34C	109.5
C13—C14—H14	108.2	H34B—C34—H34C	109.5
C13—C14—C15	109.6 (3)	C33—C35—H35A	109.5
C13—C14—C16	111.9 (4)	C33—C35—H35B	109.5
C15—C14—H14	108.2	C33—C35—H35C	109.5
C15—C14—C16	110.7 (4)	H35A—C35—H35B	109.5
C16—C14—H14	108.2	H35A—C35—H35C	109.5

C14—C15—H15A	109.5	H35B—C35—H35C	109.5
C14—C15—H15B	109.5	C28—C36—H36	108.0
C14—C15—H15C	109.5	C28—C36—C37	110.2 (3)
H15A—C15—H15B	109.5	C28—C36—C38	112.0 (3)
H15A—C15—H15C	109.5	C37—C36—H36	108.0
H15B—C15—H15C	109.5	C37—C36—C38	110.4 (4)
C14—C16—H16A	109.5	C38—C36—H36	108.0
C14—C16—H16B	109.5	C36—C37—H37A	109.5
C14—C16—H16C	109.5	C36—C37—H37B	109.5
H16A—C16—H16B	109.5	C36—C37—H37C	109.5
H16A—C16—H16C	109.5	H37A—C37—H37B	109.5
H16B—C16—H16C	109.5	H37A—C37—H37C	109.5
C9—C17—H17	107.7	H37B—C37—H37C	109.5
C9—C17—C18	111.0 (4)	C36—C38—H38A	109.5
C9—C17—C19	111.4 (4)	C36—C38—H38B	109.5
C18—C17—H17	107.7	C36—C38—H38C	109.5
C18—C17—C19	111.1 (4)	H38A—C38—H38B	109.5
C19—C17—H17	107.7	H38A—C38—H38C	109.5
C17—C18—H18A	109.5	H38B—C38—H38C	109.5
C17—C18—H18B	109.5	O2—C11—O1	102.7 (5)
C17—C18—H18C	109.5	O3—C11—O1	112.6 (4)
H18A—C18—H18B	109.5	O3—C11—O2	104.4 (4)
H18A—C18—H18C	109.5	O4—C11—O1	110.4 (4)
H18B—C18—H18C	109.5	O4—C11—O2	107.4 (6)
C17—C19—H19A	109.5	O4—C11—O3	117.9 (5)
C17—C19—H19B	109.5	C12—C39—C13	113.2 (4)
C17—C19—H19C	109.5	C12—C39—H39A	108.9
H19A—C19—H19B	109.5	C12—C39—H39B	108.9
H19A—C19—H19C	109.5	C13—C39—H39A	108.9
H19B—C19—H19C	109.5	C13—C39—H39B	108.9
S2—C20—Au1	120.80 (19)	H39A—C39—H39B	107.7

N2—C20—Au1	131.0 (3)		
S1—C2—C3—N1	-1.2 (4)	C11—C12—C13—C8	0.1 (6)
S1—C2—C3—C4	-180.0 (3)	C11—C12—C13— C14	-177.3 (4)
S1—C2—C7—C6	163.6 (3)	C12—C13—C14— C15	74.2 (5)
S2—C21—C22—C23	165.7 (3)	C12—C13—C14— C16	-49.0 (5)
S2—C21—C26—N2	-0.2 (4)	C13—C8—C9—C10	-0.1 (5)
S2—C21—C26—C25	179.6 (3)	C13—C8—C9—C17	-179.5 (4)
N1—C3—C4—C5	167.5 (3)	C17—C9—C10—C11	179.3 (4)
N1—C8—C9—C10	-179.1 (3)	C20—S2—C21—C22	-178.9 (3)
N1—C8—C9—C17	1.4 (5)	C20—S2—C21—C26	0.8 (3)
N1—C8—C13—C12	179.2 (3)	C20—N2—C26—C21	-0.7 (5)
N1—C8—C13—C14	-3.5 (5)	C20—N2—C26—C25	179.4 (3)
N2—C27—C28—C29	-176.1 (3)	C20—N2—C27—C28	89.0 (4)
N2—C27—C28—C36	2.1 (5)	C20—N2—C27—C32	-89.5 (4)
N2—C27—C32—C31	177.9 (3)	C21—S2—C20—Au1	176.3 (2)
N2—C27—C32—C33	-1.4 (6)	C21—S2—C20—N2	-1.2 (3)
C1—S1—C2—C3	0.4 (3)	C21—C22—C23— C24	44.0 (5)
C1—S1—C2—C7	-179.3 (4)	C22—C21—C26—N2	179.5 (3)
C1—N1—C3—C2	1.7 (5)	C22—C21—C26— C25	-0.7 (6)
C1—N1—C3—C4	-179.5 (3)	C22—C23—C24— C25	-62.1 (6)
C1—N1—C8—C9	-85.8 (4)	C23—C24—C25— C26	44.0 (6)
C1—N1—C8—C13	95.1 (4)	C24—C25—C26—N2	165.9 (4)
C2—S1—C1—Au1	173.1 (2)	C24—C25—C26— C21	-13.9 (6)
C2—S1—C1—N1	0.5 (3)	C26—N2—C20—Au1	-175.8 (3)

C2—C3—C4—C5	-13.9 (5)	C26—N2—C20—S2	1.3 (4)
C3—N1—C1—Au1	-173.6 (3)	C26—N2—C27—C28	-88.7 (4)
C3—N1—C1—S1	-1.3 (4)	C26—N2—C27—C32	92.7 (4)
C3—N1—C8—C9	92.0 (4)	C26—C21—C22— C23	-13.9 (6)
C3—N1—C8—C13	-87.1 (4)	C27—N2—C20—Au1	6.3 (5)
C3—C2—C7—C6	-16.1 (6)	C27—N2—C20—S2	-176.6 (3)
C3—C4—C5—C6	44.7 (5)	C27—N2—C26—C21	177.1 (3)
C4—C5—C6—C7	-64.3 (5)	C27—N2—C26—C25	-2.8 (5)
C5—C6—C7—C2	46.9 (5)	C27—C28—C29— C30	-2.2 (6)
C7—C2—C3—N1	178.5 (4)	C27—C28—C36— C37	-109.4 (4)
C7—C2—C3—C4	-0.2 (7)	C27—C28—C36— C38	127.3 (4)
C8—N1—C1—Au1	4.4 (5)	C27—C32—C33— C34	113.7 (4)
C8—N1—C1—S1	176.6 (3)	C27—C32—C33— C35	-123.4 (4)
C8—N1—C3—C2	-176.2 (3)	C28—C27—C32— C31	-0.6 (6)
C8—N1—C3—C4	2.5 (5)	C28—C27—C32— C33	-179.9 (4)
C8—C9—C10—C11	-0.2 (6)	C28—C29—C30— C31	0.4 (6)
C8—C9—C17—C18	116.5 (4)	C29—C28—C36— C37	68.8 (5)
C8—C9—C17—C19	-119.1 (4)	C29—C28—C36— C38	-54.5 (5)
C8—C13—C14—C15	-103.0 (4)	C29—C30—C31— C32	1.5 (7)
C8—C13—C14—C16	133.8 (4)	C30—C31—C32— C27	-1.4 (6)
C9—C8—C13—C12	0.1 (5)	C30—C31—C32— C33	177.9 (4)

C9—C8—C13—C14	177.4 (4)	C31—C32—C33— C34	-65.6 (5)
C9—C10—C11—C12	0.3 (6)	C31—C32—C33— C35	57.4 (5)
C10—C9—C17—C18	-62.9 (5)	C32—C27—C28— C29	2.4 (6)
C10—C9—C17—C19	61.4 (5)	C32—C27—C28— C36	-179.4 (4)
C10—C11—C12— C13	-0.3 (6)	C36—C28—C29— C30	179.5 (4)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Crystal structure of 2c.

Single crystal of complex **2c** were grown by slow evaporation in a mixture of DCM and n-hexane (DCM: n-hexane = 1:3) at low temperature.

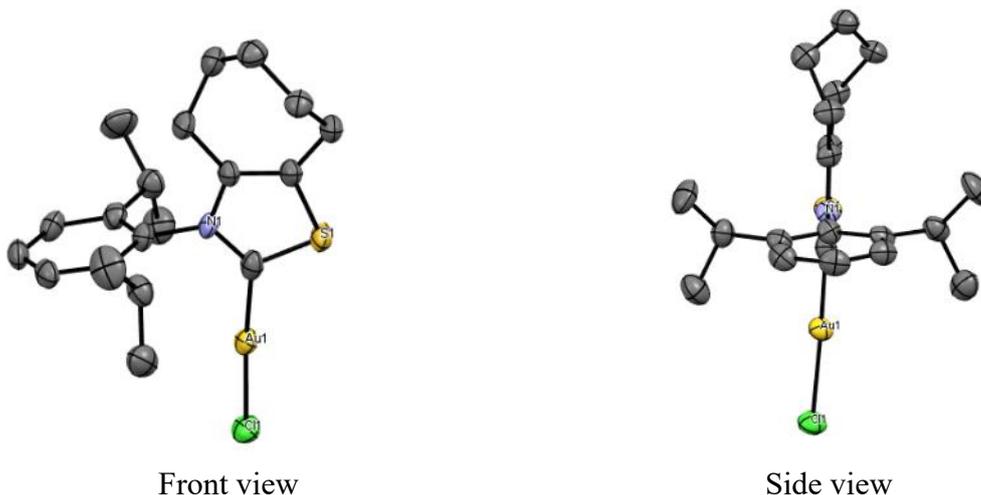


Chart S5. Crystal structure of **2c** (50% ellipsoids). (Crystallographic data has been deposited with the Cambridge Crystallographic Data Center as supplementary publication no. 2503057)

Table S7. Crystal Data and Structure Refinement Summary for **2c**.

Crystal data

$C_{20}H_{27}AuClNS$	$F(000) = 1064$
$M_r = 545.90$	$D_x = 1.801 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/n$	Cu $K\alpha$ radiation, $\lambda = 1.54184 \text{ \AA}$
$a = 8.8827 (4) \text{ \AA}$	Cell parameters from 9216 reflections
$b = 18.3827 (8) \text{ \AA}$	$\theta = 4.3\text{--}68.5^\circ$
$c = 12.3960 (6) \text{ \AA}$	$\mu = 15.92 \text{ mm}^{-1}$
$\beta = 96.015 (2)^\circ$	$T = 193 \text{ K}$
$V = 2012.97 (16) \text{ \AA}^3$	Block, colourless
$Z = 4$	

Data collection

Bruker diffractometer	$R_{\text{int}} = 0.053$
Absorption correction: multi-scan <i>SADABS2016/2</i> (Bruker,2016/2) was used for absorption correction. $wR2(\text{int})$ was 0.1386 before and 0.0753 after correction. The Ratio of minimum to maximum transmission is 0.6043. The $\lambda/2$ correction factor is Not present.	$\theta_{\text{max}} = 68.7^\circ$, $\theta_{\text{min}} = 4.3^\circ$
$T_{\text{min}} = 0.455$, $T_{\text{max}} = 0.753$	$h = -10 \rightarrow 10$
17056 measured reflections	$k = -22 \rightarrow 21$
3655 independent reflections	$l = -14 \rightarrow 14$
3063 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.047$	$w = 1/[\sigma^2(F_o^2) + (0.0956P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.132$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.05$	$\Delta_{\text{max}} = 1.72 \text{ e \AA}^{-3}$
3655 reflections	$\Delta_{\text{min}} = -2.38 \text{ e \AA}^{-3}$

222 parameters	Extinction correction: <i>SHELXL2018/3</i> (Sheldrick 2018), $F_c^* = kF_c [1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
0 restraints	Extinction coefficient: 0.00179 (14)
Primary atom site location: dual	

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2) for (cu_zzj_241125105044_aucI_0m)

	<i>x</i>	<i>y</i>	<i>z</i>	U_{iso}^*/U_{eq}
Au1	0.56941 (3)	0.32333 (2)	0.76813 (2)	0.03328 (18)
Cl1	0.68206 (18)	0.21307 (9)	0.74712 (16)	0.0431 (4)
S1	0.59347 (17)	0.48741 (9)	0.85523 (14)	0.0367 (4)
N1	0.3514 (5)	0.4506 (3)	0.7533 (4)	0.0291 (11)
C1	0.4872 (7)	0.4214 (4)	0.7871 (5)	0.0348 (14)
C2	0.4548 (7)	0.5530 (4)	0.8348 (6)	0.0348 (14)
C3	0.3309 (7)	0.5241 (3)	0.7778 (6)	0.0330 (14)
C4	0.1846 (7)	0.5629 (4)	0.7403 (6)	0.0408 (16)
H4A	0.110270	0.553309	0.792733	0.049*
H4B	0.143124	0.542689	0.669297	0.049*
C5	0.2040 (8)	0.6452 (4)	0.7290 (6)	0.0419 (16)
H5A	0.295168	0.654523	0.691519	0.050*
H5B	0.115675	0.664587	0.682492	0.050*
C6	0.2192 (9)	0.6867 (4)	0.8352 (7)	0.0438 (18)
H6A	0.248493	0.737326	0.820206	0.053*
H6B	0.118379	0.688434	0.862404	0.053*
C7	0.3311 (8)	0.6570 (4)	0.9245 (6)	0.0386 (15)
H7A	0.281902	0.617477	0.962246	0.046*
H7B	0.357937	0.696094	0.977958	0.046*
C8	0.4779 (7)	0.6272 (4)	0.8842 (6)	0.0393 (16)
H8A	0.512276	0.660935	0.829613	0.047*
H8B	0.558077	0.624695	0.945889	0.047*
C9	0.2299 (7)	0.4075 (4)	0.6966 (6)	0.0336 (14)

C10	0.2184 (7)	0.4022 (4)	0.5836 (6)	0.0348 (14)
C11	0.0988 (8)	0.3629 (4)	0.5329 (6)	0.0404 (16)
H11	0.089703	0.356988	0.456389	0.048*
C12	-0.0091 (9)	0.3317 (4)	0.5930 (7)	0.0411 (18)
H12	-0.092069	0.305704	0.556976	0.049*
C13	0.0040 (8)	0.3386 (4)	0.7041 (7)	0.0398 (16)
H13	-0.070030	0.316721	0.743705	0.048*
C14	0.1222 (7)	0.3765 (4)	0.7594 (6)	0.0333 (14)
C15	0.1378 (8)	0.3797 (4)	0.8819 (6)	0.0415 (16)
H15	0.220715	0.414811	0.905583	0.050*
C16	0.1839 (11)	0.3048 (5)	0.9294 (7)	0.053 (2)
H16A	0.104336	0.269274	0.906975	0.080*
H16B	0.197720	0.307818	1.008703	0.080*
H16C	0.278885	0.289399	0.902658	0.080*
C17	-0.0084 (9)	0.4072 (5)	0.9251 (8)	0.065 (3)
H17A	-0.039202	0.453303	0.889714	0.098*
H17B	0.009907	0.414702	1.003699	0.098*
H17C	-0.088956	0.371114	0.909528	0.098*
C18	0.3323 (8)	0.4377 (4)	0.5175 (6)	0.0413 (16)
H18	0.397390	0.471012	0.566116	0.050*
C19	0.4338 (9)	0.3802 (5)	0.4729 (7)	0.056 (2)
H19A	0.484492	0.351845	0.533037	0.084*
H19B	0.509985	0.404228	0.433450	0.084*
H19C	0.372094	0.347766	0.423529	0.084*
C20	0.2522 (10)	0.4827 (5)	0.4248 (7)	0.061 (2)
H20A	0.197877	0.450181	0.371508	0.091*
H20B	0.327311	0.510816	0.389810	0.091*
H20C	0.180185	0.516023	0.453693	0.091*

Atomic displacement parameters (\AA^2) for (cu_zzj_241125105044_auc1_0m)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
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Au1	0.0218 (2)	0.0367 (2)	0.0415 (2)	0.00198 (9)	0.00378 (13)	0.00044 (10)
Cl1	0.0314 (8)	0.0408 (9)	0.0577 (11)	0.0071 (7)	0.0077 (7)	0.0003 (8)
S1	0.0218 (7)	0.0420 (9)	0.0453 (10)	-0.0003 (6)	-0.0015 (6)	-0.0028 (7)
N1	0.016 (2)	0.035 (3)	0.035 (3)	0.001 (2)	-0.001 (2)	0.001 (2)
C1	0.024 (3)	0.047 (4)	0.034 (3)	-0.006 (3)	0.005 (3)	0.002 (3)
C2	0.024 (3)	0.036 (3)	0.044 (4)	-0.004 (3)	0.004 (3)	0.002 (3)
C3	0.023 (3)	0.032 (3)	0.044 (4)	-0.004 (3)	0.003 (3)	0.001 (3)
C4	0.023 (3)	0.041 (4)	0.057 (5)	0.000 (3)	-0.003 (3)	-0.001 (3)
C5	0.029 (3)	0.048 (4)	0.047 (4)	0.001 (3)	-0.003 (3)	0.002 (3)
C6	0.045 (4)	0.040 (4)	0.047 (5)	0.006 (3)	0.004 (4)	-0.001 (3)
C7	0.038 (4)	0.036 (3)	0.042 (4)	0.005 (3)	0.005 (3)	-0.007 (3)
C8	0.027 (3)	0.038 (4)	0.052 (4)	-0.004 (3)	-0.002 (3)	0.001 (3)
C9	0.020 (3)	0.041 (4)	0.039 (4)	-0.002 (3)	0.002 (2)	-0.001 (3)
C10	0.024 (3)	0.039 (4)	0.041 (4)	0.003 (3)	0.002 (3)	-0.002 (3)
C11	0.032 (3)	0.051 (4)	0.036 (4)	0.004 (3)	-0.007 (3)	-0.005 (3)
C12	0.028 (4)	0.041 (4)	0.052 (5)	-0.006 (3)	-0.006 (3)	-0.008 (3)
C13	0.024 (3)	0.038 (3)	0.058 (5)	-0.004 (3)	0.008 (3)	-0.001 (3)
C14	0.020 (3)	0.034 (3)	0.048 (4)	0.001 (2)	0.009 (3)	-0.005 (3)
C15	0.037 (4)	0.041 (4)	0.048 (4)	-0.005 (3)	0.012 (3)	-0.009 (3)
C16	0.061 (5)	0.053 (4)	0.044 (5)	-0.004 (4)	0.000 (4)	-0.001 (4)
C17	0.051 (5)	0.081 (6)	0.069 (6)	-0.004 (5)	0.033 (4)	-0.021 (5)
C18	0.036 (3)	0.047 (4)	0.041 (4)	-0.006 (3)	0.007 (3)	0.003 (3)
C19	0.046 (4)	0.066 (5)	0.059 (5)	0.001 (4)	0.017 (4)	-0.008 (4)
C20	0.057 (5)	0.071 (6)	0.054 (5)	0.004 (4)	0.005 (4)	0.032 (4)

Geometric parameters (Å, °) for (cu_zzj_241125105044_auc1_0m)

Au1—Cl1	2.2874 (16)	C10—C18	1.514 (9)
Au1—C1	1.969 (7)	C11—H11	0.9500
S1—C1	1.705 (7)	C11—C12	1.397 (11)
S1—C2	1.723 (7)	C12—H12	0.9500
N1—C1	1.346 (8)	C12—C13	1.375 (12)

N1—C3	1.401 (8)	C13—H13	0.9500
N1—C9	1.459 (8)	C13—C14	1.380 (10)
C2—C3	1.352 (9)	C14—C15	1.512 (10)
C2—C8	1.500 (9)	C15—H15	1.0000
C3—C4	1.512 (9)	C15—C16	1.537 (11)
C4—H4A	0.9900	C15—C17	1.541 (9)
C4—H4B	0.9900	C16—H16A	0.9800
C4—C5	1.531 (10)	C16—H16B	0.9800
C5—H5A	0.9900	C16—H16C	0.9800
C5—H5B	0.9900	C17—H17A	0.9800
C5—C6	1.514 (11)	C17—H17B	0.9800
C6—H6A	0.9900	C17—H17C	0.9800
C6—H6B	0.9900	C18—H18	1.0000
C6—C7	1.510 (11)	C18—C19	1.530 (10)
C7—H7A	0.9900	C18—C20	1.530 (11)
C7—H7B	0.9900	C19—H19A	0.9800
C7—C8	1.545 (9)	C19—H19B	0.9800
C8—H8A	0.9900	C19—H19C	0.9800
C8—H8B	0.9900	C20—H20A	0.9800
C9—C10	1.397 (9)	C20—H20B	0.9800
C9—C14	1.415 (9)	C20—H20C	0.9800
C10—C11	1.381 (9)		
C1—Au1—C11	175.83 (18)	C11—C10—C18	120.3 (7)
C1—S1—C2	94.3 (3)	C10—C11—H11	119.7
C1—N1—C3	116.7 (5)	C10—C11—C12	120.7 (7)
C1—N1—C9	121.8 (5)	C12—C11—H11	119.7
C3—N1—C9	121.5 (5)	C11—C12—H12	119.8
S1—C1—Au1	121.2 (4)	C13—C12—C11	120.4 (7)
N1—C1—Au1	131.2 (5)	C13—C12—H12	119.8
N1—C1—S1	107.6 (5)	C12—C13—H13	119.2

C3—C2—S1	109.4 (5)	C12—C13—C14	121.6 (7)
C3—C2—C8	129.7 (6)	C14—C13—H13	119.2
C8—C2—S1	120.7 (5)	C9—C14—C15	122.7 (6)
N1—C3—C4	121.0 (6)	C13—C14—C9	117.0 (7)
C2—C3—N1	112.0 (6)	C13—C14—C15	120.2 (6)
C2—C3—C4	127.0 (6)	C14—C15—H15	107.9
C3—C4—H4A	109.0	C14—C15—C16	110.0 (6)
C3—C4—H4B	109.0	C14—C15—C17	111.7 (7)
C3—C4—C5	113.1 (5)	C16—C15—H15	107.9
H4A—C4—H4B	107.8	C16—C15—C17	111.2 (7)
C5—C4—H4A	109.0	C17—C15—H15	107.9
C5—C4—H4B	109.0	C15—C16—H16A	109.5
C4—C5—H5A	108.6	C15—C16—H16B	109.5
C4—C5—H5B	108.6	C15—C16—H16C	109.5
H5A—C5—H5B	107.6	H16A—C16—H16B	109.5
C6—C5—C4	114.7 (7)	H16A—C16—H16C	109.5
C6—C5—H5A	108.6	H16B—C16—H16C	109.5
C6—C5—H5B	108.6	C15—C17—H17A	109.5
C5—C6—H6A	108.2	C15—C17—H17B	109.5
C5—C6—H6B	108.2	C15—C17—H17C	109.5
H6A—C6—H6B	107.3	H17A—C17—H17B	109.5
C7—C6—C5	116.6 (6)	H17A—C17—H17C	109.5
C7—C6—H6A	108.2	H17B—C17—H17C	109.5
C7—C6—H6B	108.2	C10—C18—H18	108.4
C6—C7—H7A	108.8	C10—C18—C19	110.5 (6)
C6—C7—H7B	108.8	C10—C18—C20	110.8 (6)
C6—C7—C8	113.8 (6)	C19—C18—H18	108.4
H7A—C7—H7B	107.7	C20—C18—H18	108.4
C8—C7—H7A	108.8	C20—C18—C19	110.3 (7)
C8—C7—H7B	108.8	C18—C19—H19A	109.5
C2—C8—C7	111.7 (6)	C18—C19—H19B	109.5

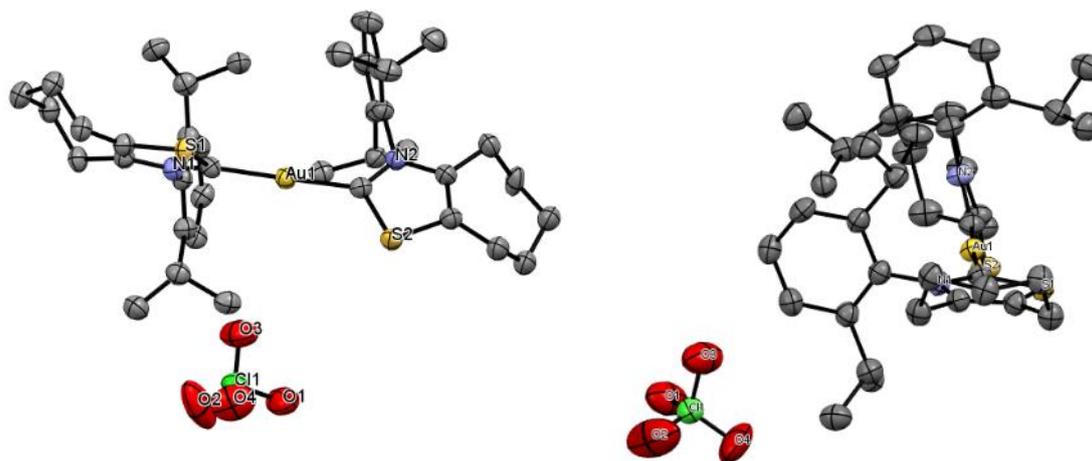
C2—C8—H8A	109.3	C18—C19—H19C	109.5
C2—C8—H8B	109.3	H19A—C19—H19B	109.5
C7—C8—H8A	109.3	H19A—C19—H19C	109.5
C7—C8—H8B	109.3	H19B—C19—H19C	109.5
H8A—C8—H8B	107.9	C18—C20—H20A	109.5
C10—C9—N1	119.5 (5)	C18—C20—H20B	109.5
C10—C9—C14	122.7 (6)	C18—C20—H20C	109.5
C14—C9—N1	117.6 (6)	H20A—C20—H20B	109.5
C9—C10—C18	122.0 (6)	H20A—C20—H20C	109.5
C11—C10—C9	117.7 (6)	H20B—C20—H20C	109.5
S1—C2—C3—N1	0.3 (7)	C6—C7—C8—C2	-78.3 (8)
S1—C2—C3—C4	-178.6 (6)	C8—C2—C3—N1	-175.1 (7)
S1—C2—C8—C7	-141.6 (5)	C8—C2—C3—C4	5.9 (12)
N1—C3—C4—C5	-154.7 (6)	C9—N1—C1—Au1	3.8 (9)
N1—C9—C10—C11	-177.8 (6)	C9—N1—C1—S1	-176.8 (5)
N1—C9—C10—C18	2.3 (9)	C9—N1—C3—C2	177.1 (6)
N1—C9—C14—C13	177.1 (6)	C9—N1—C3—C4	-3.9 (9)
N1—C9—C14—C15	-6.5 (9)	C9—C10—C11—C12	2.0 (10)
C1—S1—C2—C3	0.4 (5)	C9—C10—C18—C19	107.7 (8)
C1—S1—C2—C8	176.3 (6)	C9—C10—C18—C20	-129.7 (8)
C1—N1—C3—C2	-1.2 (8)	C9—C14—C15—C16	-106.1 (8)
C1—N1—C3—C4	177.9 (6)	C9—C14—C15—C17	129.9 (7)
C1—N1—C9—C10	-89.4 (8)	C10—C9—C14—C13	1.2 (10)
C1—N1—C9—C14	94.5 (7)	C10—C9—C14—C15	177.5 (6)
C2—S1—C1—Au1	178.4 (4)	C10—C11—C12— C13	-1.3 (11)
C2—S1—C1—N1	-1.0 (5)	C11—C10—C18— C19	-72.2 (8)
C2—C3—C4—C5	24.2 (10)	C11—C10—C18— C20	50.4 (9)
C3—N1—C1—Au1	-177.9 (5)	C11—C12—C13—	0.5 (11)

		C14	
C3—N1—C1—S1	1.4 (7)	C12—C13—C14—C9	-0.4 (10)
C3—N1—C9—C10	92.4 (7)	C12—C13—C14—C15	-176.9 (7)
C3—N1—C9—C14	-83.7 (8)	C13—C14—C15—C16	70.1 (8)
C3—C2—C8—C7	33.4 (11)	C13—C14—C15—C17	-53.9 (9)
C3—C4—C5—C6	-76.8 (8)	C14—C9—C10—C11	-2.0 (10)
C4—C5—C6—C7	48.4 (9)	C14—C9—C10—C18	178.1 (6)
C5—C6—C7—C8	38.7 (10)	C18—C10—C11—C12	-178.1 (6)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Crystal structure of 3c.



Front view

Side view

Chart S6. Crystal structure of **3c** (50% ellipsoids). (Crystallographic data has been deposited with the Cambridge Crystallographic Data Center as supplementary publication no. 2503060)

Table S8. Crystal Data and Structure Refinement Summary for **3c**.

Crystal data

$C_{40}H_{54}AuN_2S_2ClO_4$	$F(000) = 1872$
$M_r = 923.39$	$D_x = 1.487 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/n$	Cu $K\alpha$ radiation, $\lambda = 1.54184 \text{ \AA}$
$a = 14.983 (4) \text{ \AA}$	Cell parameters from 364 reflections
$b = 14.190 (5) \text{ \AA}$	$\theta = 28.4\text{--}63.0^\circ$
$c = 19.781 (10) \text{ \AA}$	$\mu = 8.56 \text{ mm}^{-1}$
$\beta = 101.23 (2)^\circ$	$T = 193 \text{ K}$
$V = 4125 (3) \text{ \AA}^3$	Block, colourless
$Z = 4$	

Data collection

Bruker diffractometer	$R_{\text{int}} = 0.102$
Absorption correction: multi-scan <i>SADABS2016/2</i> (Bruker,2016/2) was used for absorption correction. $wR2(\text{int})$ was 0.1389 before and 0.0955 after correction. The Ratio of minimum to maximum transmission is 0.2129. The $\lambda/2$ correction factor is Not present.	$\theta_{\text{max}} = 69.0^\circ$, $\theta_{\text{min}} = 3.4^\circ$
$T_{\text{min}} = 0.023$, $T_{\text{max}} = 0.110$	$h = -18 \rightarrow 18$
38220 measured reflections	$k = -17 \rightarrow 17$
7594 independent reflections	$l = -23 \rightarrow 23$
4968 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Primary atom site location: dual
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.069$	H-atom parameters constrained
$wR(F^2) = 0.210$	$w = 1/[\sigma^2(F_o^2) + (0.0931P)^2 + 4.9274P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.08$	$(\Delta/\sigma)_{\text{max}} = 0.001$

7594 reflections	$\Delta\rho_{\max} = 1.89 \text{ e } \text{\AA}^{-3}$
459 parameters	$\Delta\rho_{\min} = -0.76 \text{ e } \text{\AA}^{-3}$
0 restraints	

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2) for (mo_240422160078)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Au1	0.39339 (2)	0.65386 (2)	0.65014 (2)	0.02388 (4)
S1	0.61194 (6)	0.63868 (7)	0.70855 (6)	0.0354 (2)
S2	0.26019 (6)	0.79819 (6)	0.54695 (6)	0.02809 (19)
N1	0.53588 (19)	0.60488 (18)	0.80502 (17)	0.0230 (6)
N2	0.20414 (19)	0.65083 (18)	0.52778 (17)	0.0240 (6)
C1	0.5154 (2)	0.6258 (2)	0.7284 (2)	0.0258 (7)
C2	0.6787 (2)	0.6146 (3)	0.8043 (2)	0.0307 (8)
C3	0.6266 (2)	0.5970 (2)	0.8484 (2)	0.0261 (7)
C4	0.6612 (3)	0.5733 (3)	0.9348 (2)	0.0321 (8)
H4A	0.627238	0.524229	0.943995	0.039*
H4B	0.652887	0.621126	0.967239	0.039*
C5	0.7605 (3)	0.5510 (3)	0.9592 (2)	0.0368 (9)
H5A	0.786803	0.549640	1.017938	0.044*
H5B	0.766954	0.493940	0.939071	0.044*
C6	0.8112 (3)	0.6145 (3)	0.9270 (3)	0.0392 (10)
H6A	0.875959	0.601241	0.948151	0.047*
H6B	0.802663	0.671845	0.945321	0.047*
C7	0.7791 (3)	0.6132 (3)	0.8359 (3)	0.0442 (11)
H7A	0.802858	0.663073	0.816186	0.053*
H7B	0.801290	0.561666	0.817357	0.053*
C8	0.4674 (2)	0.5940 (2)	0.8411 (2)	0.0239 (7)
C9	0.4383 (2)	0.6661 (2)	0.8708 (2)	0.0273 (7)
C10	0.3735 (3)	0.6539 (3)	0.9061 (2)	0.0335 (8)
H10	0.352020	0.701055	0.927141	0.040*
C11	0.3400 (3)	0.5744 (3)	0.9109 (2)	0.0351 (9)

H11	0.295528	0.567706	0.935018	0.042*
C12	0.3701 (3)	0.5047 (3)	0.8813 (2)	0.0326 (8)
H12	0.346308	0.450475	0.885433	0.039*
C13	0.4351 (2)	0.5128 (2)	0.8453 (2)	0.0269 (7)
C14	0.4651 (3)	0.4367 (2)	0.8095 (3)	0.0348 (9)
H14	0.520076	0.452776	0.797558	0.042*
C15	0.3923 (3)	0.4126 (3)	0.7315 (3)	0.0504 (12)
H15A	0.337692	0.396804	0.741978	0.076*
H15B	0.412811	0.364709	0.707522	0.076*
H15C	0.379772	0.460897	0.695062	0.076*
C16	0.4882 (3)	0.3617 (3)	0.8668 (3)	0.0524 (12)
H16A	0.531350	0.379656	0.917916	0.079*
H16B	0.514458	0.316410	0.844455	0.079*
H16C	0.433677	0.341024	0.874669	0.079*
C17	0.4733 (3)	0.7544 (2)	0.8654 (3)	0.0364 (9)
H17	0.519341	0.749706	0.839001	0.044*
C18	0.3988 (3)	0.8115 (3)	0.8144 (3)	0.0472 (11)
H18A	0.353136	0.818052	0.839526	0.071*
H18B	0.371672	0.786234	0.761647	0.071*
H18C	0.423691	0.866986	0.809244	0.071*
C19	0.5188 (4)	0.7925 (3)	0.9480 (3)	0.0590 (14)
H19A	0.542843	0.848366	0.942634	0.089*
H19B	0.567662	0.755523	0.978965	0.089*
H19C	0.474905	0.798164	0.975179	0.089*
C20	0.2771 (2)	0.6938 (2)	0.5715 (2)	0.0252 (7)
C21	0.1560 (2)	0.7814 (2)	0.4767 (2)	0.0265 (7)
C22	0.0964 (3)	0.8478 (3)	0.4256 (2)	0.0355 (9)
H22A	0.131928	0.885622	0.403755	0.043*
H22B	0.069692	0.882315	0.457983	0.043*
C23	0.0225 (3)	0.8058 (3)	0.3580 (3)	0.0478 (11)
H23A	-0.025051	0.847745	0.333294	0.057*

H23B	0.047388	0.786978	0.316992	0.057*
C24	-0.0178 (3)	0.7311 (3)	0.3853 (3)	0.0523 (13)
H24A	-0.067648	0.708468	0.339785	0.063*
H24B	-0.043054	0.750049	0.426097	0.063*
C25	0.0507 (3)	0.6601 (3)	0.4204 (3)	0.0366 (9)
H25A	0.026678	0.620077	0.450656	0.044*
H25B	0.062071	0.628641	0.377003	0.044*
C26	0.1359 (2)	0.6982 (2)	0.4741 (2)	0.0261 (7)
C27	0.1966 (2)	0.5601 (2)	0.5388 (2)	0.0263 (7)
C28	0.1590 (2)	0.5339 (2)	0.5952 (2)	0.0284 (8)
C29	0.1575 (3)	0.4475 (2)	0.6084 (2)	0.0339 (9)
H29	0.134435	0.427236	0.647534	0.041*
C30	0.1888 (3)	0.3904 (3)	0.5655 (3)	0.0395 (10)
H30	0.186766	0.331603	0.575354	0.047*
C31	0.2231 (3)	0.4183 (2)	0.5086 (3)	0.0366 (9)
H31	0.243082	0.378237	0.478729	0.044*
C32	0.2289 (3)	0.5044 (2)	0.4941 (2)	0.0309 (8)
C33	0.2696 (3)	0.5338 (3)	0.4333 (2)	0.0394 (10)
H33	0.263886	0.596705	0.428914	0.047*
C34	0.3689 (3)	0.5115 (3)	0.4602 (3)	0.0474 (11)
H34A	0.399821	0.537403	0.512040	0.071*
H34B	0.394669	0.532750	0.421246	0.071*
H34C	0.375949	0.449951	0.464540	0.071*
C35	0.2206 (4)	0.4959 (4)	0.3514 (3)	0.0568 (13)
H35A	0.227113	0.434265	0.354045	0.085*
H35B	0.246381	0.518415	0.312907	0.085*
H35C	0.156978	0.510725	0.334773	0.085*
C36	0.1236 (3)	0.5955 (3)	0.6424 (2)	0.0339 (8)
H36	0.123888	0.653310	0.619905	0.041*
C37	0.1851 (3)	0.5967 (3)	0.7294 (3)	0.0495 (11)
H37A	0.185250	0.540723	0.752900	0.074*

H37B	0.163416	0.638767	0.758660	0.074*
H37C	0.246125	0.611279	0.732202	0.074*
C38	0.0274 (3)	0.5747 (4)	0.6366 (3)	0.0566 (13)
H38A	-0.010288	0.569914	0.580579	0.085*
H38B	0.004264	0.619848	0.661799	0.085*
H38C	0.026550	0.521053	0.663727	0.085*
Cl1	0.80257 (8)	0.79170 (8)	0.65554 (8)	0.0512 (3)
O1	0.8347 (3)	0.8747 (3)	0.6725 (4)	0.1064 (18)
O2	0.7753 (5)	0.7722 (6)	0.7200 (4)	0.206 (5)
O3	0.7253 (4)	0.7872 (4)	0.5906 (3)	0.133 (2)
O4	0.8689 (4)	0.7396 (4)	0.6582 (6)	0.214 (5)
Cl2	1.13883 (14)	0.82571 (12)	0.70528 (14)	0.1011 (6)
Cl3	1.02859 (15)	0.95185 (13)	0.60283 (13)	0.1069 (7)
C39	1.0324 (5)	0.8640 (5)	0.6603 (6)	0.112 (3)
H39A	1.006420	0.878407	0.701800	0.134*
H39B	0.994847	0.819084	0.626584	0.134*

Atomic displacement parameters (\AA^2) for (mo_240422160078)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Au1	0.01963 (7)	0.02657 (7)	0.02309 (7)	0.00039 (5)	0.00422 (5)	0.00223 (6)
S1	0.0235 (5)	0.0576 (7)	0.0259 (4)	0.0058 (4)	0.0092 (4)	0.0096 (4)
S2	0.0252 (5)	0.0236 (4)	0.0314 (5)	-0.0034 (3)	0.0042 (4)	0.0021 (4)
N1	0.0204 (14)	0.0254 (15)	0.0238 (14)	0.0017 (11)	0.0081 (12)	0.0019 (12)
N2	0.0213 (14)	0.0218 (14)	0.0263 (14)	0.0017 (12)	0.0046 (12)	0.0023 (12)
C1	0.0207 (17)	0.0297 (18)	0.0260 (17)	0.0022 (14)	0.0065 (14)	0.0034 (14)
C2	0.0243 (19)	0.041 (2)	0.0269 (18)	0.0023 (16)	0.0084 (15)	0.0055 (16)
C3	0.0221 (18)	0.0278 (18)	0.0252 (17)	-0.0010 (14)	0.0039 (14)	0.0005 (14)
C4	0.028 (2)	0.040 (2)	0.0248 (18)	-0.0019 (16)	0.0051 (16)	0.0041 (16)
C5	0.031 (2)	0.040 (2)	0.032 (2)	0.0001 (17)	0.0005 (17)	0.0083 (17)
C6	0.0206 (19)	0.046 (2)	0.042 (2)	-0.0046 (17)	-0.0008 (17)	0.0064 (19)
C7	0.024 (2)	0.068 (3)	0.039 (2)	0.002 (2)	0.0089 (18)	0.013 (2)

C8	0.0210 (17)	0.0270 (17)	0.0239 (16)	0.0006 (13)	0.0079 (14)	0.0019 (14)
C9	0.0271 (18)	0.0272 (18)	0.0274 (17)	-0.0001 (14)	0.0090 (15)	-0.0004 (14)
C10	0.035 (2)	0.038 (2)	0.0316 (19)	0.0022 (17)	0.0166 (17)	-0.0025 (17)
C11	0.032 (2)	0.045 (2)	0.032 (2)	0.0004 (17)	0.0166 (17)	0.0043 (17)
C12	0.029 (2)	0.034 (2)	0.035 (2)	-0.0032 (16)	0.0115 (17)	0.0061 (16)
C13	0.0233 (18)	0.0261 (18)	0.0287 (18)	0.0009 (14)	0.0055 (15)	0.0005 (14)
C14	0.028 (2)	0.0268 (19)	0.047 (2)	-0.0007 (15)	0.0095 (18)	-0.0039 (17)
C15	0.053 (3)	0.045 (3)	0.045 (3)	0.008 (2)	0.007 (2)	-0.014 (2)
C16	0.050 (3)	0.031 (2)	0.067 (3)	0.009 (2)	0.008 (2)	0.003 (2)
C17	0.041 (2)	0.0255 (19)	0.048 (2)	-0.0048 (17)	0.022 (2)	-0.0056 (17)
C18	0.064 (3)	0.030 (2)	0.049 (3)	0.004 (2)	0.021 (2)	0.0003 (19)
C19	0.060 (3)	0.040 (3)	0.065 (3)	-0.007 (2)	0.004 (3)	-0.015 (2)
C20	0.0207 (17)	0.0280 (18)	0.0252 (17)	-0.0020 (14)	0.0055 (14)	0.0026 (14)
C21	0.0196 (17)	0.0276 (18)	0.0286 (18)	0.0003 (14)	0.0035 (14)	0.0023 (14)
C22	0.0273 (19)	0.0303 (19)	0.043 (2)	0.0059 (16)	0.0042 (17)	0.0124 (18)
C23	0.034 (2)	0.044 (3)	0.052 (3)	0.0031 (19)	-0.002 (2)	0.017 (2)
C24	0.030 (2)	0.045 (3)	0.063 (3)	-0.0040 (19)	-0.009 (2)	0.015 (2)
C25	0.0267 (19)	0.031 (2)	0.041 (2)	-0.0055 (16)	-0.0019 (17)	0.0003 (18)
C26	0.0212 (17)	0.0279 (18)	0.0265 (17)	0.0004 (14)	0.0047 (14)	0.0033 (14)
C27	0.0227 (18)	0.0207 (17)	0.0289 (18)	0.0000 (13)	0.0003 (14)	0.0009 (14)
C28	0.0244 (18)	0.0277 (18)	0.0293 (18)	-0.0017 (14)	0.0042 (15)	0.0024 (15)
C29	0.028 (2)	0.030 (2)	0.041 (2)	-0.0034 (16)	0.0091 (17)	0.0051 (17)
C30	0.040 (2)	0.0227 (19)	0.053 (3)	-0.0039 (17)	0.011 (2)	0.0019 (18)
C31	0.039 (2)	0.0249 (19)	0.044 (2)	0.0022 (16)	0.0118 (19)	-0.0048 (17)
C32	0.030 (2)	0.0285 (19)	0.0323 (19)	0.0032 (15)	0.0081 (16)	0.0008 (15)
C33	0.051 (3)	0.032 (2)	0.040 (2)	0.0087 (19)	0.021 (2)	0.0026 (18)
C34	0.046 (3)	0.051 (3)	0.051 (3)	0.002 (2)	0.024 (2)	0.004 (2)
C35	0.063 (3)	0.068 (3)	0.039 (3)	0.011 (3)	0.018 (2)	0.000 (2)
C36	0.035 (2)	0.032 (2)	0.035 (2)	-0.0015 (16)	0.0134 (18)	-0.0006 (16)
C37	0.050 (3)	0.059 (3)	0.037 (2)	0.004 (2)	0.012 (2)	-0.003 (2)
C38	0.037 (3)	0.066 (3)	0.072 (4)	0.000 (2)	0.026 (3)	-0.014 (3)

C11	0.0377 (6)	0.0514 (7)	0.0582 (7)	0.0028 (5)	0.0082 (5)	0.0166 (6)
O1	0.094 (4)	0.063 (3)	0.170 (6)	-0.009 (3)	0.056 (4)	-0.025 (3)
O2	0.154 (6)	0.319 (11)	0.117 (5)	-0.098 (7)	0.009 (5)	0.105 (6)
O3	0.098 (4)	0.166 (6)	0.085 (4)	0.005 (4)	-0.032 (3)	0.009 (4)
O4	0.069 (4)	0.107 (5)	0.441 (14)	0.008 (3)	0.055 (6)	-0.132 (7)
C12	0.0872 (13)	0.0713 (11)	0.1349 (18)	0.0189 (9)	0.0251 (12)	-0.0066 (11)
C13	0.1039 (15)	0.0787 (12)	0.1099 (15)	-0.0136 (11)	-0.0004 (12)	0.0244 (11)
C39	0.062 (4)	0.109 (6)	0.160 (8)	-0.007 (4)	0.031 (5)	0.057 (6)

Geometric parameters (Å, °) for (mo_240422160078)

Au1—C1	2.016 (4)	C19—H19B	0.9800
Au1—C20	2.006 (3)	C19—H19C	0.9800
S1—C1	1.699 (4)	C21—C22	1.499 (5)
S1—C2	1.724 (4)	C21—C26	1.351 (5)
S2—C20	1.706 (4)	C22—H22A	0.9900
S2—C21	1.724 (4)	C22—H22B	0.9900
N1—C1	1.339 (4)	C22—C23	1.522 (6)
N1—C3	1.390 (4)	C23—H23A	0.9900
N1—C8	1.451 (4)	C23—H23B	0.9900
N2—C20	1.341 (4)	C23—C24	1.503 (6)
N2—C26	1.396 (4)	C24—H24A	0.9900
N2—C27	1.459 (4)	C24—H24B	0.9900
C2—C3	1.352 (5)	C24—C25	1.541 (6)
C2—C7	1.500 (5)	C25—H25A	0.9900
C3—C4	1.501 (5)	C25—H25B	0.9900
C4—H4A	0.9900	C25—C26	1.494 (5)
C4—H4B	0.9900	C27—C28	1.398 (5)
C4—C5	1.528 (5)	C27—C32	1.399 (5)
C5—H5A	0.9900	C28—C29	1.390 (5)
C5—H5B	0.9900	C28—C36	1.517 (5)
C5—C6	1.518 (6)	C29—H29	0.9500

C6—H6A	0.9900	C29—C30	1.381 (6)
C6—H6B	0.9900	C30—H30	0.9500
C6—C7	1.533 (6)	C30—C31	1.382 (6)
C7—H7A	0.9900	C31—H31	0.9500
C7—H7B	0.9900	C31—C32	1.395 (5)
C8—C9	1.401 (5)	C32—C33	1.516 (5)
C8—C13	1.395 (5)	C33—H33	1.0000
C9—C10	1.391 (5)	C33—C34	1.524 (6)
C9—C17	1.518 (5)	C33—C35	1.528 (6)
C10—H10	0.9500	C34—H34A	0.9800
C10—C11	1.379 (6)	C34—H34B	0.9800
C11—H11	0.9500	C34—H34C	0.9800
C11—C12	1.378 (6)	C35—H35A	0.9800
C12—H12	0.9500	C35—H35B	0.9800
C12—C13	1.396 (5)	C35—H35C	0.9800
C13—C14	1.514 (5)	C36—H36	1.0000
C14—H14	1.0000	C36—C37	1.530 (6)
C14—C15	1.526 (6)	C36—C38	1.532 (6)
C14—C16	1.529 (6)	C37—H37A	0.9800
C15—H15A	0.9800	C37—H37B	0.9800
C15—H15B	0.9800	C37—H37C	0.9800
C15—H15C	0.9800	C38—H38A	0.9800
C16—H16A	0.9800	C38—H38B	0.9800
C16—H16B	0.9800	C38—H38C	0.9800
C16—H16C	0.9800	C11—O1	1.404 (5)
C17—H17	1.0000	C11—O2	1.397 (7)
C17—C18	1.521 (6)	C11—O3	1.375 (5)
C17—C19	1.530 (6)	C11—O4	1.325 (5)
C18—H18A	0.9800	C12—C39	1.717 (7)
C18—H18B	0.9800	C13—C39	1.718 (7)
C18—H18C	0.9800	C39—H39A	0.9900

C19—H19A	0.9800	C39—H39B	0.9900
C20—Au1—C1	174.01 (14)	N2—C20—S2	108.2 (3)
C1—S1—C2	93.37 (17)	C22—C21—S2	125.9 (3)
C20—S2—C21	93.77 (17)	C26—C21—S2	109.4 (3)
C1—N1—C3	116.0 (3)	C26—C21—C22	124.7 (3)
C1—N1—C8	121.8 (3)	C21—C22—H22A	109.8
C3—N1—C8	122.1 (3)	C21—C22—H22B	109.8
C20—N2—C26	116.3 (3)	C21—C22—C23	109.5 (3)
C20—N2—C27	121.0 (3)	H22A—C22—H22B	108.2
C26—N2—C27	122.7 (3)	C23—C22—H22A	109.8
S1—C1—Au1	123.41 (19)	C23—C22—H22B	109.8
N1—C1—Au1	127.4 (3)	C22—C23—H23A	109.1
N1—C1—S1	108.8 (3)	C22—C23—H23B	109.1
C3—C2—S1	109.5 (3)	H23A—C23—H23B	107.8
C3—C2—C7	124.1 (3)	C24—C23—C22	112.5 (4)
C7—C2—S1	126.4 (3)	C24—C23—H23A	109.1
N1—C3—C4	123.0 (3)	C24—C23—H23B	109.1
C2—C3—N1	112.3 (3)	C23—C24—H24A	109.1
C2—C3—C4	124.7 (3)	C23—C24—H24B	109.1
C3—C4—H4A	109.8	C23—C24—C25	112.6 (4)
C3—C4—H4B	109.8	H24A—C24—H24B	107.8
C3—C4—C5	109.5 (3)	C25—C24—H24A	109.1
H4A—C4—H4B	108.2	C25—C24—H24B	109.1
C5—C4—H4A	109.8	C24—C25—H25A	109.9
C5—C4—H4B	109.8	C24—C25—H25B	109.9
C4—C5—H5A	109.3	H25A—C25—H25B	108.3
C4—C5—H5B	109.3	C26—C25—C24	109.1 (3)
H5A—C5—H5B	108.0	C26—C25—H25A	109.9
C6—C5—C4	111.6 (3)	C26—C25—H25B	109.9
C6—C5—H5A	109.3	N2—C26—C25	123.2 (3)

C6—C5—H5B	109.3	C21—C26—N2	112.3 (3)
C5—C6—H6A	109.3	C21—C26—C25	124.5 (3)
C5—C6—H6B	109.3	C28—C27—N2	117.6 (3)
C5—C6—C7	111.6 (3)	C28—C27—C32	123.7 (3)
H6A—C6—H6B	108.0	C32—C27—N2	118.7 (3)
C7—C6—H6A	109.3	C27—C28—C36	122.8 (3)
C7—C6—H6B	109.3	C29—C28—C27	116.8 (4)
C2—C7—C6	109.1 (3)	C29—C28—C36	120.4 (3)
C2—C7—H7A	109.9	C28—C29—H29	119.4
C2—C7—H7B	109.9	C30—C29—C28	121.2 (4)
C6—C7—H7A	109.9	C30—C29—H29	119.4
C6—C7—H7B	109.9	C29—C30—H30	119.7
H7A—C7—H7B	108.3	C29—C30—C31	120.5 (4)
C9—C8—N1	117.8 (3)	C31—C30—H30	119.7
C13—C8—N1	118.6 (3)	C30—C31—H31	119.5
C13—C8—C9	123.6 (3)	C30—C31—C32	121.1 (4)
C8—C9—C17	123.3 (3)	C32—C31—H31	119.5
C10—C9—C8	116.7 (3)	C27—C32—C33	123.1 (3)
C10—C9—C17	119.9 (3)	C31—C32—C27	116.7 (4)
C9—C10—H10	119.5	C31—C32—C33	120.3 (4)
C11—C10—C9	121.0 (4)	C32—C33—H33	108.2
C11—C10—H10	119.5	C32—C33—C34	110.5 (3)
C10—C11—H11	119.5	C32—C33—C35	111.4 (4)
C12—C11—C10	120.9 (4)	C34—C33—H33	108.2
C12—C11—H11	119.5	C34—C33—C35	110.2 (4)
C11—C12—H12	119.6	C35—C33—H33	108.2
C11—C12—C13	120.7 (4)	C33—C34—H34A	109.5
C13—C12—H12	119.6	C33—C34—H34B	109.5
C8—C13—C12	116.9 (3)	C33—C34—H34C	109.5
C8—C13—C14	122.3 (3)	H34A—C34—H34B	109.5
C12—C13—C14	120.7 (3)	H34A—C34—H34C	109.5

C13—C14—H14	108.2	H34B—C34—H34C	109.5
C13—C14—C15	109.6 (3)	C33—C35—H35A	109.5
C13—C14—C16	111.9 (4)	C33—C35—H35B	109.5
C15—C14—H14	108.2	C33—C35—H35C	109.5
C15—C14—C16	110.7 (4)	H35A—C35—H35B	109.5
C16—C14—H14	108.2	H35A—C35—H35C	109.5
C14—C15—H15A	109.5	H35B—C35—H35C	109.5
C14—C15—H15B	109.5	C28—C36—H36	108.0
C14—C15—H15C	109.5	C28—C36—C37	110.2 (3)
H15A—C15—H15B	109.5	C28—C36—C38	112.0 (3)
H15A—C15—H15C	109.5	C37—C36—H36	108.0
H15B—C15—H15C	109.5	C37—C36—C38	110.4 (4)
C14—C16—H16A	109.5	C38—C36—H36	108.0
C14—C16—H16B	109.5	C36—C37—H37A	109.5
C14—C16—H16C	109.5	C36—C37—H37B	109.5
H16A—C16—H16B	109.5	C36—C37—H37C	109.5
H16A—C16—H16C	109.5	H37A—C37—H37B	109.5
H16B—C16—H16C	109.5	H37A—C37—H37C	109.5
C9—C17—H17	107.7	H37B—C37—H37C	109.5
C9—C17—C18	111.0 (4)	C36—C38—H38A	109.5
C9—C17—C19	111.4 (4)	C36—C38—H38B	109.5
C18—C17—H17	107.7	C36—C38—H38C	109.5
C18—C17—C19	111.1 (4)	H38A—C38—H38B	109.5
C19—C17—H17	107.7	H38A—C38—H38C	109.5
C17—C18—H18A	109.5	H38B—C38—H38C	109.5
C17—C18—H18B	109.5	O2—C11—O1	102.7 (5)
C17—C18—H18C	109.5	O3—C11—O1	112.6 (4)
H18A—C18—H18B	109.5	O3—C11—O2	104.4 (4)
H18A—C18—H18C	109.5	O4—C11—O1	110.4 (4)
H18B—C18—H18C	109.5	O4—C11—O2	107.4 (6)
C17—C19—H19A	109.5	O4—C11—O3	117.9 (5)

C17—C19—H19B	109.5	C12—C39—C13	113.2 (4)
C17—C19—H19C	109.5	C12—C39—H39A	108.9
H19A—C19—H19B	109.5	C12—C39—H39B	108.9
H19A—C19—H19C	109.5	C13—C39—H39A	108.9
H19B—C19—H19C	109.5	C13—C39—H39B	108.9
S2—C20—Au1	120.80 (19)	H39A—C39—H39B	107.7
N2—C20—Au1	131.0 (3)		
S1—C2—C3—N1	-1.2 (4)	C11—C12—C13—C8	0.1 (6)
S1—C2—C3—C4	-180.0 (3)	C11—C12—C13— C14	-177.3 (4)
S1—C2—C7—C6	163.6 (3)	C12—C13—C14— C15	74.2 (5)
S2—C21—C22—C23	165.7 (3)	C12—C13—C14— C16	-49.0 (5)
S2—C21—C26—N2	-0.2 (4)	C13—C8—C9—C10	-0.1 (5)
S2—C21—C26—C25	179.6 (3)	C13—C8—C9—C17	-179.5 (4)
N1—C3—C4—C5	167.5 (3)	C17—C9—C10—C11	179.3 (4)
N1—C8—C9—C10	-179.1 (3)	C20—S2—C21—C22	-178.9 (3)
N1—C8—C9—C17	1.4 (5)	C20—S2—C21—C26	0.8 (3)
N1—C8—C13—C12	179.2 (3)	C20—N2—C26—C21	-0.7 (5)
N1—C8—C13—C14	-3.5 (5)	C20—N2—C26—C25	179.4 (3)
N2—C27—C28—C29	-176.1 (3)	C20—N2—C27—C28	89.0 (4)
N2—C27—C28—C36	2.1 (5)	C20—N2—C27—C32	-89.5 (4)
N2—C27—C32—C31	177.9 (3)	C21—S2—C20—Au1	176.3 (2)
N2—C27—C32—C33	-1.4 (6)	C21—S2—C20—N2	-1.2 (3)
C1—S1—C2—C3	0.4 (3)	C21—C22—C23— C24	44.0 (5)
C1—S1—C2—C7	-179.3 (4)	C22—C21—C26—N2	179.5 (3)
C1—N1—C3—C2	1.7 (5)	C22—C21—C26— C25	-0.7 (6)
C1—N1—C3—C4	-179.5 (3)	C22—C23—C24— C25	-62.1 (6)

C1—N1—C8—C9	-85.8 (4)	C23—C24—C25— C26	44.0 (6)
C1—N1—C8—C13	95.1 (4)	C24—C25—C26—N2	165.9 (4)
C2—S1—C1—Au1	173.1 (2)	C24—C25—C26— C21	-13.9 (6)
C2—S1—C1—N1	0.5 (3)	C26—N2—C20—Au1	-175.8 (3)
C2—C3—C4—C5	-13.9 (5)	C26—N2—C20—S2	1.3 (4)
C3—N1—C1—Au1	-173.6 (3)	C26—N2—C27—C28	-88.7 (4)
C3—N1—C1—S1	-1.3 (4)	C26—N2—C27—C32	92.7 (4)
C3—N1—C8—C9	92.0 (4)	C26—C21—C22— C23	-13.9 (6)
C3—N1—C8—C13	-87.1 (4)	C27—N2—C20—Au1	6.3 (5)
C3—C2—C7—C6	-16.1 (6)	C27—N2—C20—S2	-176.6 (3)
C3—C4—C5—C6	44.7 (5)	C27—N2—C26—C21	177.1 (3)
C4—C5—C6—C7	-64.3 (5)	C27—N2—C26—C25	-2.8 (5)
C5—C6—C7—C2	46.9 (5)	C27—C28—C29— C30	-2.2 (6)
C7—C2—C3—N1	178.5 (4)	C27—C28—C36— C37	-109.4 (4)
C7—C2—C3—C4	-0.2 (7)	C27—C28—C36— C38	127.3 (4)
C8—N1—C1—Au1	4.4 (5)	C27—C32—C33— C34	113.7 (4)
C8—N1—C1—S1	176.6 (3)	C27—C32—C33— C35	-123.4 (4)
C8—N1—C3—C2	-176.2 (3)	C28—C27—C32— C31	-0.6 (6)
C8—N1—C3—C4	2.5 (5)	C28—C27—C32— C33	-179.9 (4)
C8—C9—C10—C11	-0.2 (6)	C28—C29—C30— C31	0.4 (6)
C8—C9—C17—C18	116.5 (4)	C29—C28—C36— C37	68.8 (5)
C8—C9—C17—C19	-119.1 (4)	C29—C28—C36— C38	-54.5 (5)

C8—C13—C14—C15	-103.0 (4)	C29—C30—C31— C32	1.5 (7)
C8—C13—C14—C16	133.8 (4)	C30—C31—C32— C27	-1.4 (6)
C9—C8—C13—C12	0.1 (5)	C30—C31—C32— C33	177.9 (4)
C9—C8—C13—C14	177.4 (4)	C31—C32—C33— C34	-65.6 (5)
C9—C10—C11—C12	0.3 (6)	C31—C32—C33— C35	57.4 (5)
C10—C9—C17—C18	-62.9 (5)	C32—C27—C28— C29	2.4 (6)
C10—C9—C17—C19	61.4 (5)	C32—C27—C28— C36	-179.4 (4)
C10—C11—C12— C13	-0.3 (6)	C36—C28—C29— C30	179.5 (4)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

4. NMR spectra

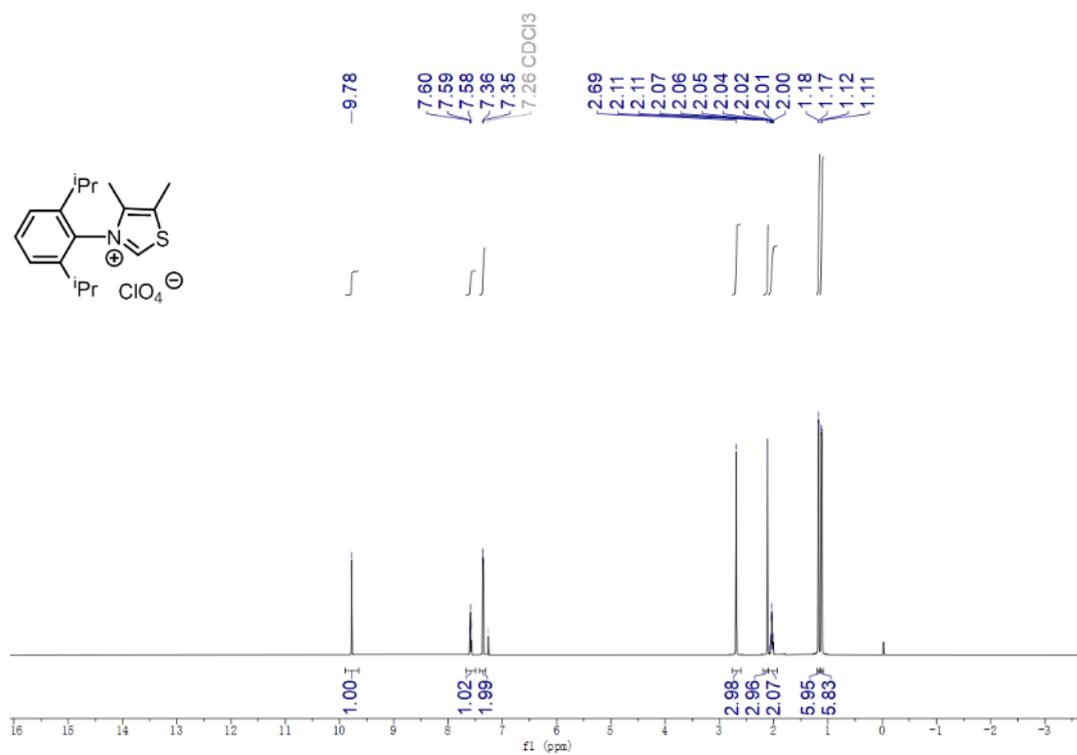


Figure S1. $^1\text{H NMR}$ (600 MHz, CDCl_3) Spectrum of Compound **1a**

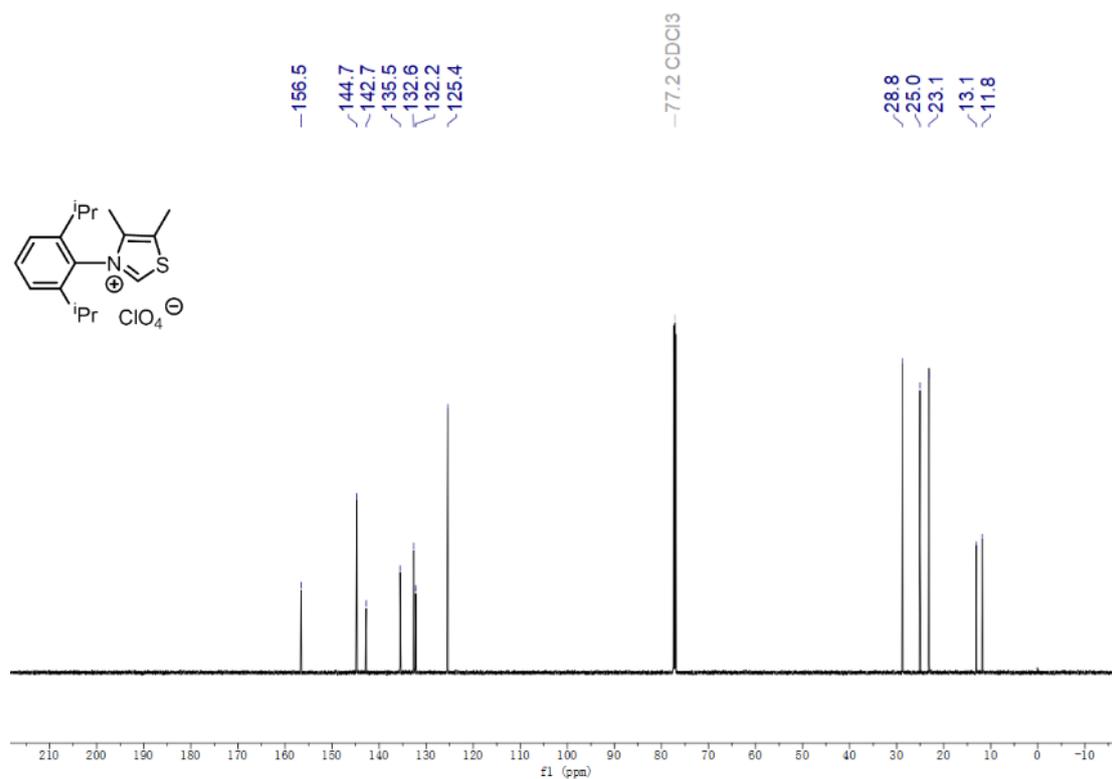


Figure S2. $^{13}\text{C NMR}$ (151 MHz, CDCl_3) Spectrum of Compound **1a**

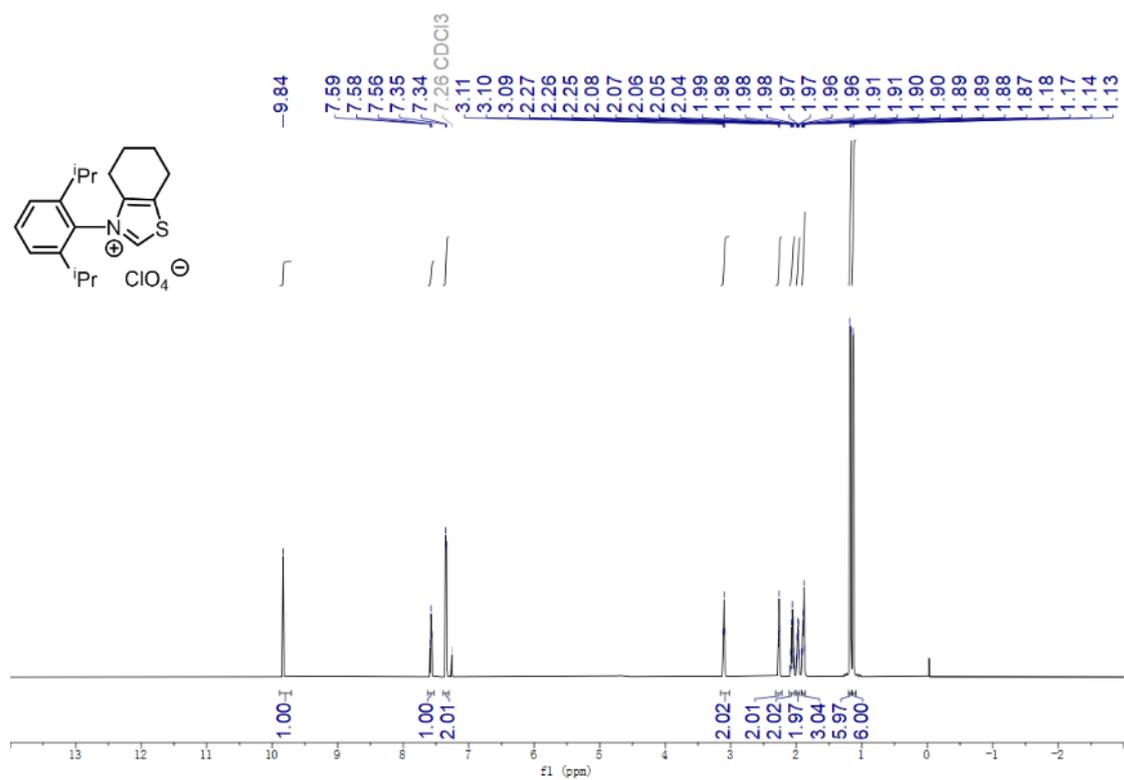


Figure S3. ¹H NMR (600 MHz, CDCl₃) Spectrum of Compound **1b**

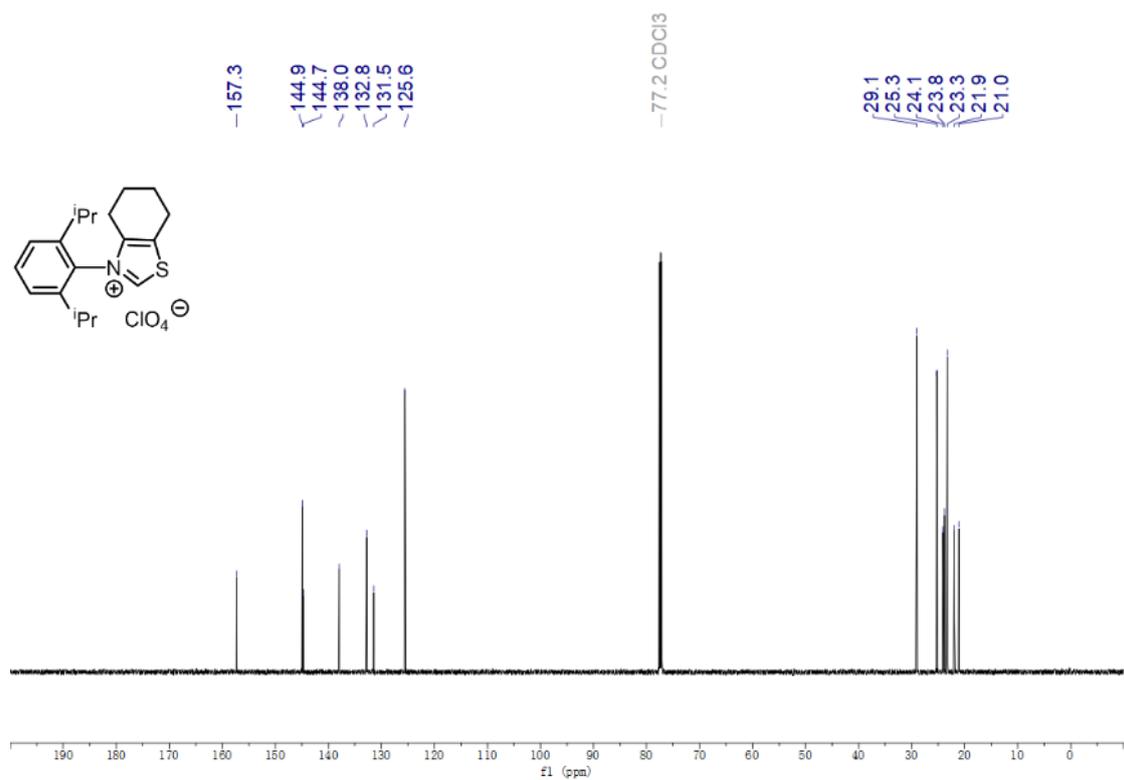


Figure S4. ¹³C NMR (151 MHz, CDCl₃) Spectrum of Compound **1b**

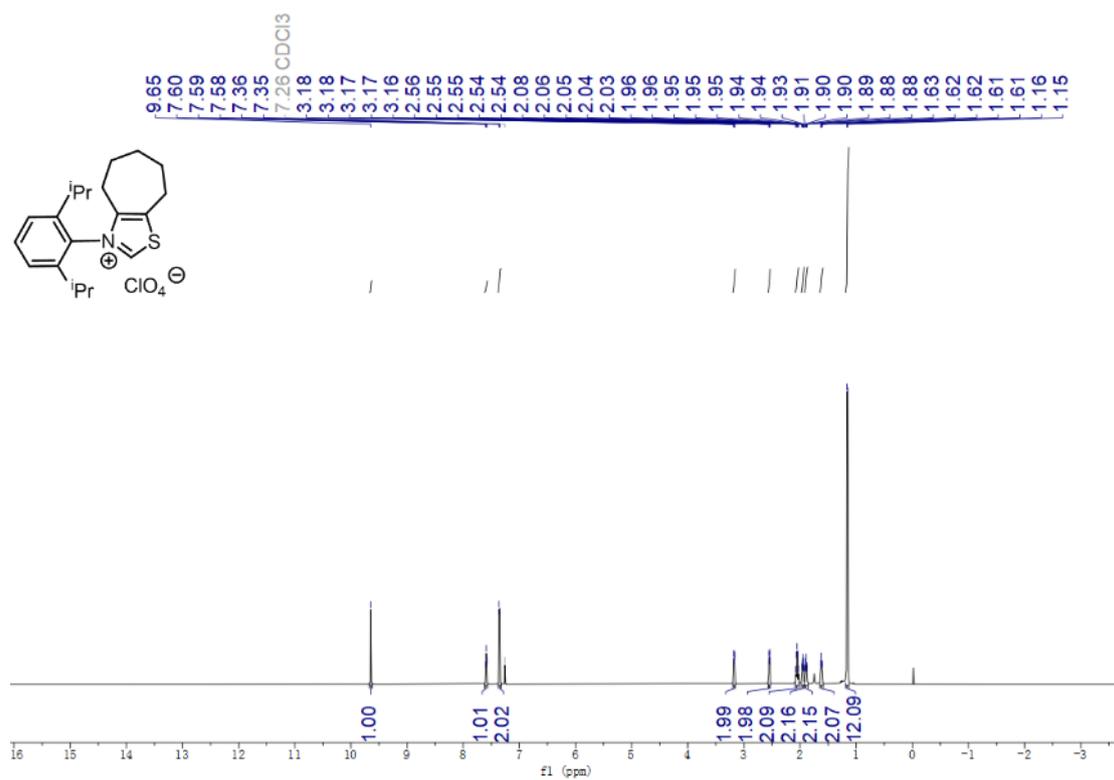


Figure S5. ¹H NMR (600 MHz, CDCl₃) Spectrum of Compound **1c**

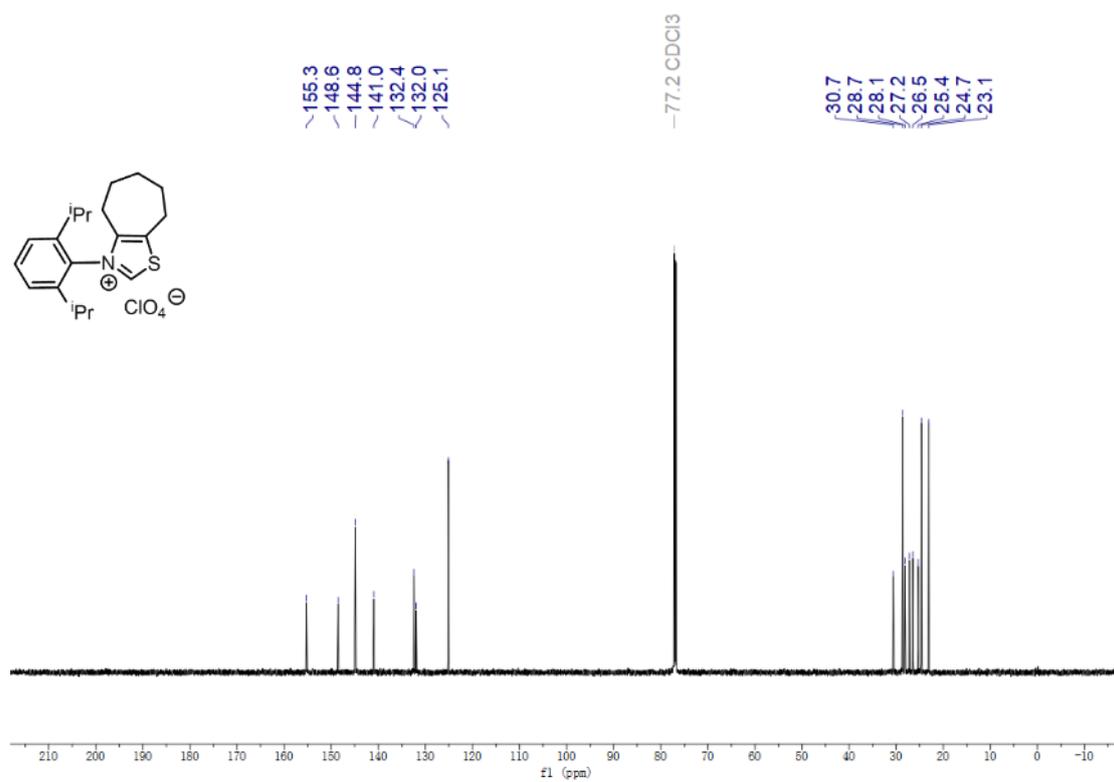


Figure S6. ¹³C NMR (151 MHz, CDCl₃) Spectrum of Compound **1c**

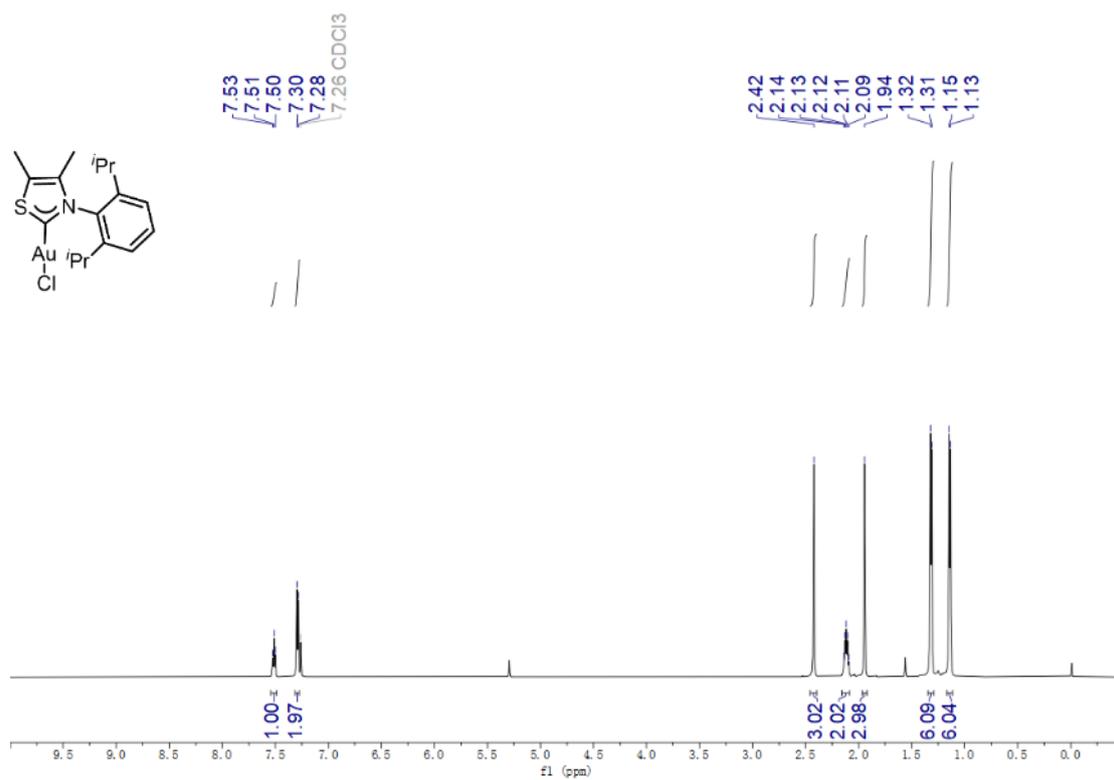


Figure S7. ^1H NMR (600 MHz, CDCl_3) Spectrum of Compound **2a**

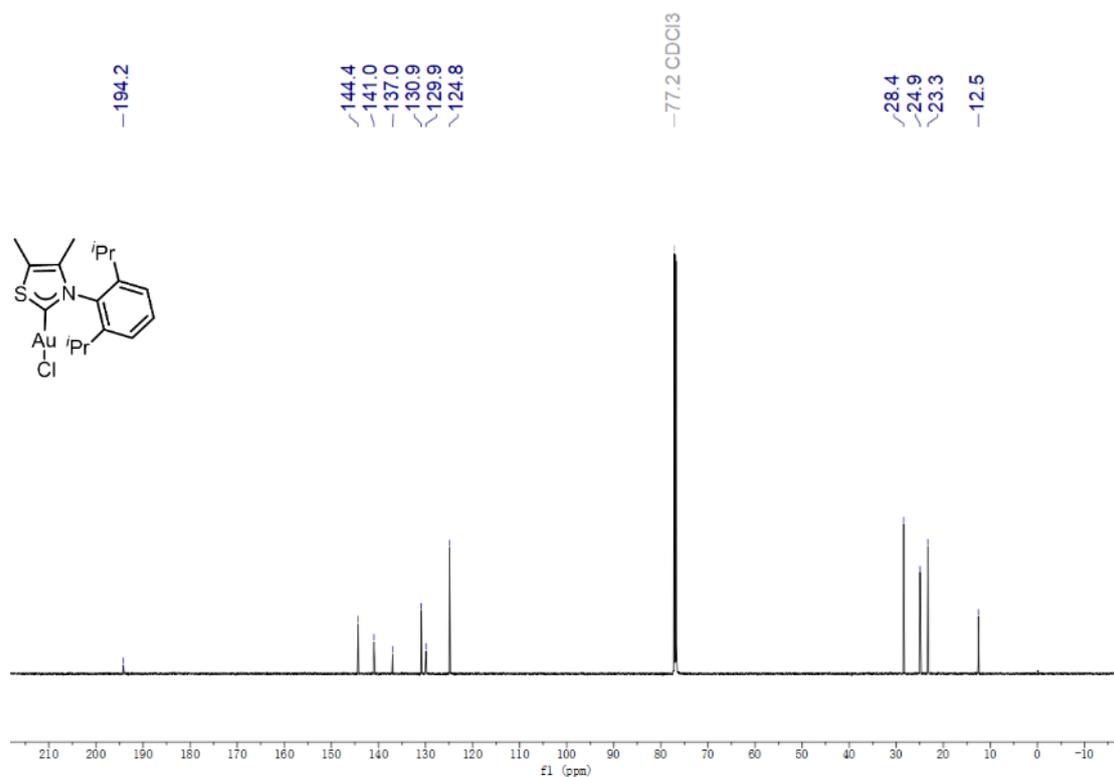


Figure S8. ^{13}C NMR (151 MHz, CDCl_3) Spectrum of Compound **2a**

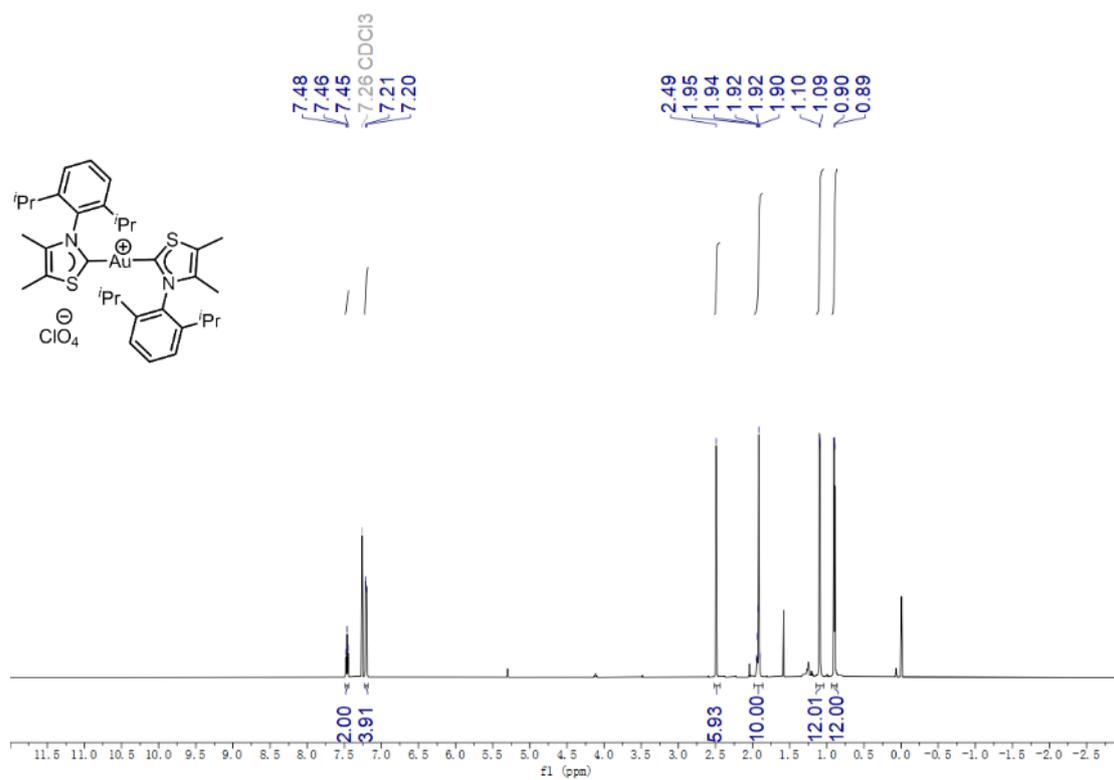


Figure S9. ¹H NMR (600 MHz, CDCl₃) Spectrum of Compound 3a

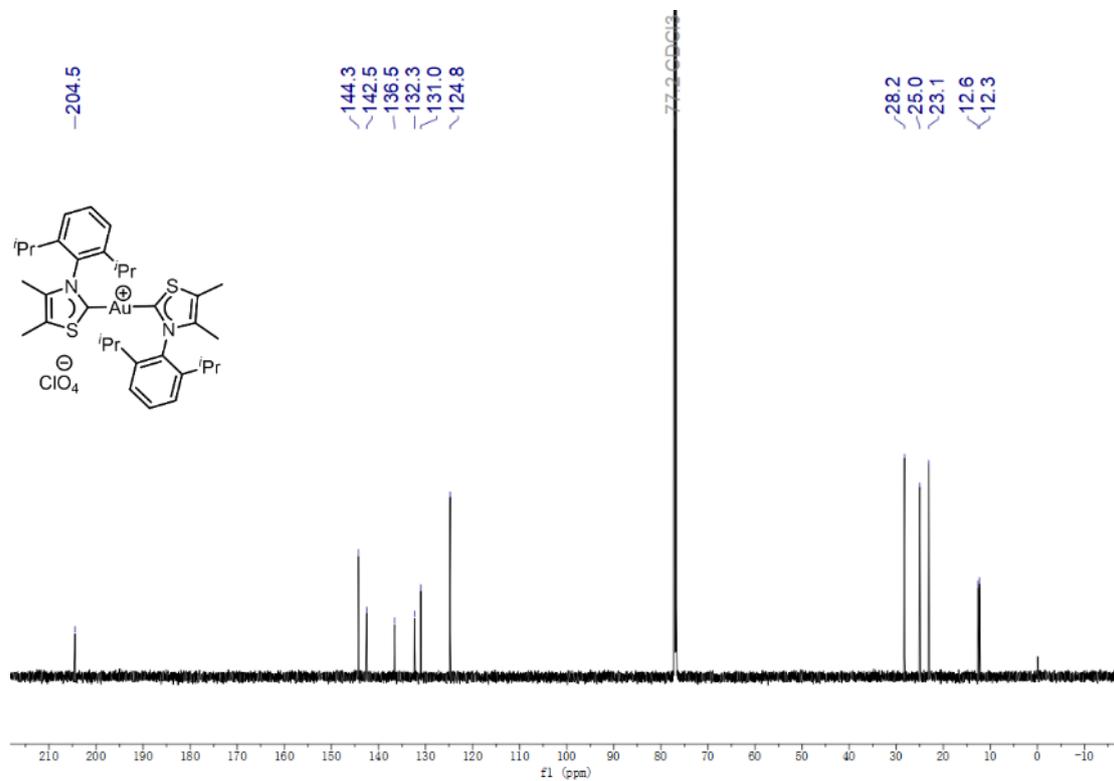


Figure S10. ¹³C NMR (151 MHz, CDCl₃) Spectrum of Compound 3a

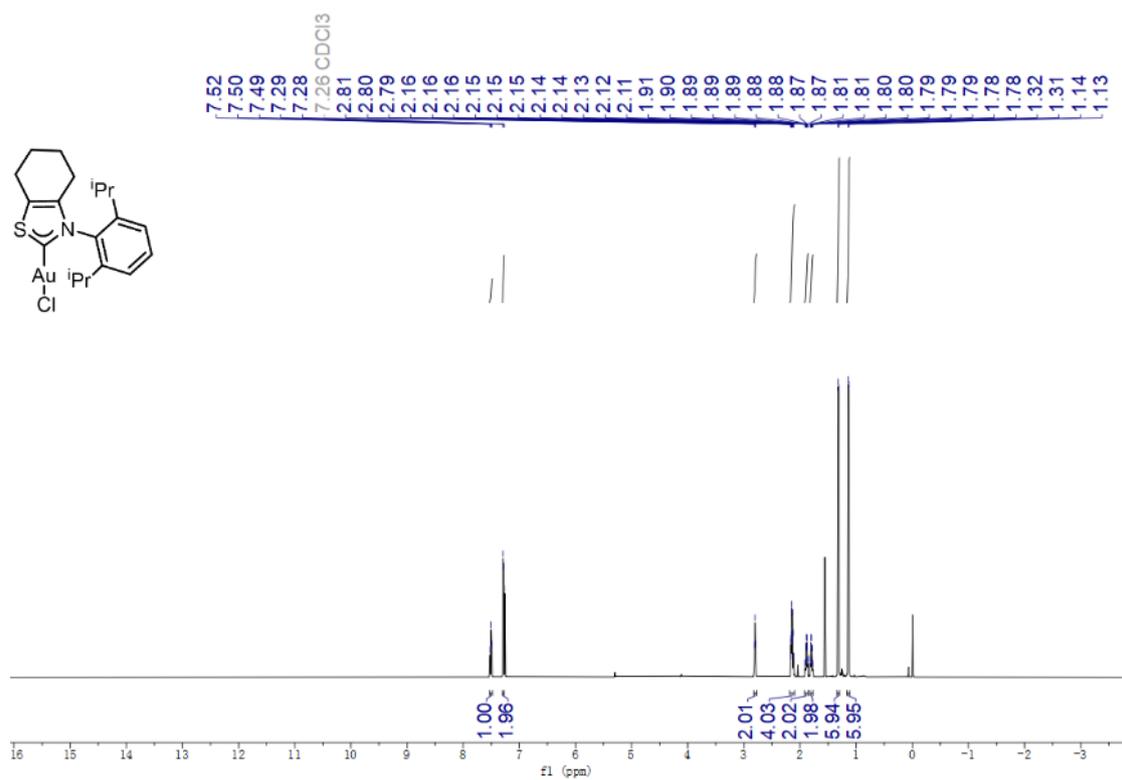


Figure S11. ¹H NMR (600 MHz, CDCl₃) Spectrum of Compound **2b**

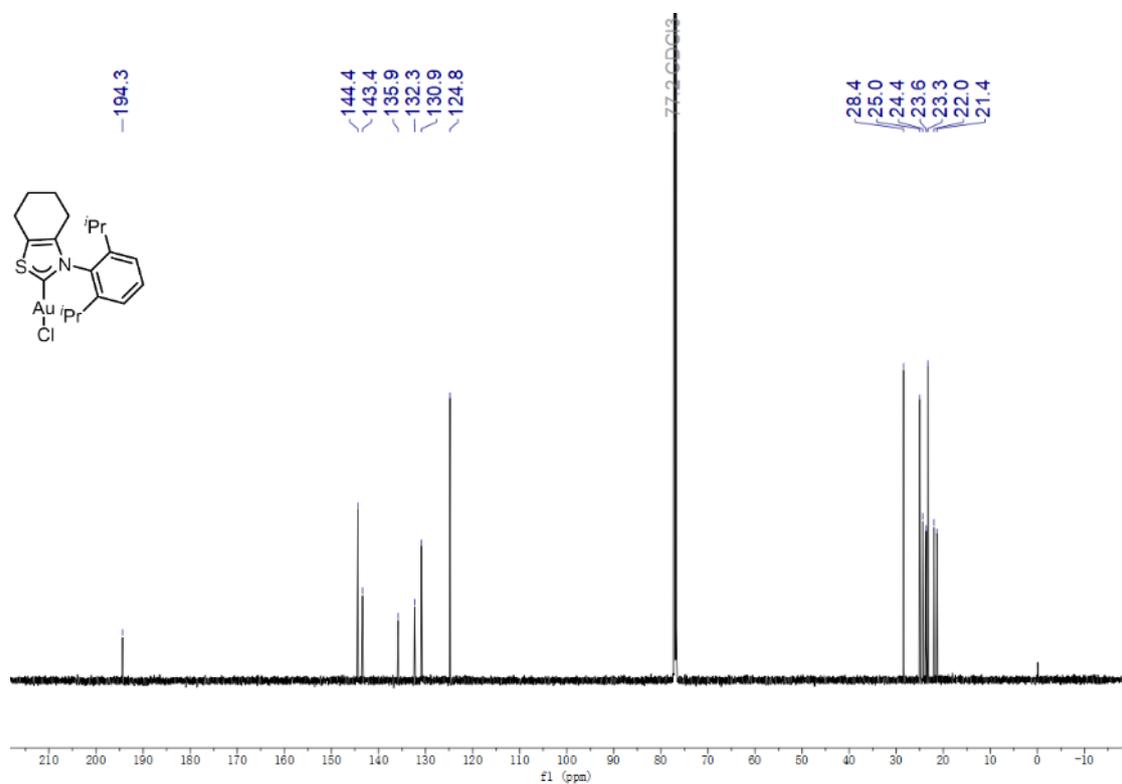


Figure S12. ¹³C NMR (151 MHz, CDCl₃) Spectrum of Compound **2b**

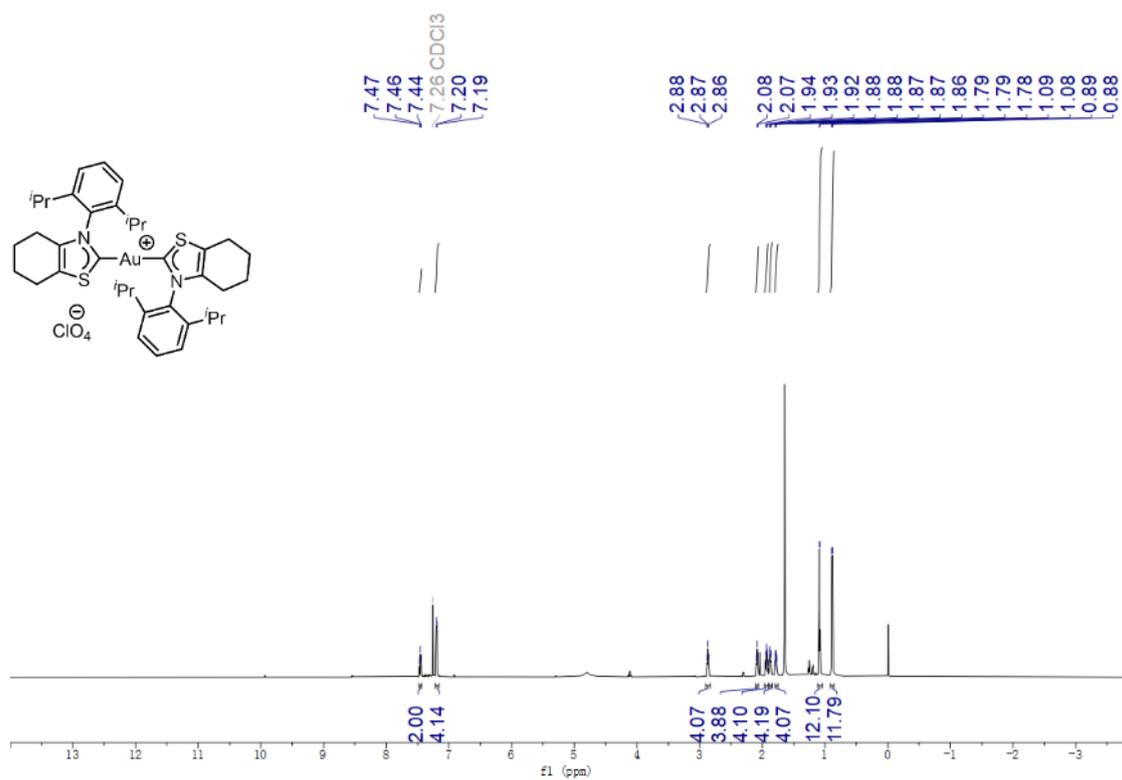


Figure S13. ¹H NMR (600 MHz, CDCl₃) Spectrum of Compound 3b

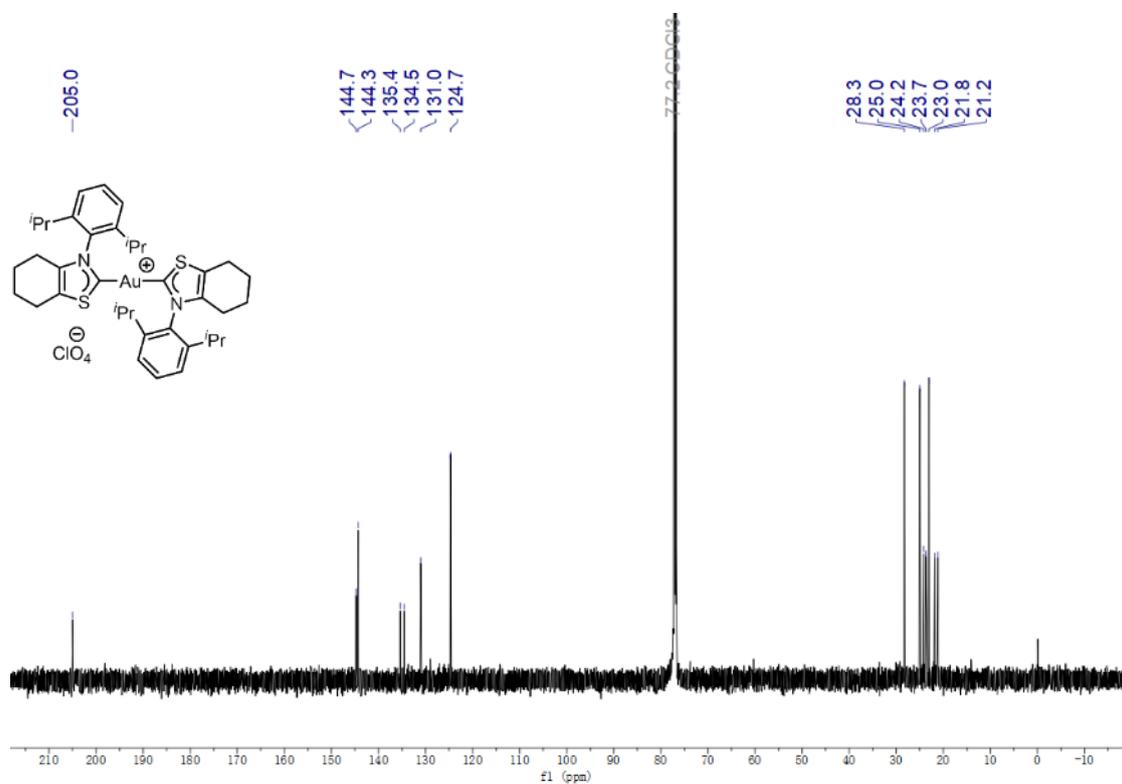


Figure S14. ¹³C NMR (151 MHz, CDCl₃) Spectrum of Compound 3b

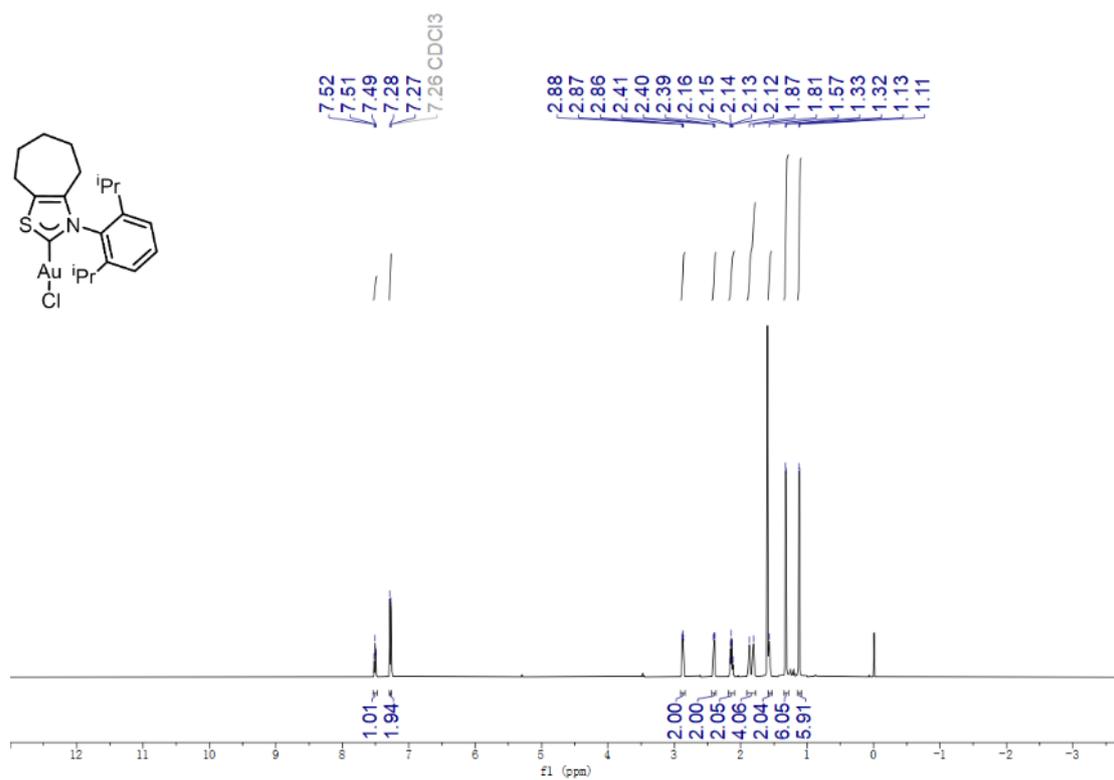


Figure S15. ¹H NMR (600 MHz, CDCl₃) Spectrum of Compound 2c

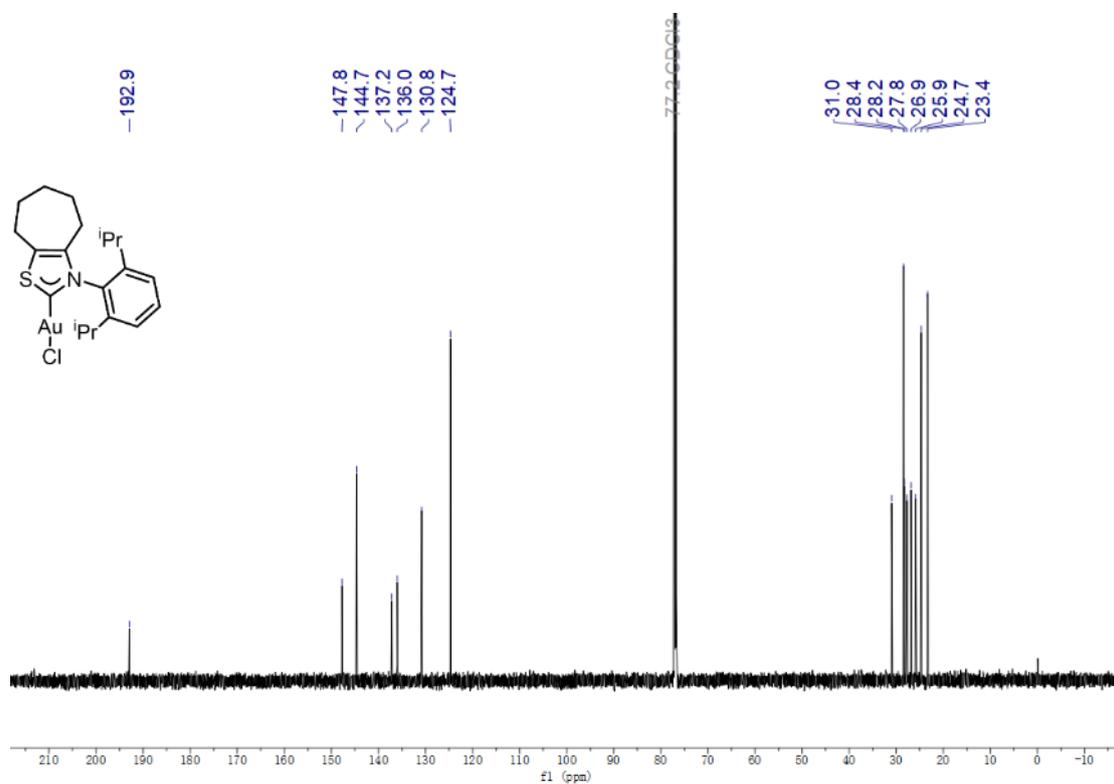


Figure S16. ¹³C NMR (151 MHz, CDCl₃) Spectrum of Compound 2c

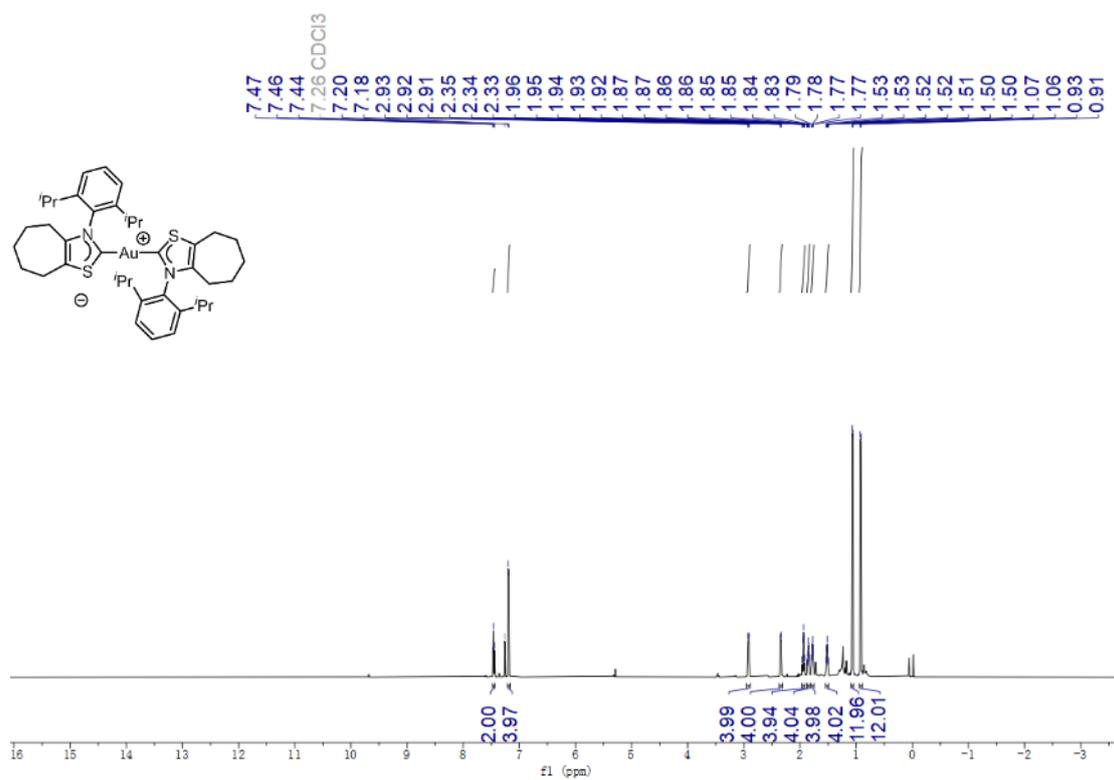


Figure S17. $^1\text{H NMR}$ (600 MHz, CDCl_3) Spectrum of Compound 3c

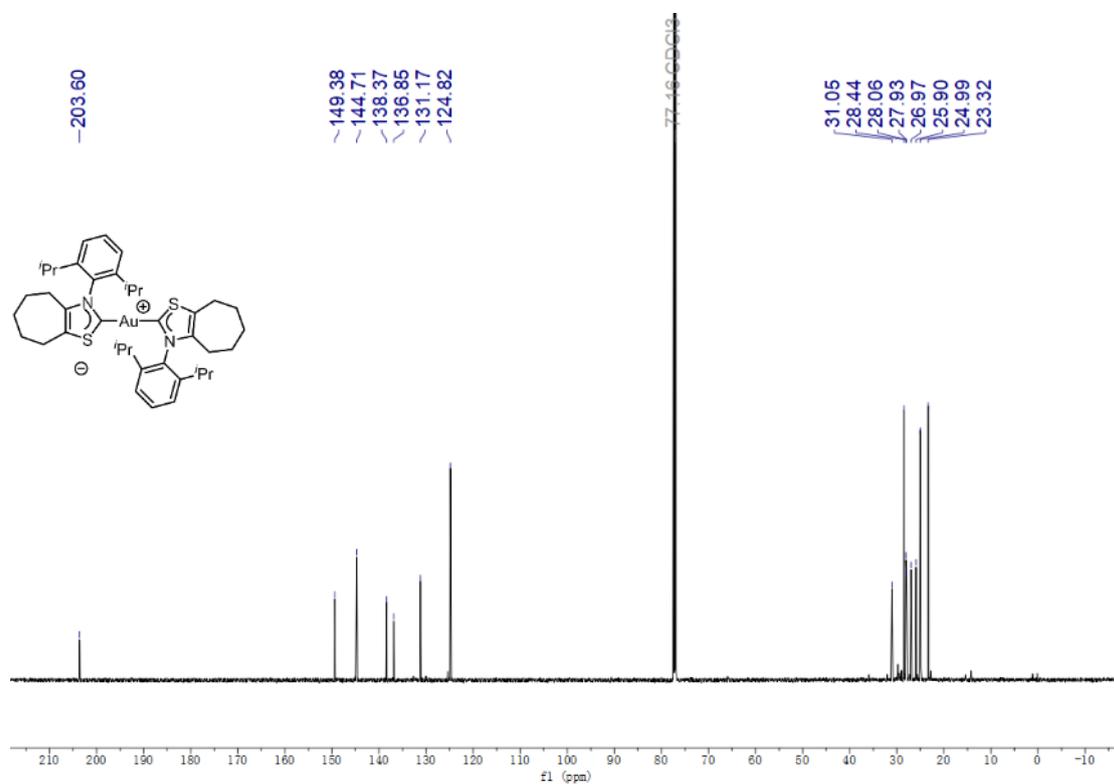


Figure S18. $^{13}\text{C NMR}$ (151 MHz, CDCl_3) Spectrum of Compound 3c

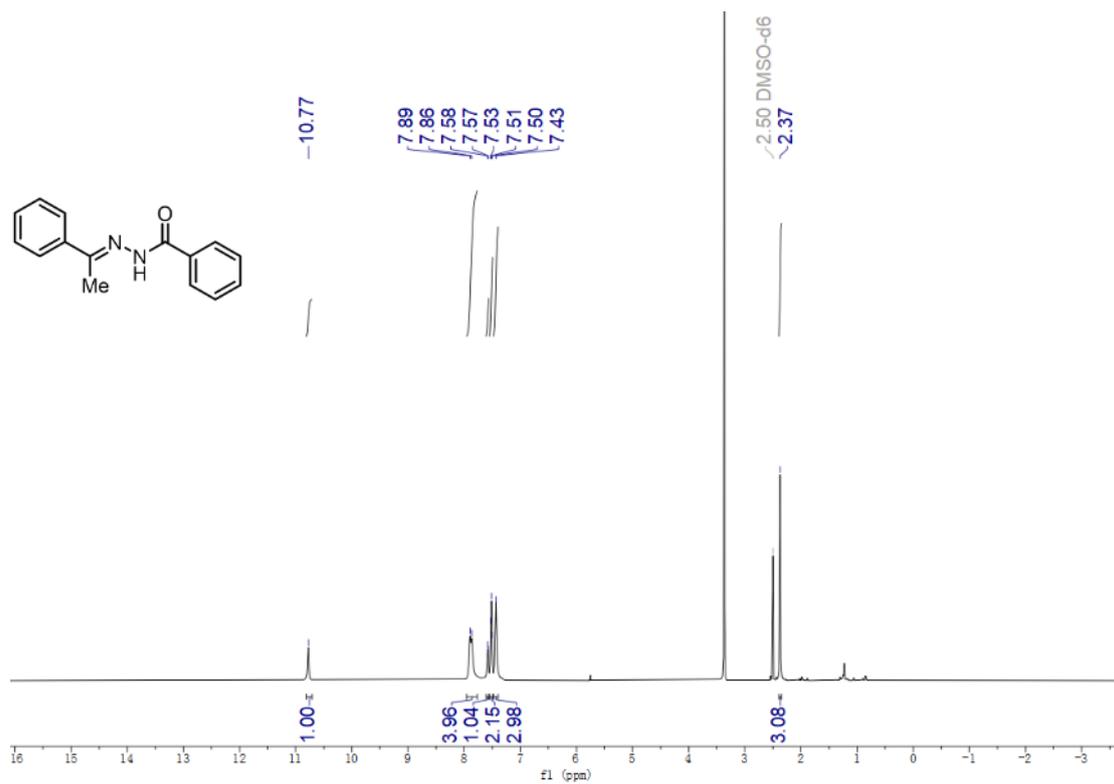


Figure S19. ¹H NMR (600 MHz, DMSO) Spectrum of Compound 6a

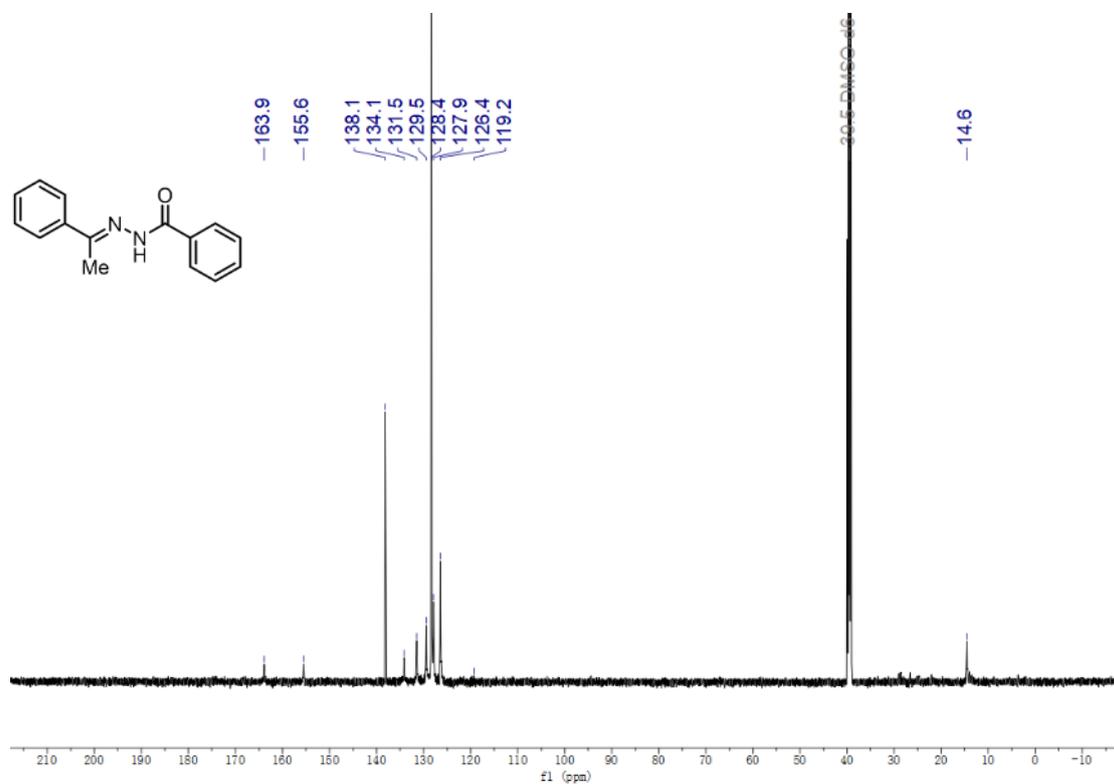


Figure S20. ¹³C NMR (151 MHz, DMSO) Spectrum of Compound 6a

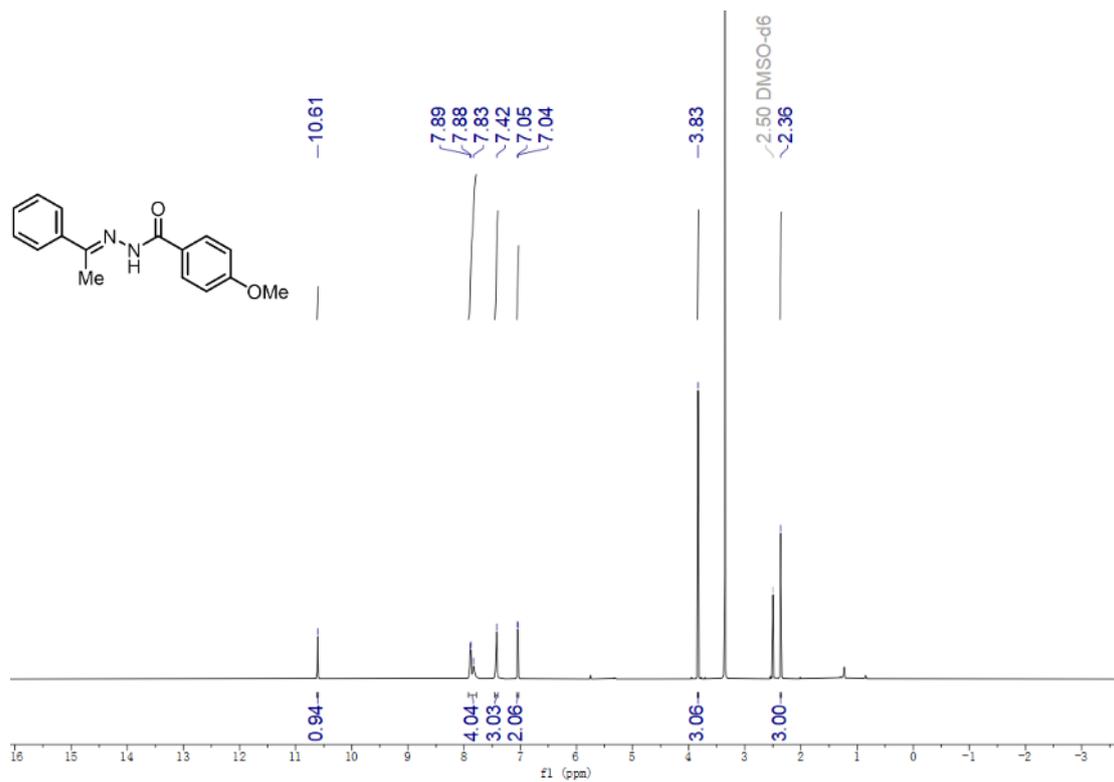


Figure S21. ¹H NMR (600 MHz, DMSO) Spectrum of Compound **6b**

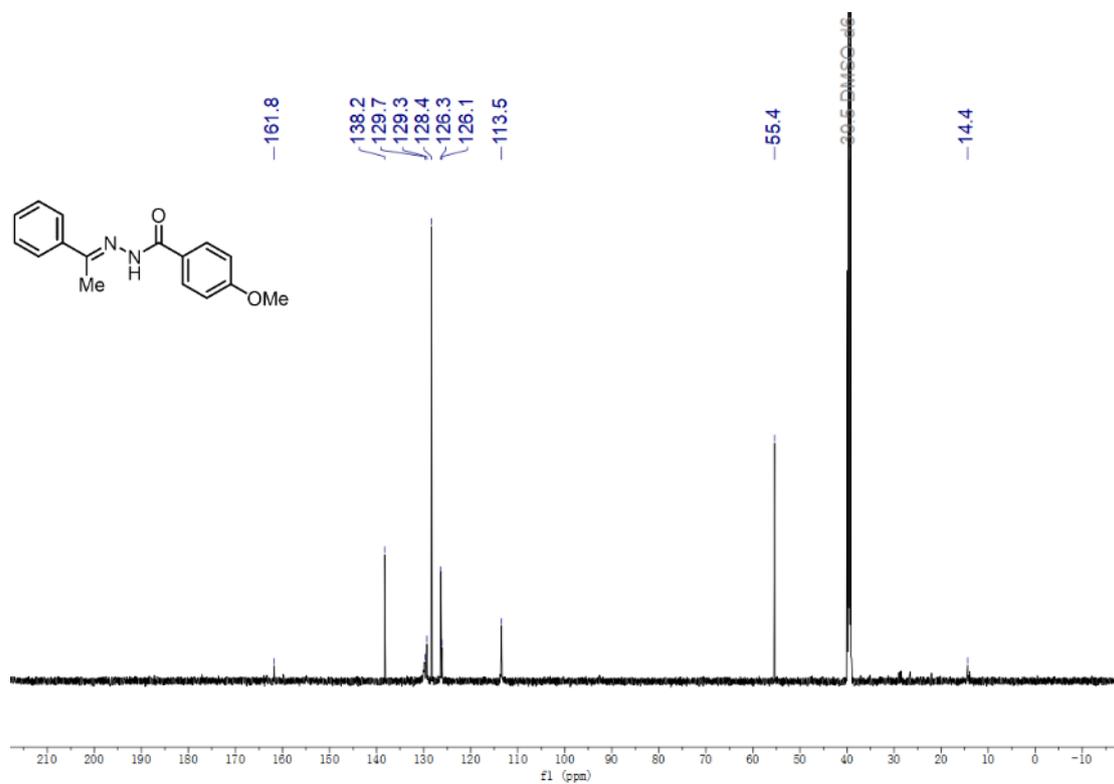


Figure S22. ¹³C NMR (151 MHz, DMSO) Spectrum of Compound **6b**

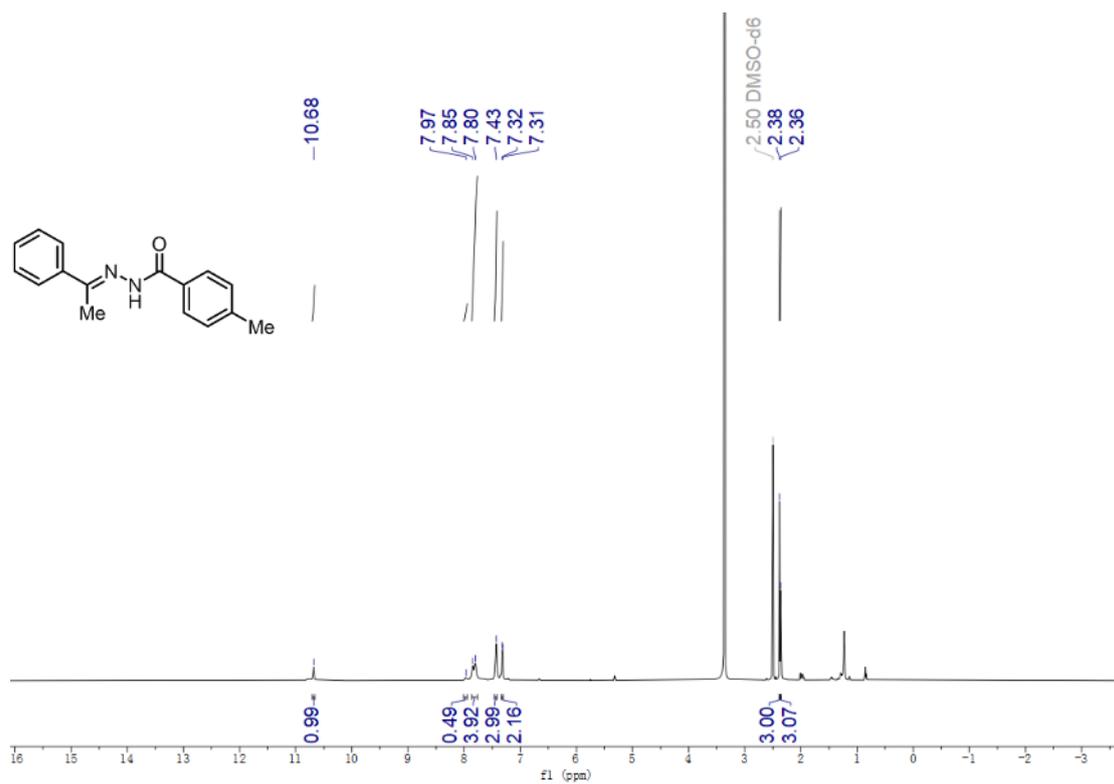


Figure S23. ¹H NMR (600 MHz, DMSO) Spectrum of Compound 6c

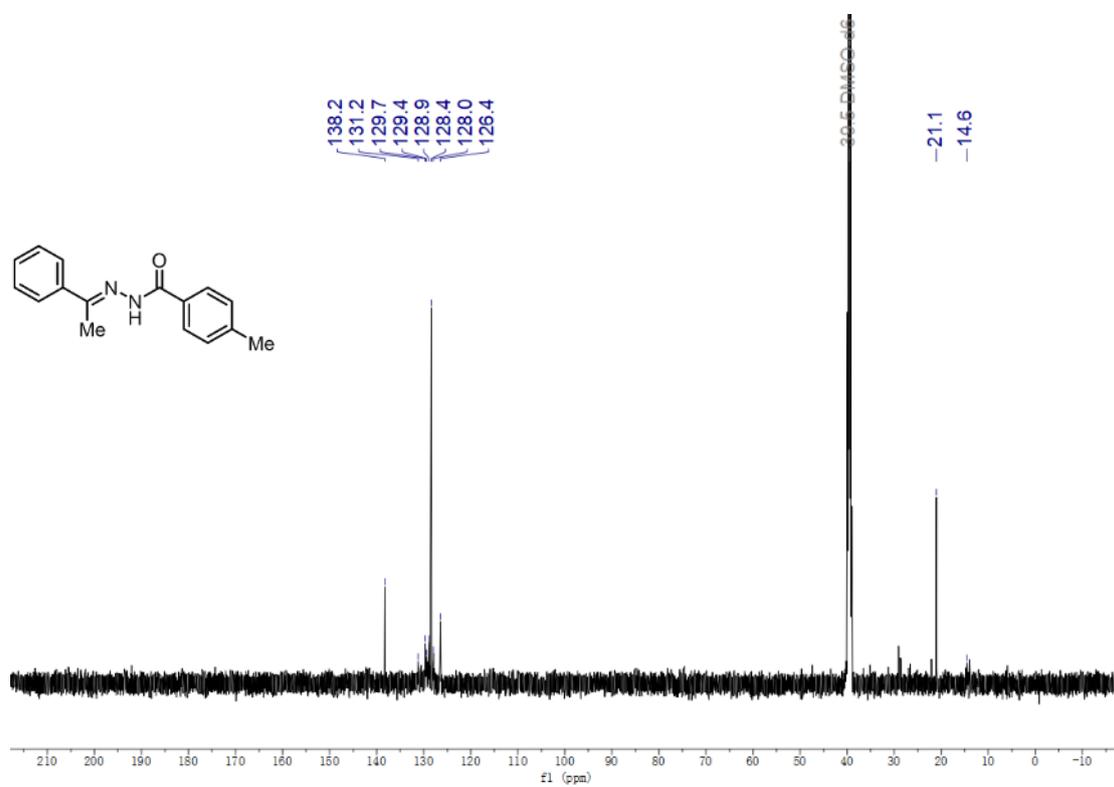


Figure S24. ¹³C NMR (151 MHz, DMSO) Spectrum of Compound 6c

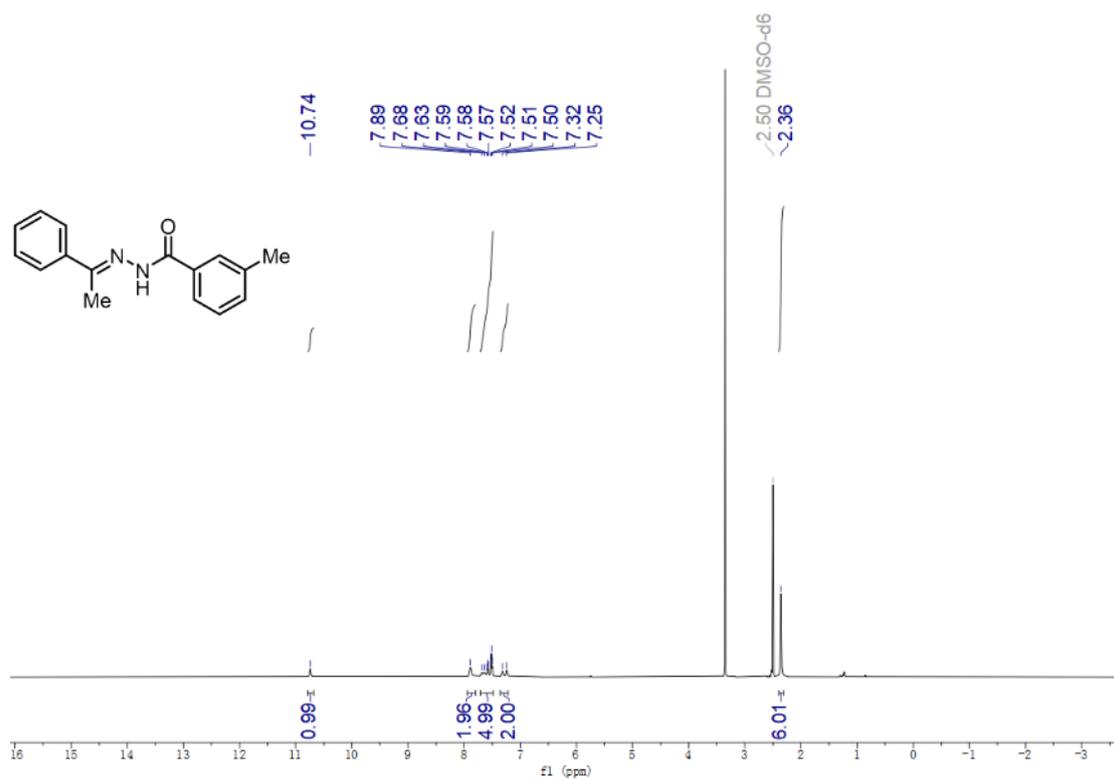


Figure S25. ¹H NMR (600 MHz, DMSO) Spectrum of Compound 6d

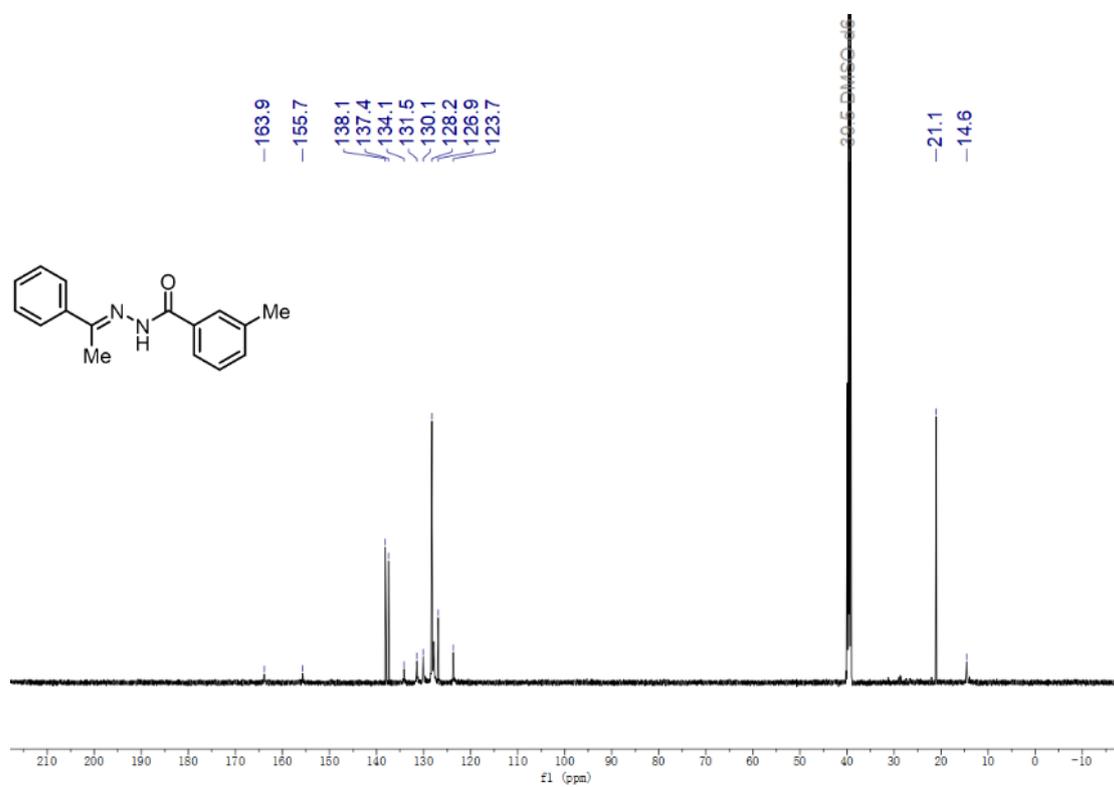


Figure S26. ¹³C NMR (151 MHz, DMSO) Spectrum of Compound 6d

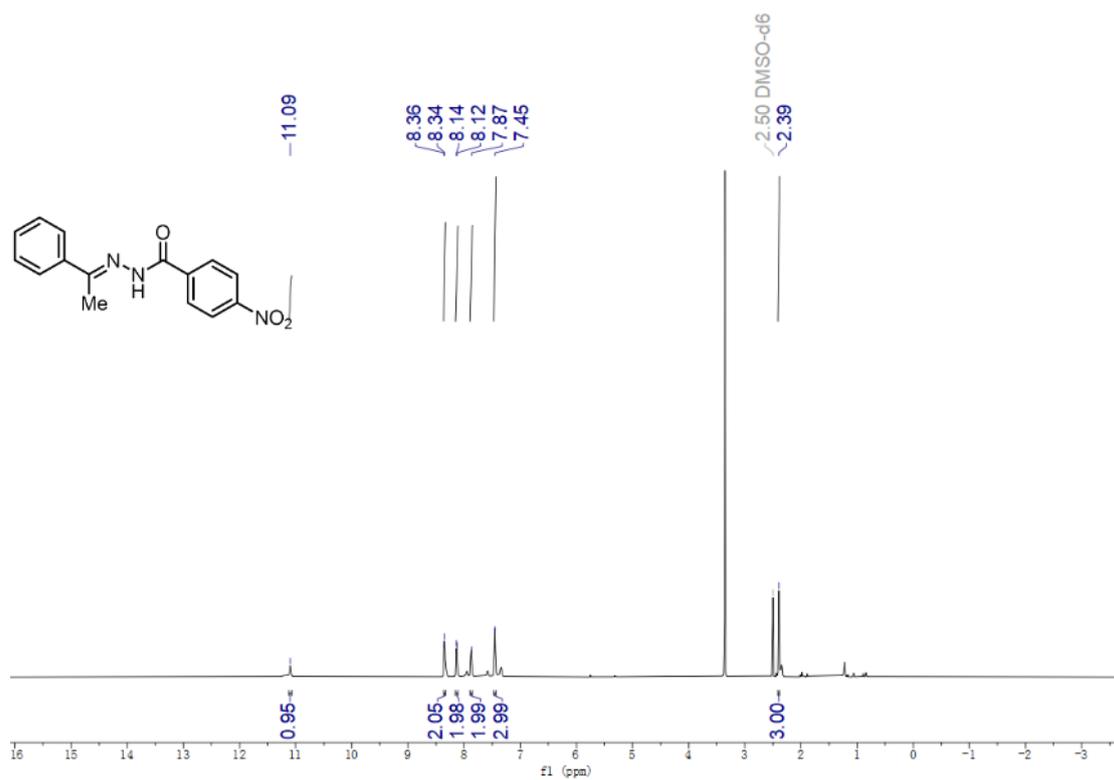


Figure S27. ¹H NMR (600 MHz, DMSO) Spectrum of Compound 6e

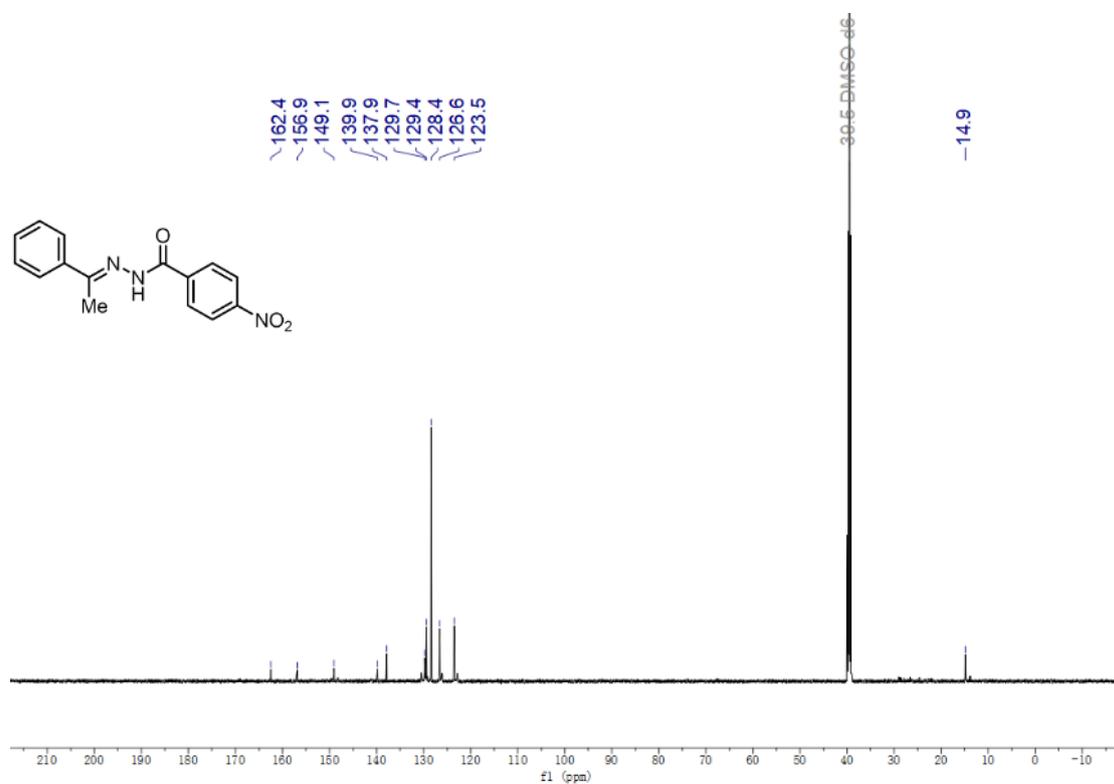


Figure S28. ¹³C NMR (151 MHz, DMSO) Spectrum of Compound 6e

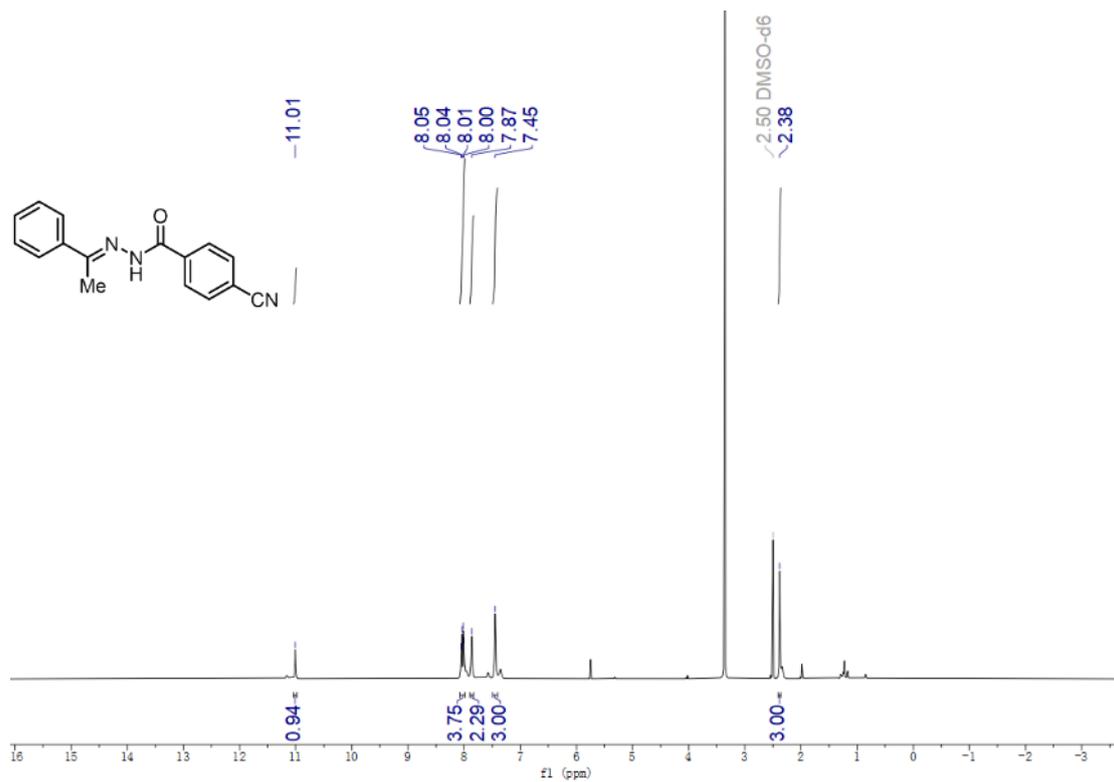


Figure S29. ¹H NMR (600 MHz, DMSO) Spectrum of Compound **6f**

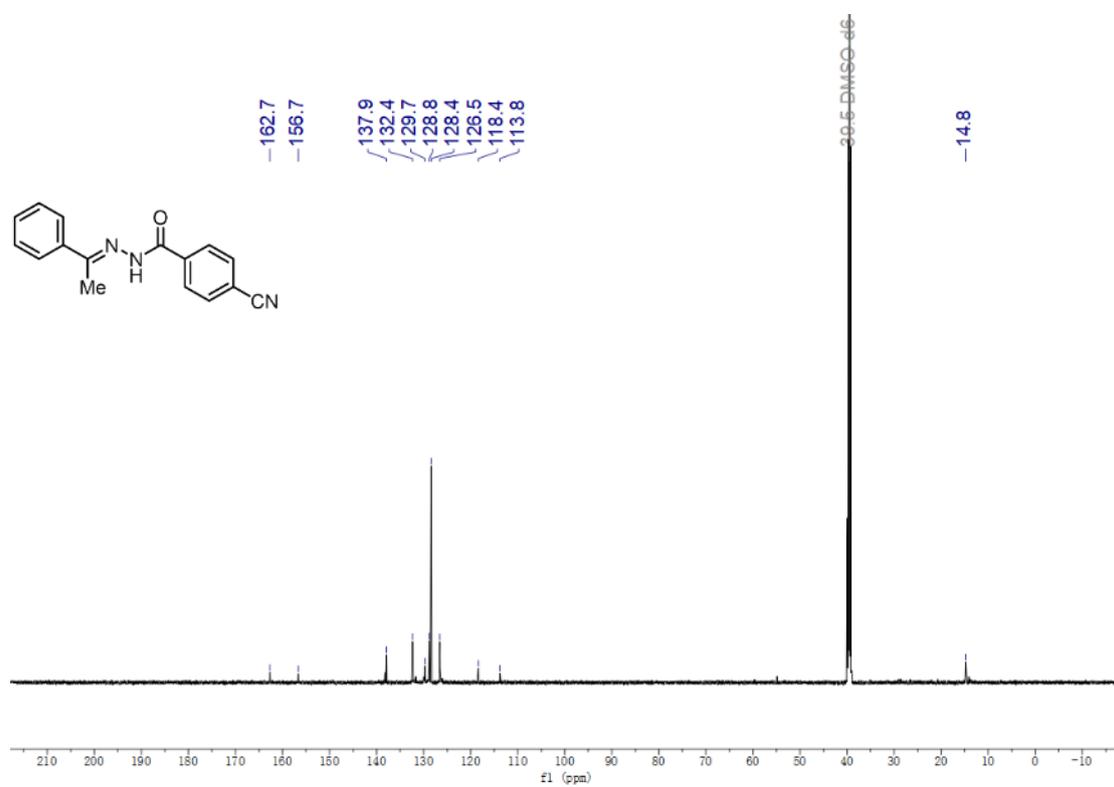


Figure S30. ¹³C NMR (151 MHz, DMSO) Spectrum of Compound **6f**

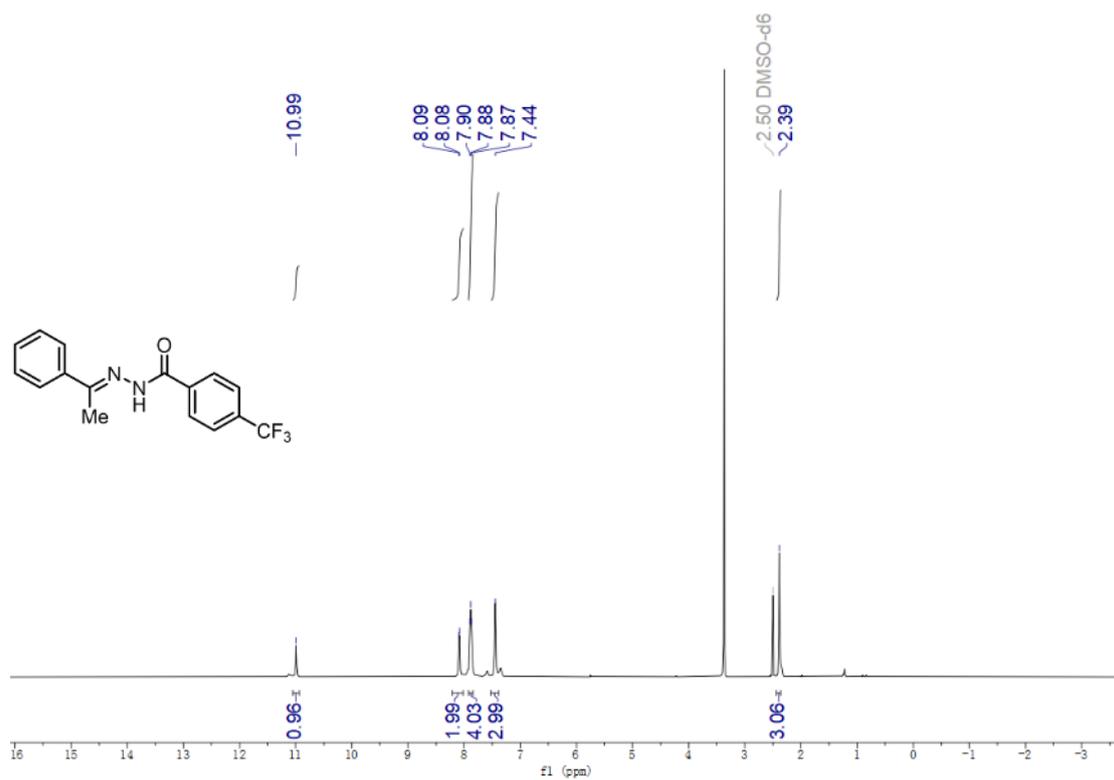


Figure S31. ¹H NMR (600 MHz, DMSO) Spectrum of Compound **6g**

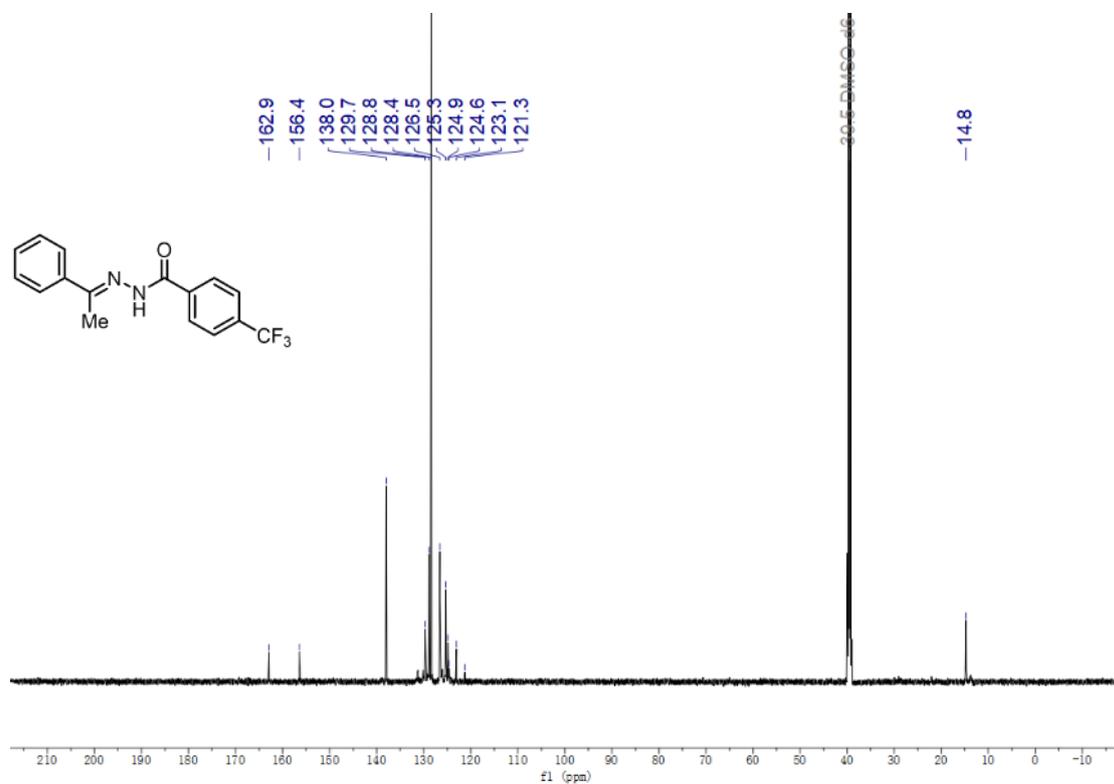


Figure S32. ¹³C NMR (151 MHz, DMSO) Spectrum of Compound **6g**

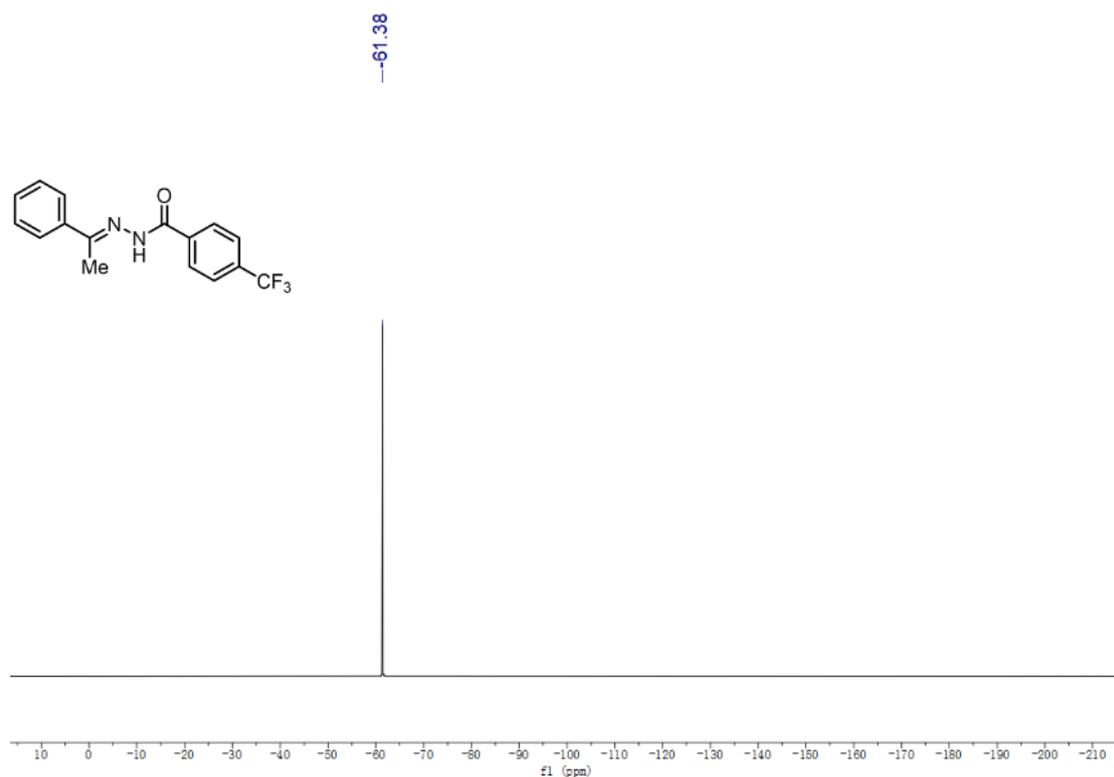


Figure S33. ^{19}F NMR (565 MHz, DMSO- d_6) Spectrum of Compound **6g**

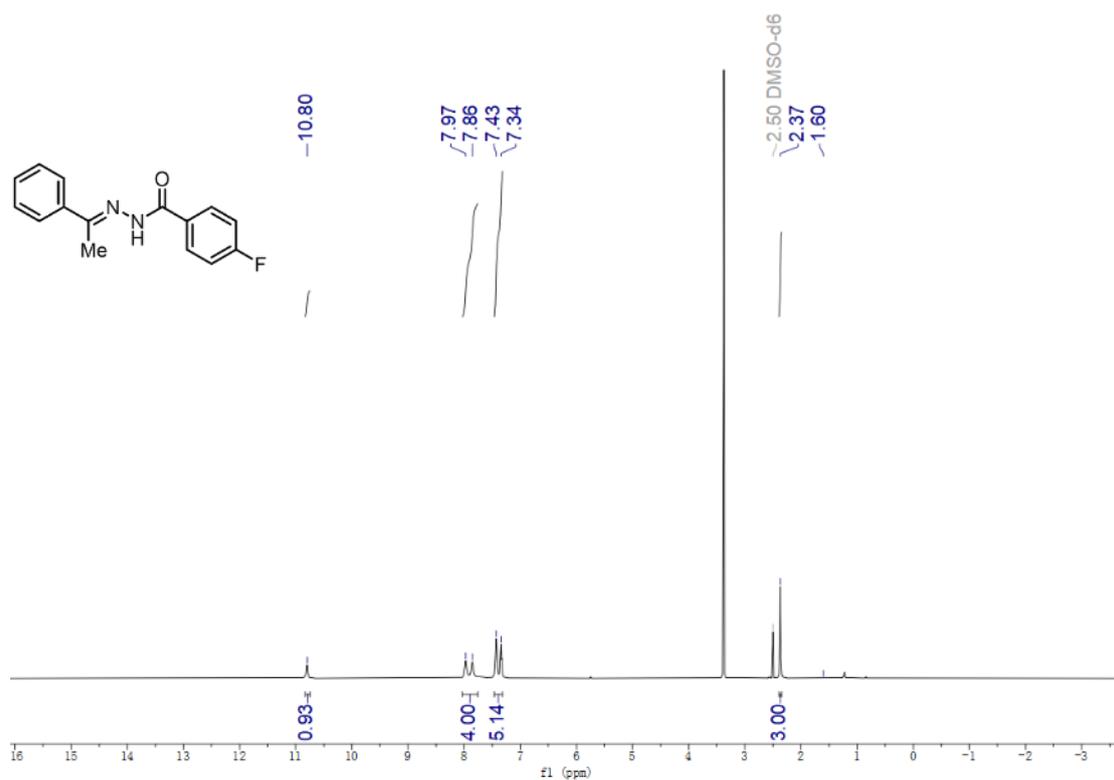


Figure S34. ^1H NMR (600 MHz, DMSO) Spectrum of Compound **6h**

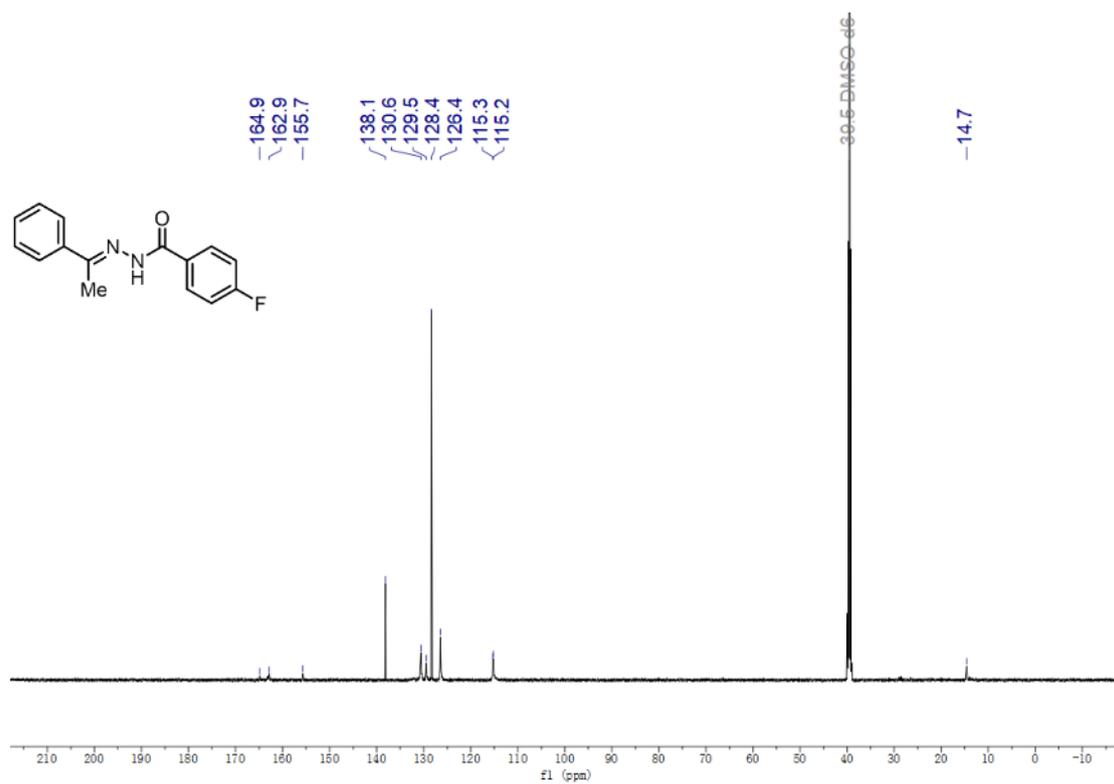


Figure S35. ¹³C NMR (151 MHz, DMSO) Spectrum of Compound **6h**

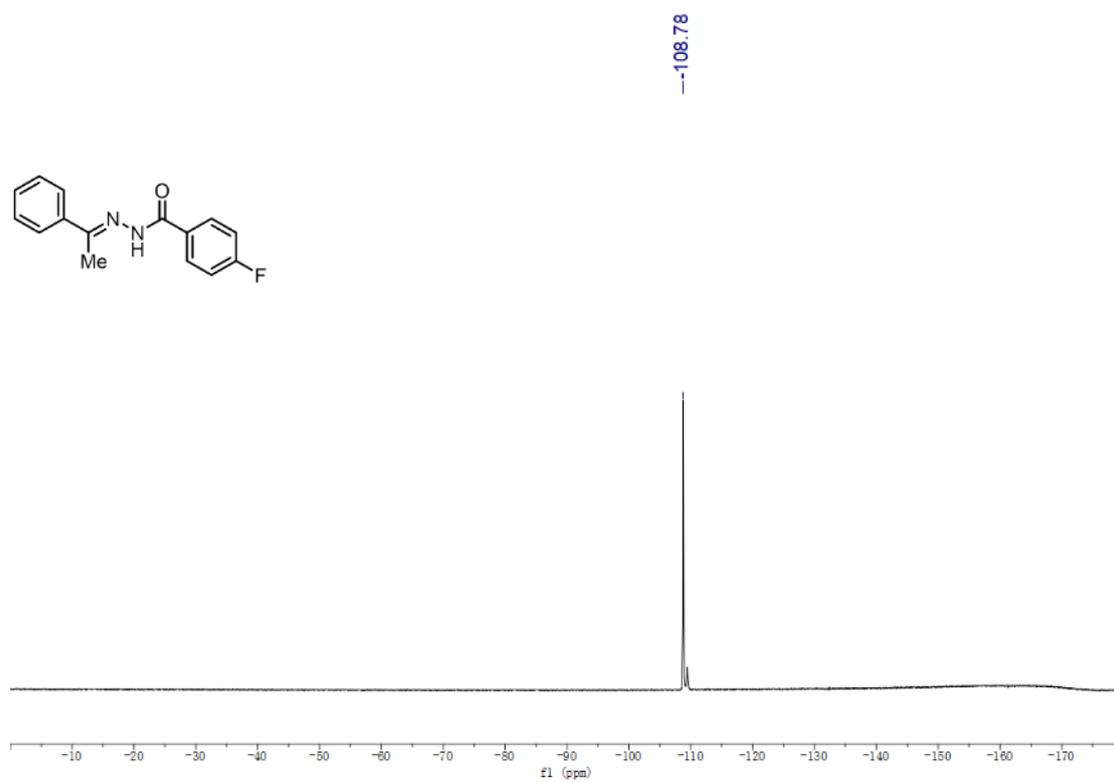


Figure S36. ¹⁹F NMR (565 MHz, DMSO-*d*₆) Spectrum of Compound **6h**

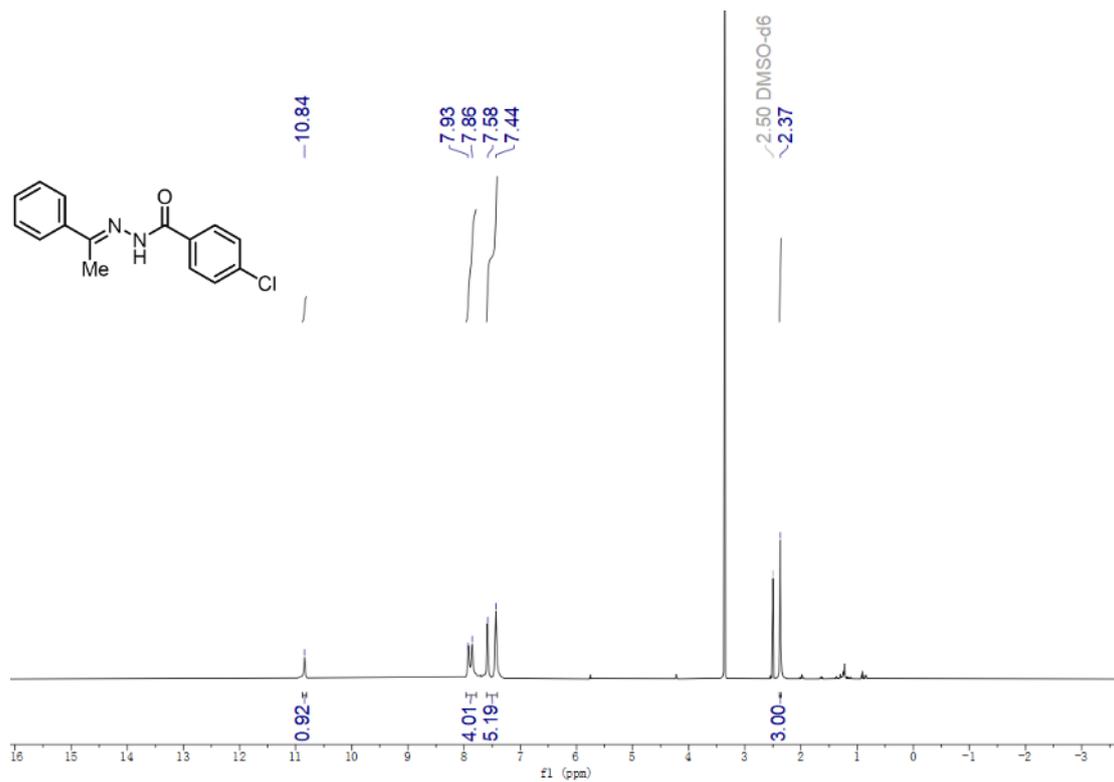


Figure S37. ¹H NMR (600 MHz, DMSO) Spectrum of Compound **6i**

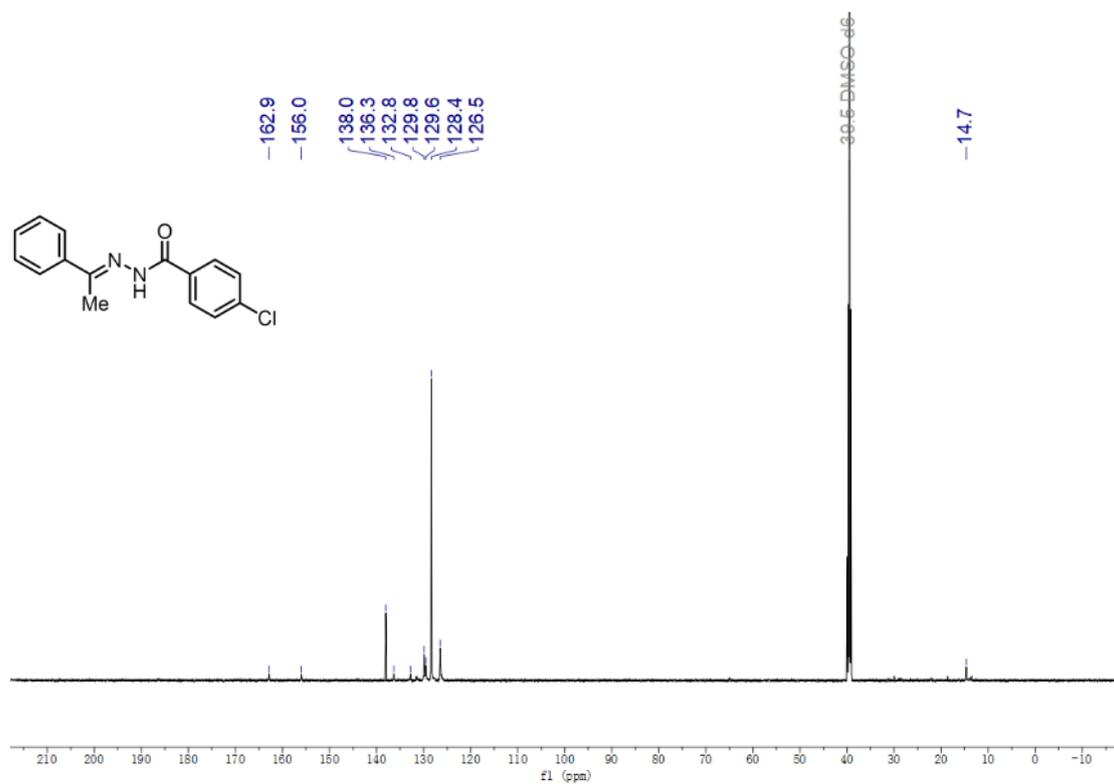


Figure S38. ¹³C NMR (151 MHz, DMSO) Spectrum of Compound **6i**

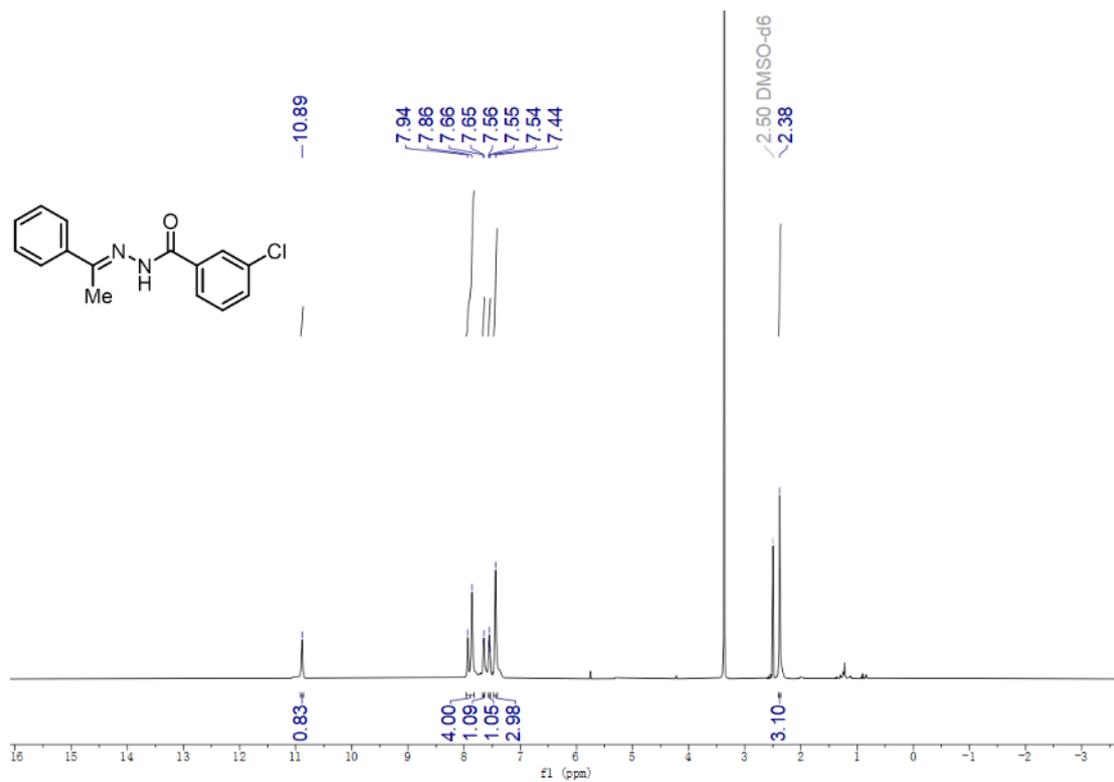


Figure S39. ¹H NMR (600 MHz, DMSO) Spectrum of Compound 6j

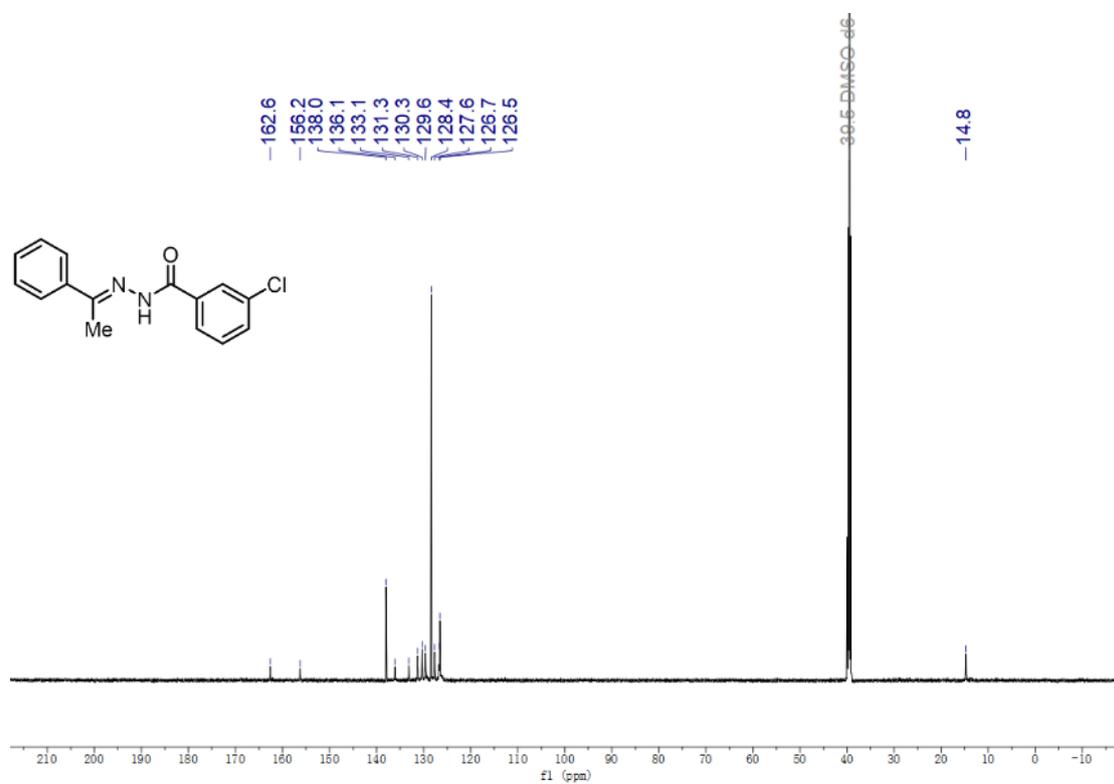


Figure S40. ¹³C NMR (151 MHz, DMSO) Spectrum of Compound 6j

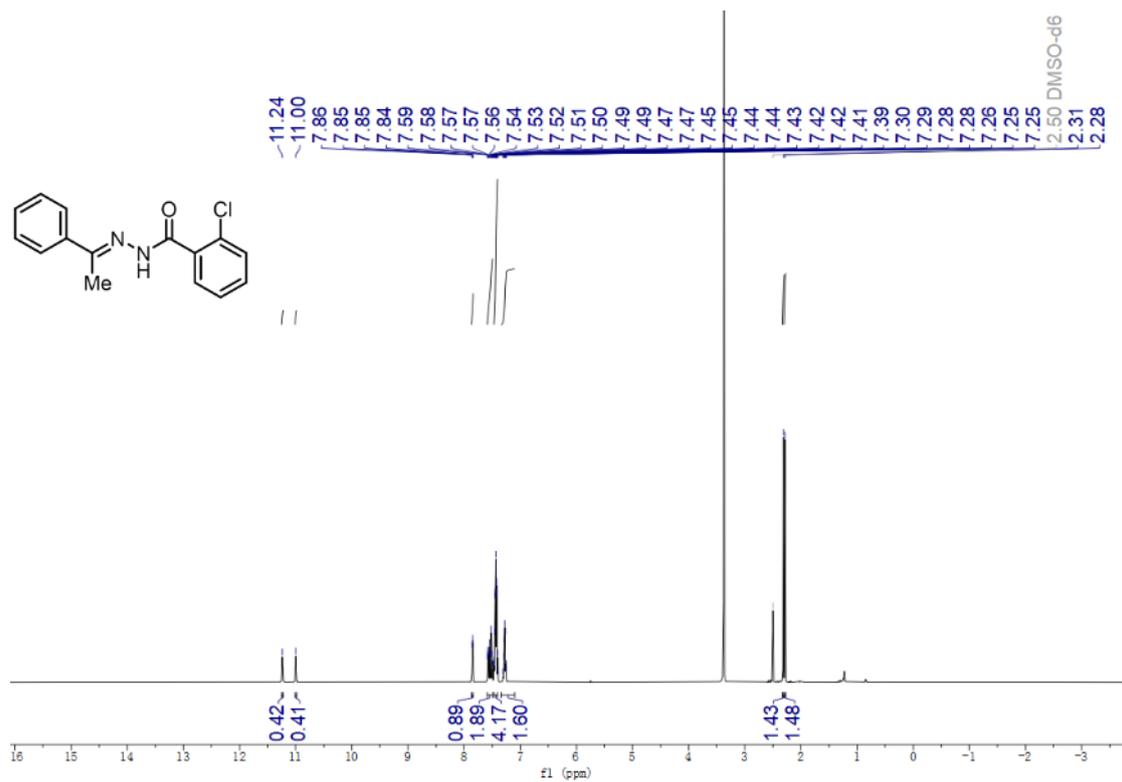


Figure S41. ¹H NMR (600 MHz, DMSO) Spectrum of Compound **6k**

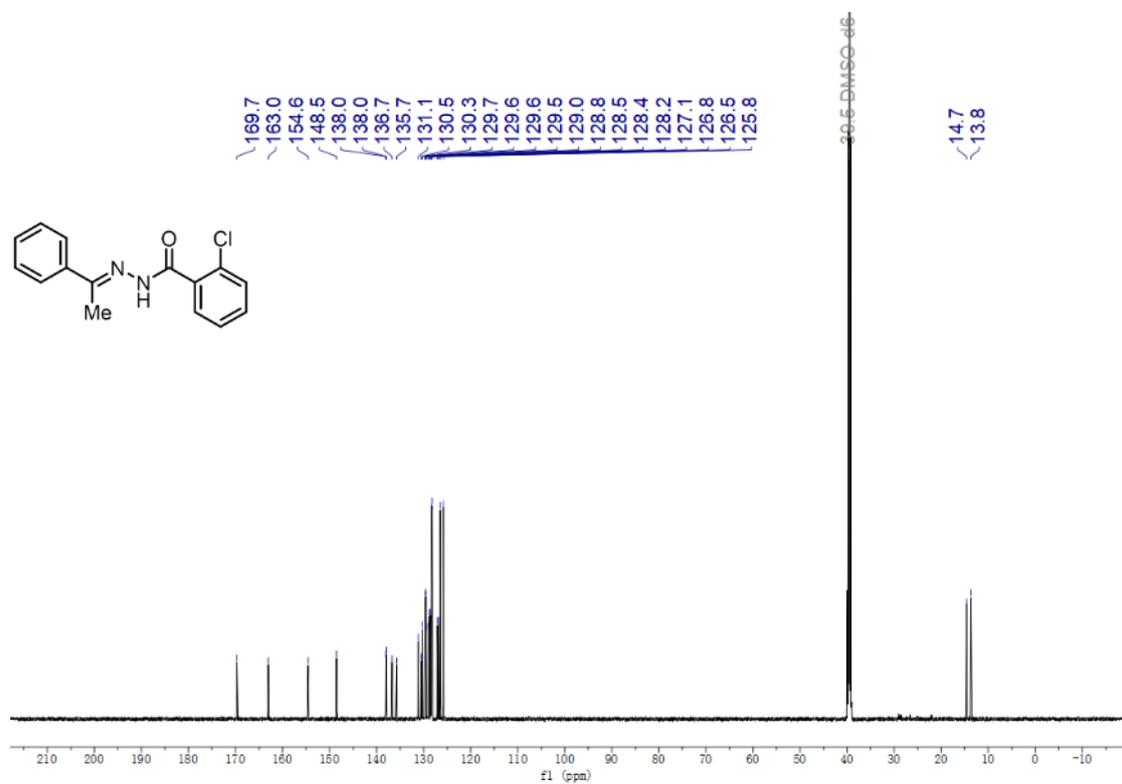


Figure S42. ¹³C NMR (151 MHz, DMSO) Spectrum of Compound **6k**

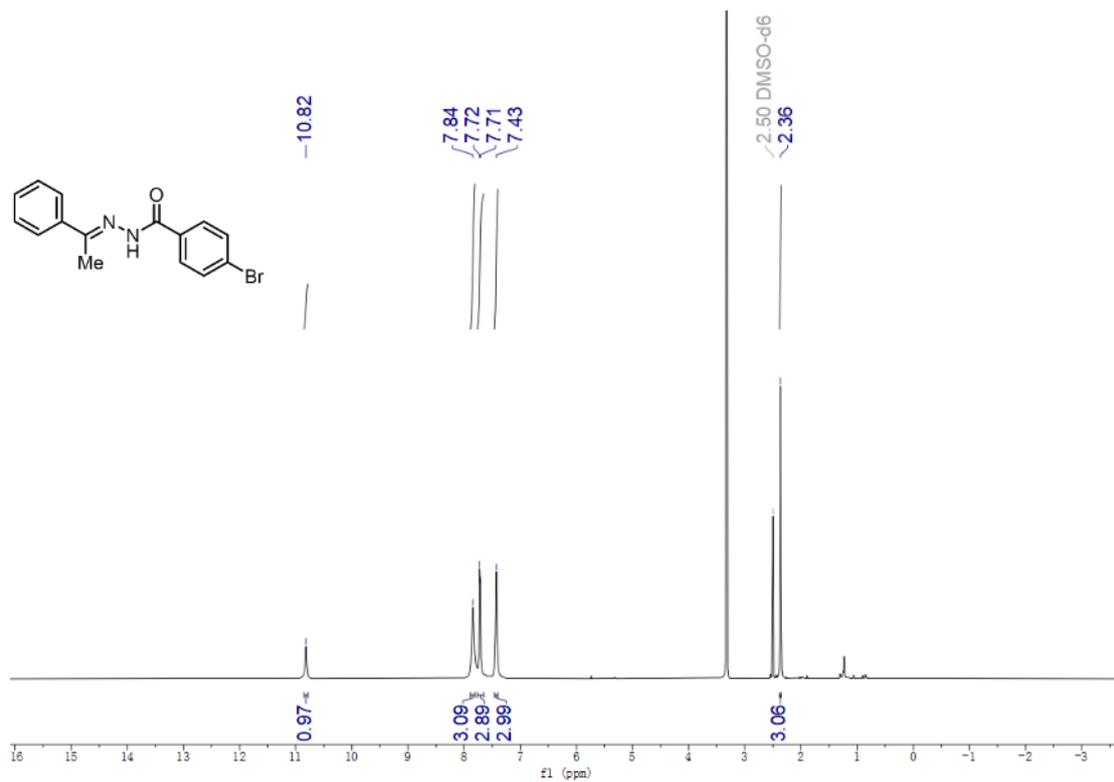


Figure S43. ¹H NMR (600 MHz, DMSO) Spectrum of Compound **6I**

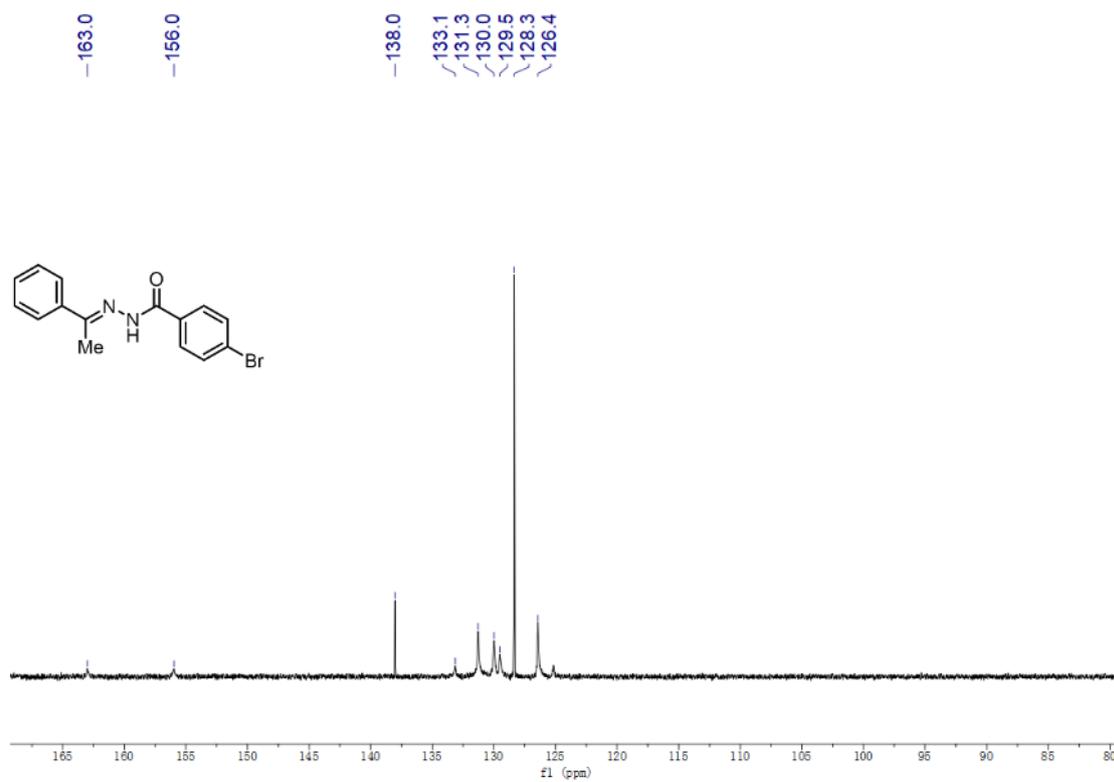


Figure S44. ¹³C NMR (151 MHz, DMSO) Spectrum of Compound **6I**

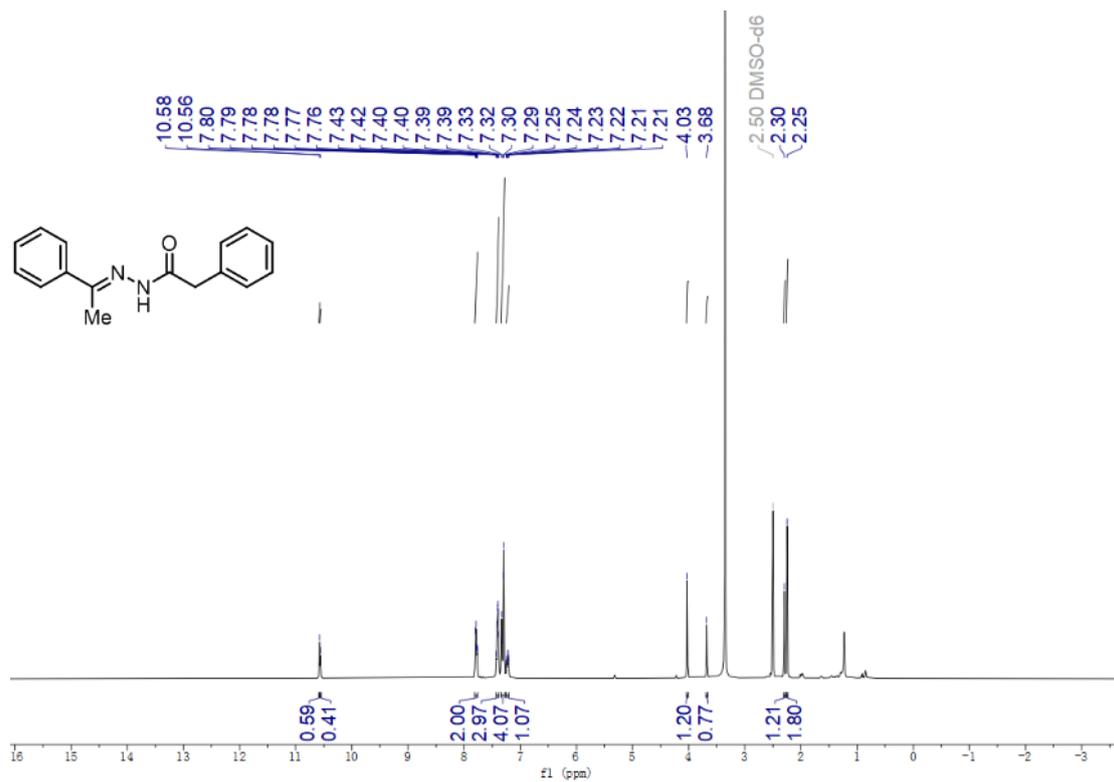


Figure S45. ¹H NMR (600 MHz, DMSO) Spectrum of Compound **6m**

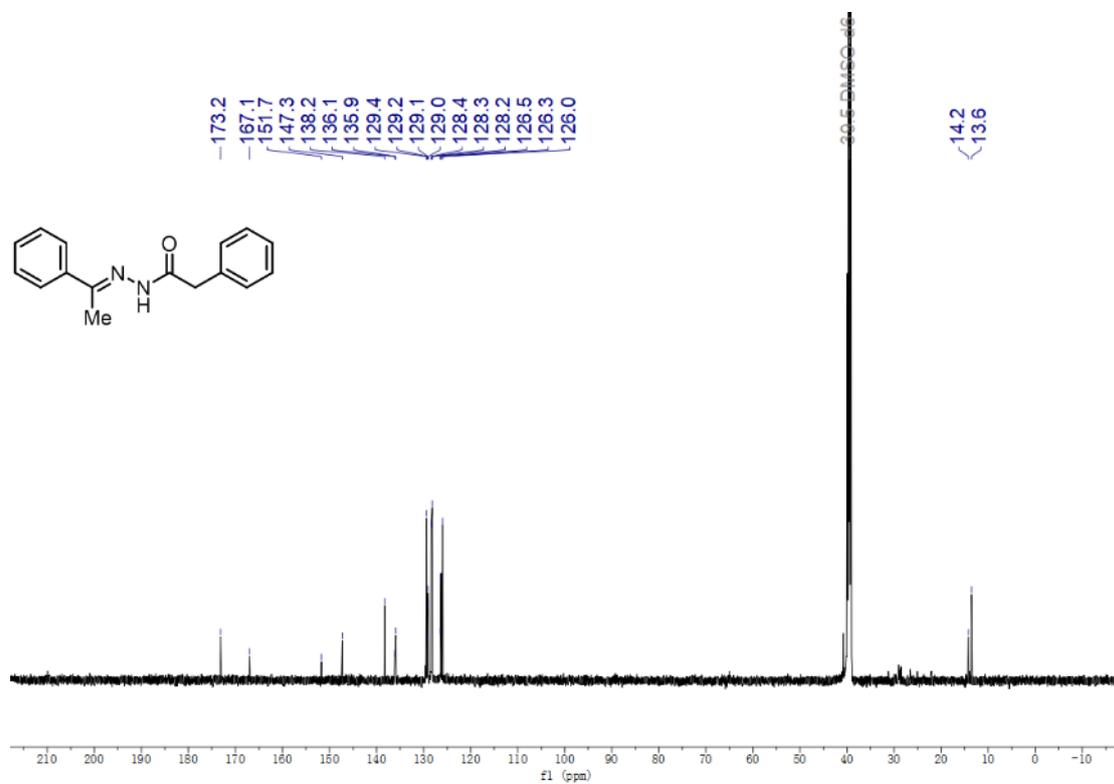


Figure S46. ¹³C NMR (151 MHz, DMSO) Spectrum of Compound **6m**

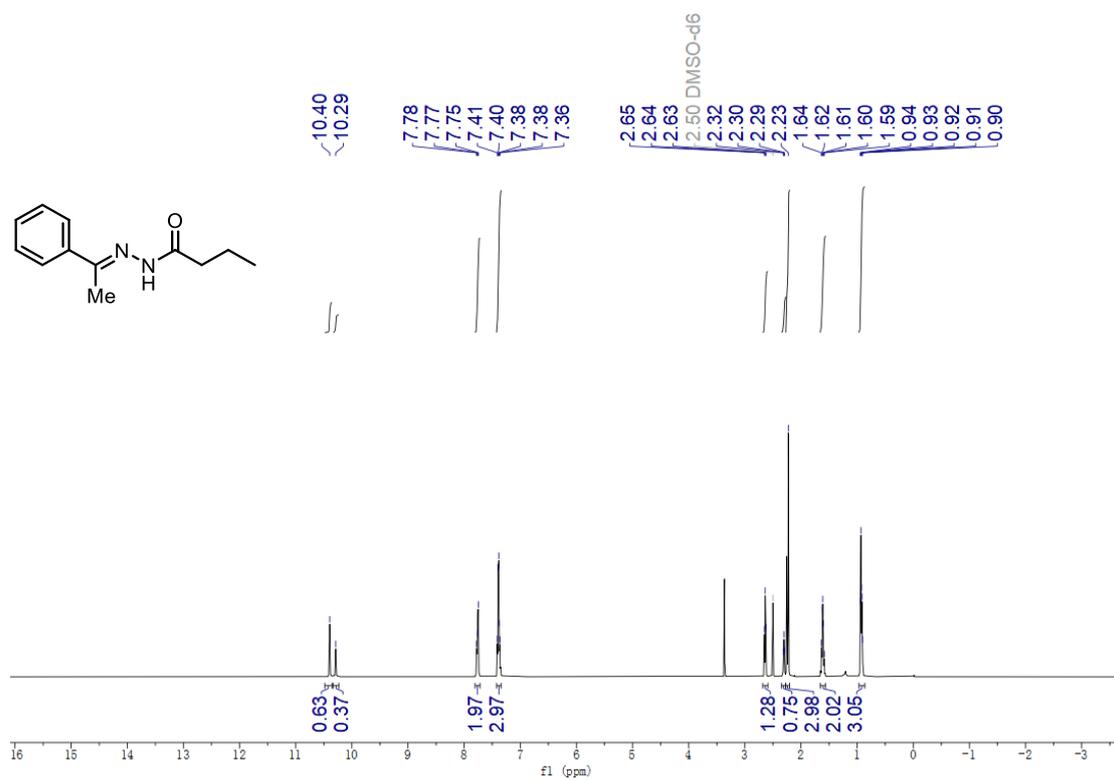


Figure S47. ¹H NMR (600 MHz, DMSO) Spectrum of Compound **6n**

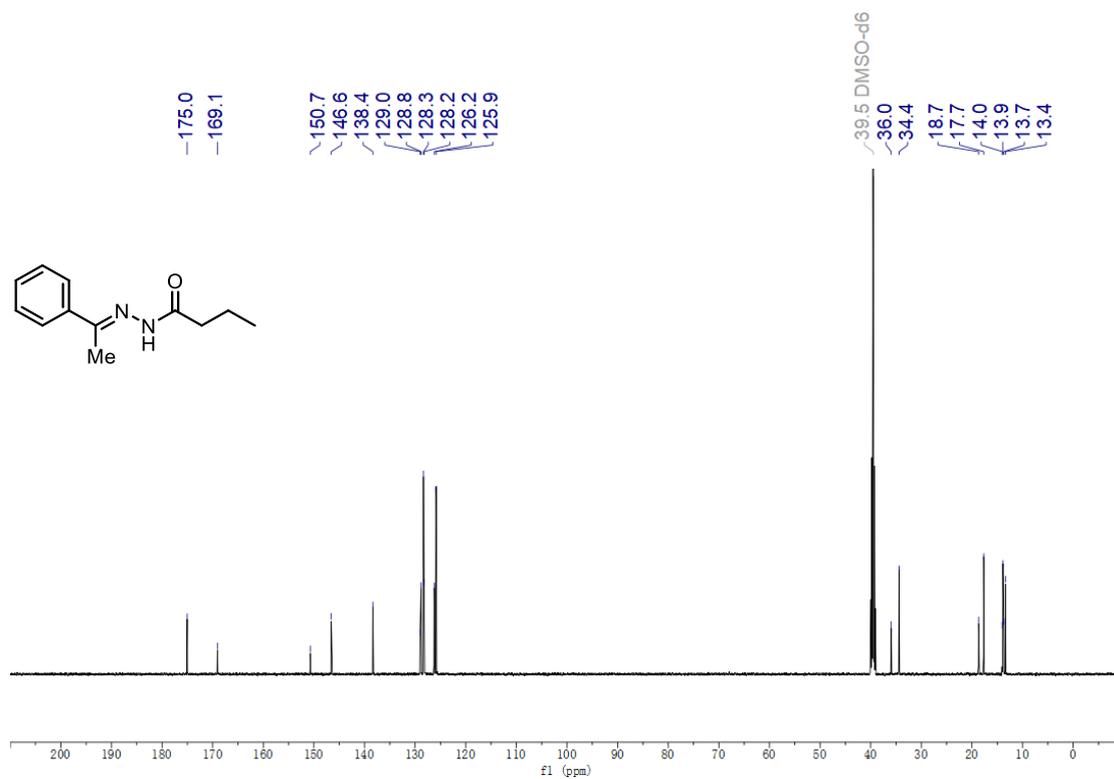


Figure S48. ¹³C NMR (151 MHz, DMSO) Spectrum of Compound **6n**

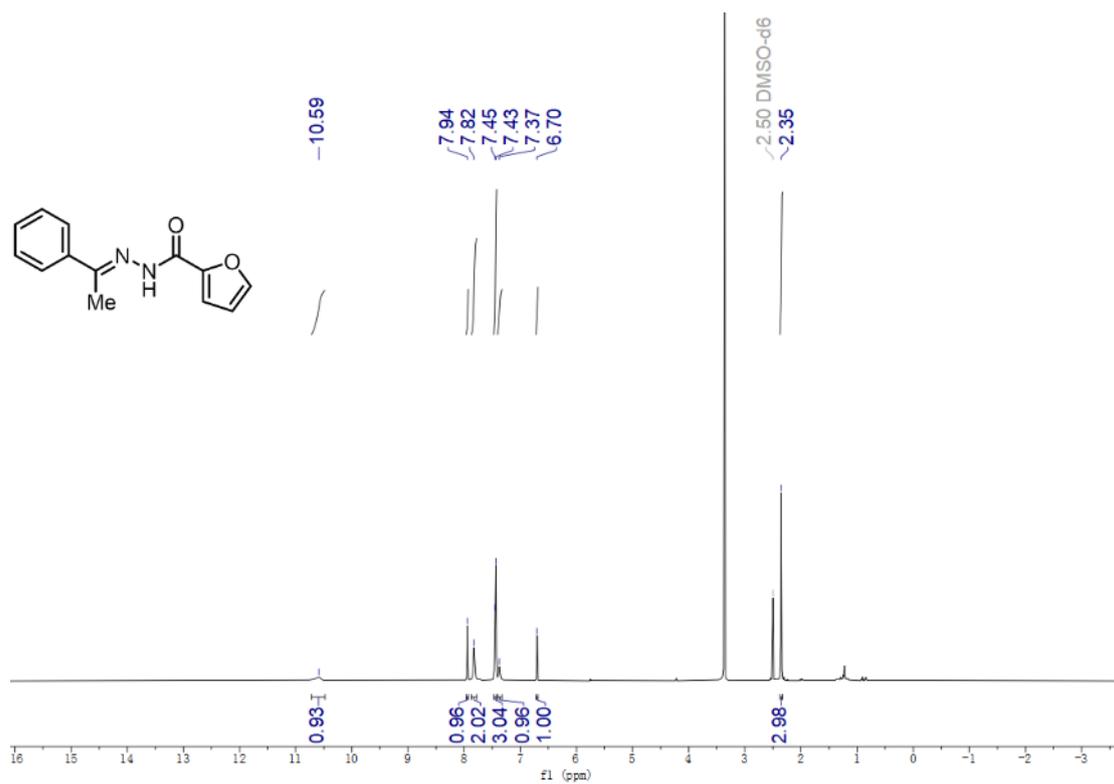


Figure S49. ¹H NMR (600 MHz, DMSO) Spectrum of Compound **60**

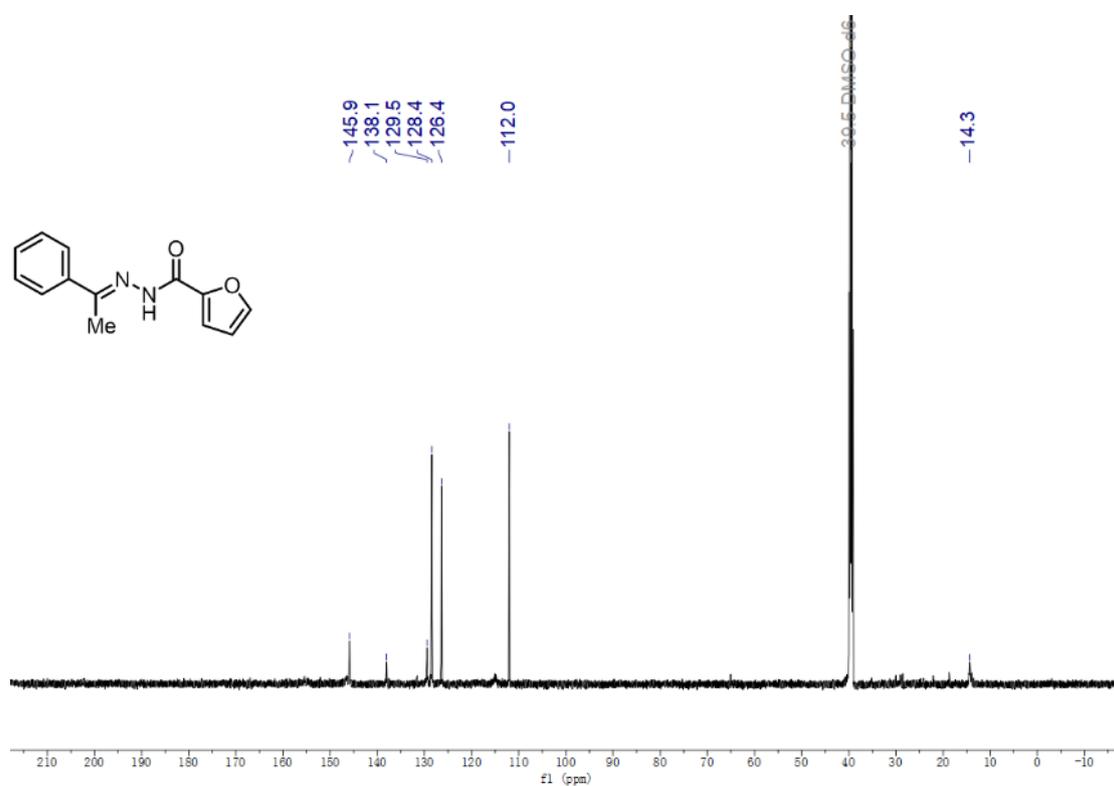


Figure S50. ¹³C NMR (151 MHz, DMSO) Spectrum of Compound **60**

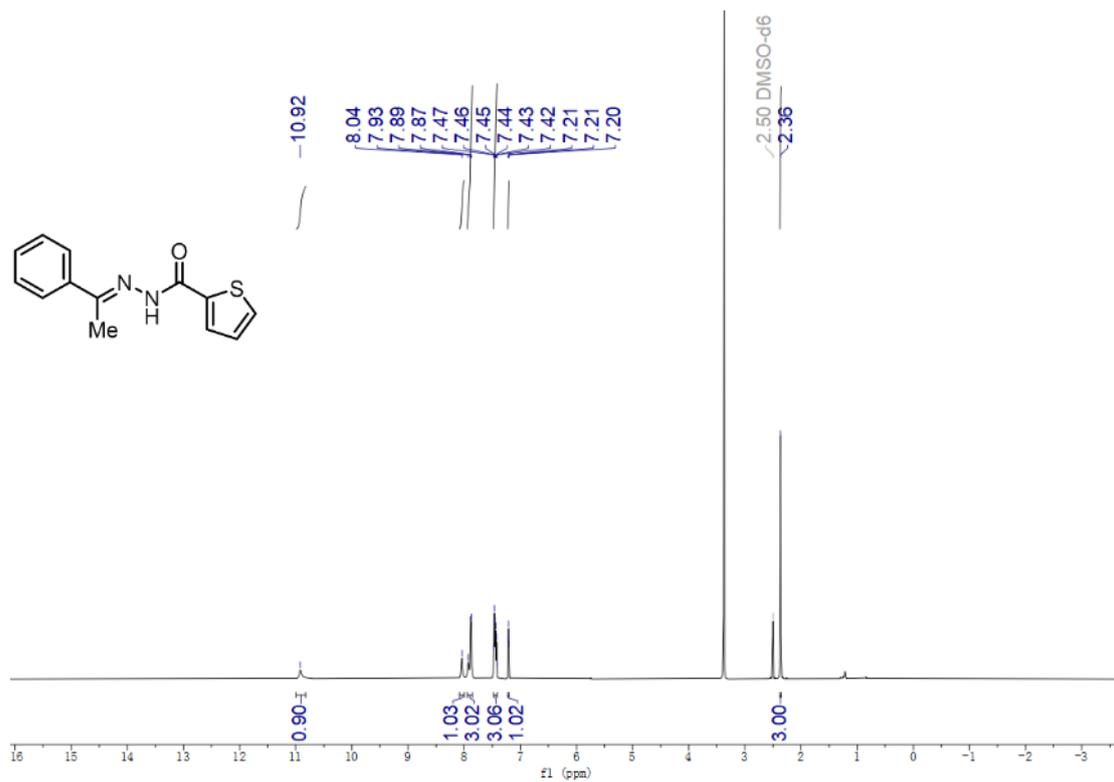


Figure S51. $^1\text{H NMR}$ (600 MHz, DMSO) Spectrum of Compound **6p**

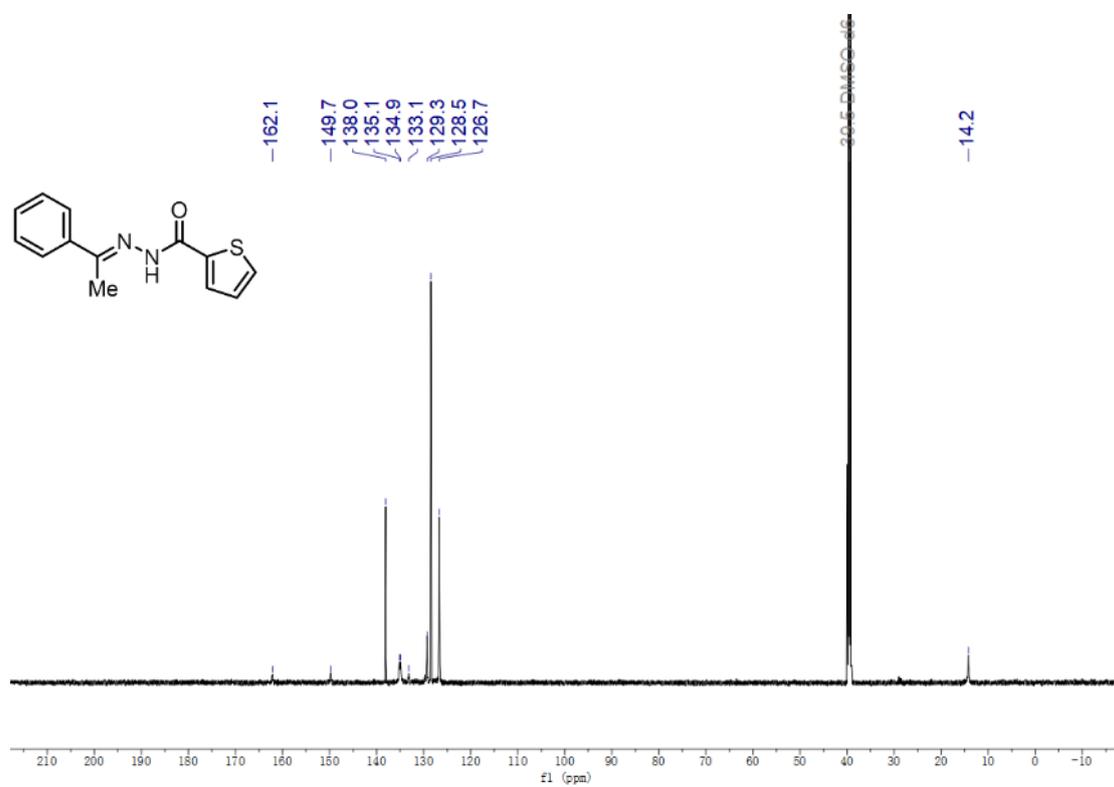


Figure S52. $^{13}\text{C NMR}$ (151 MHz, DMSO) Spectrum of Compound **6p**

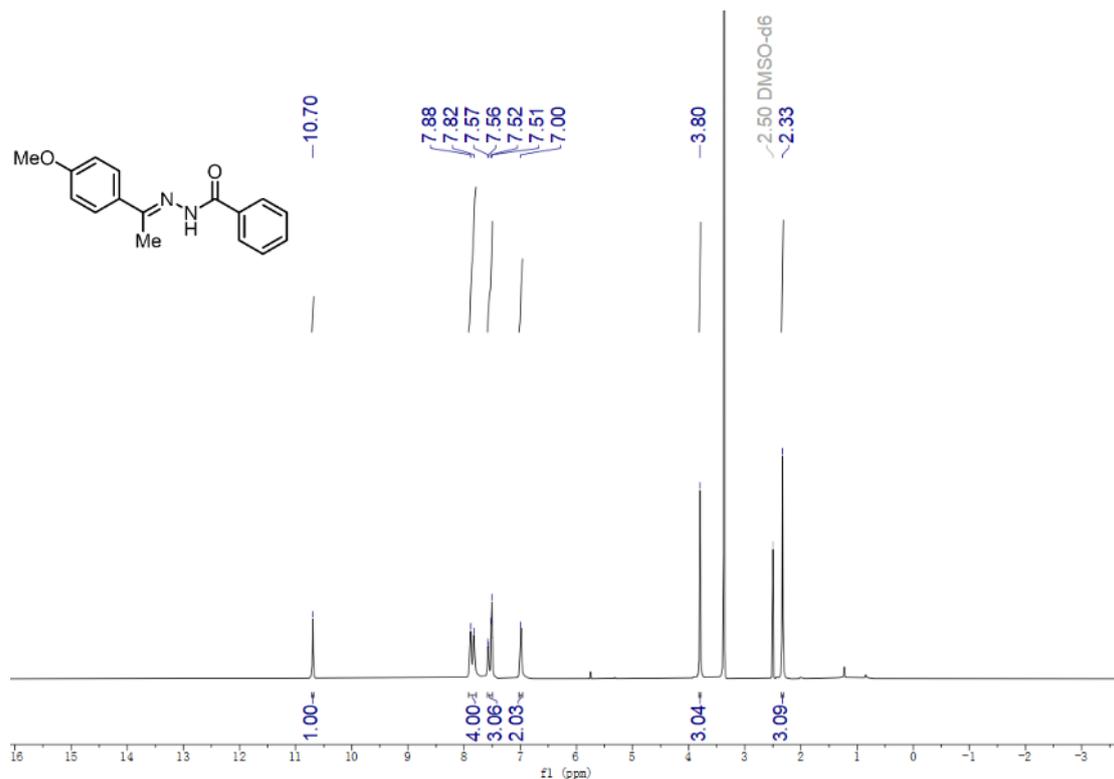


Figure S53. ¹H NMR (600 MHz, DMSO) Spectrum of Compound 6aa

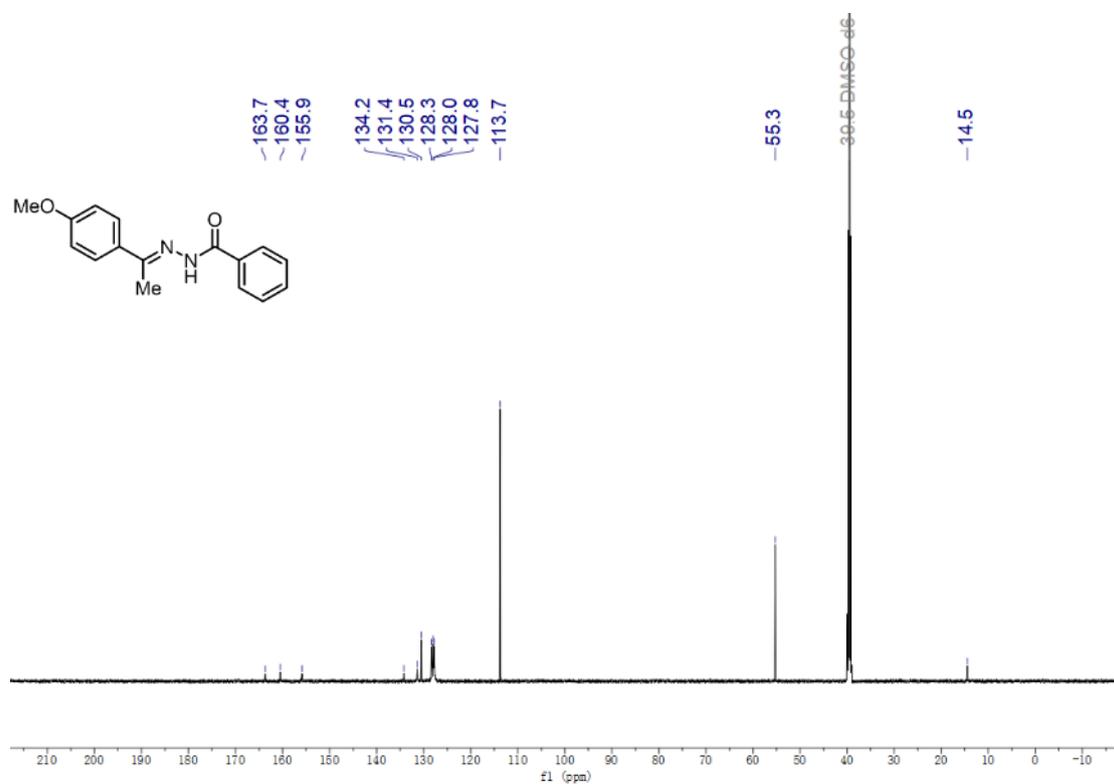


Figure S54. ¹³C NMR (151 MHz, DMSO) Spectrum of Compound 6aa

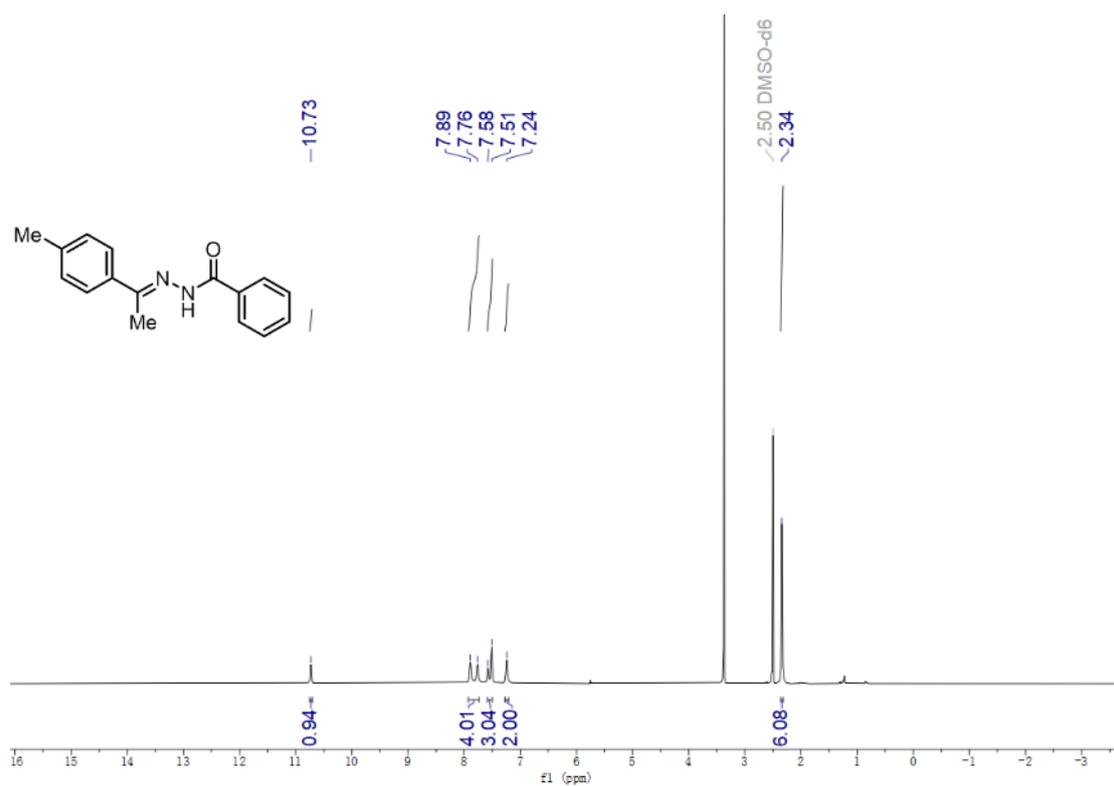


Figure S53. ¹H NMR (600 MHz, DMSO) Spectrum of Compound **6ab**

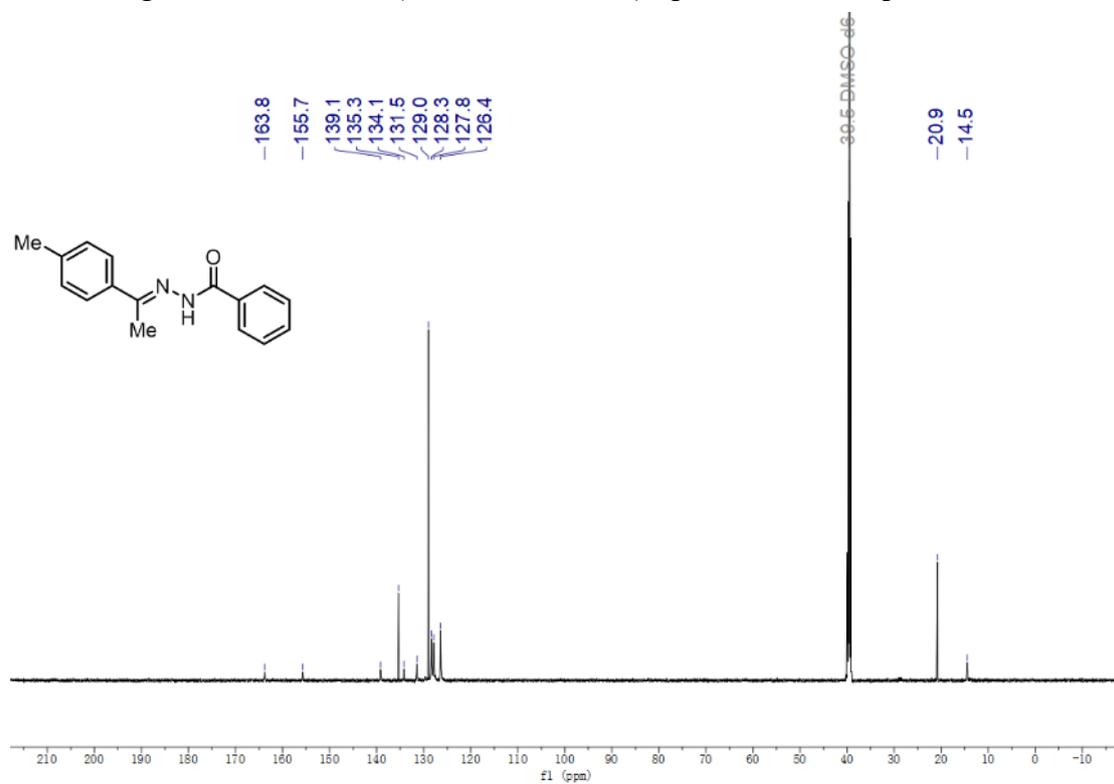


Figure S54. ¹³C NMR (151 MHz, DMSO) Spectrum of Compound **6ab**

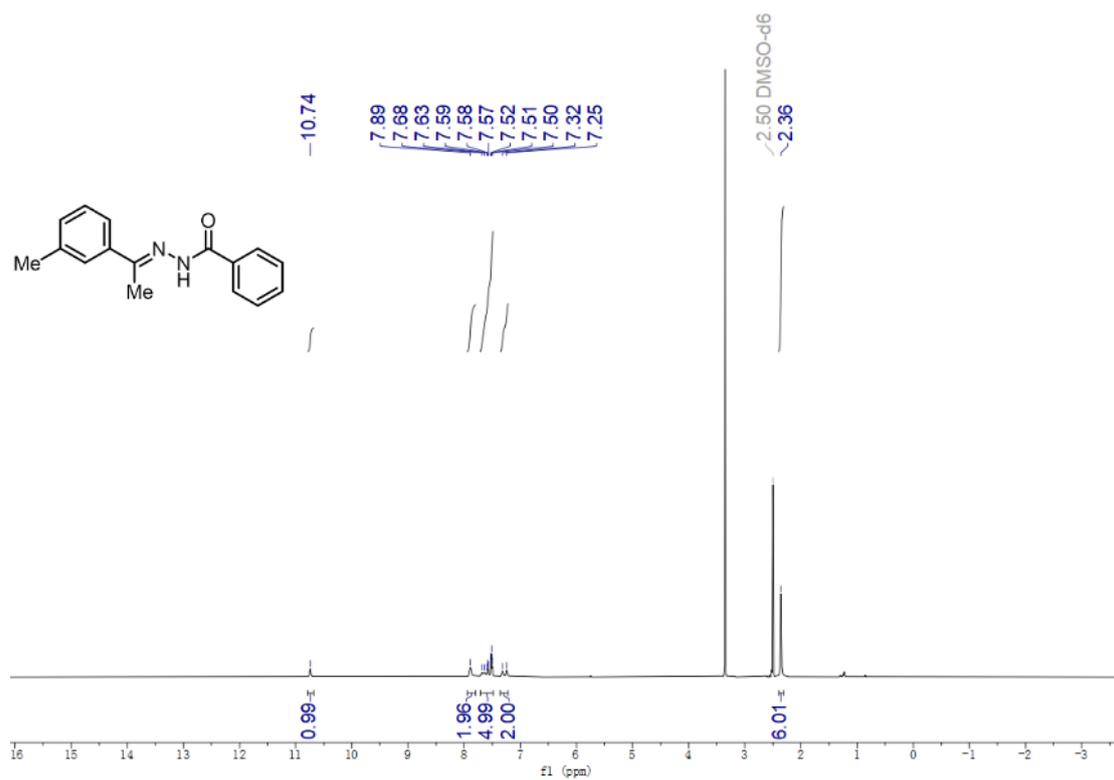


Figure S55. ¹H NMR (600 MHz, DMSO) Spectrum of Compound **6ac**

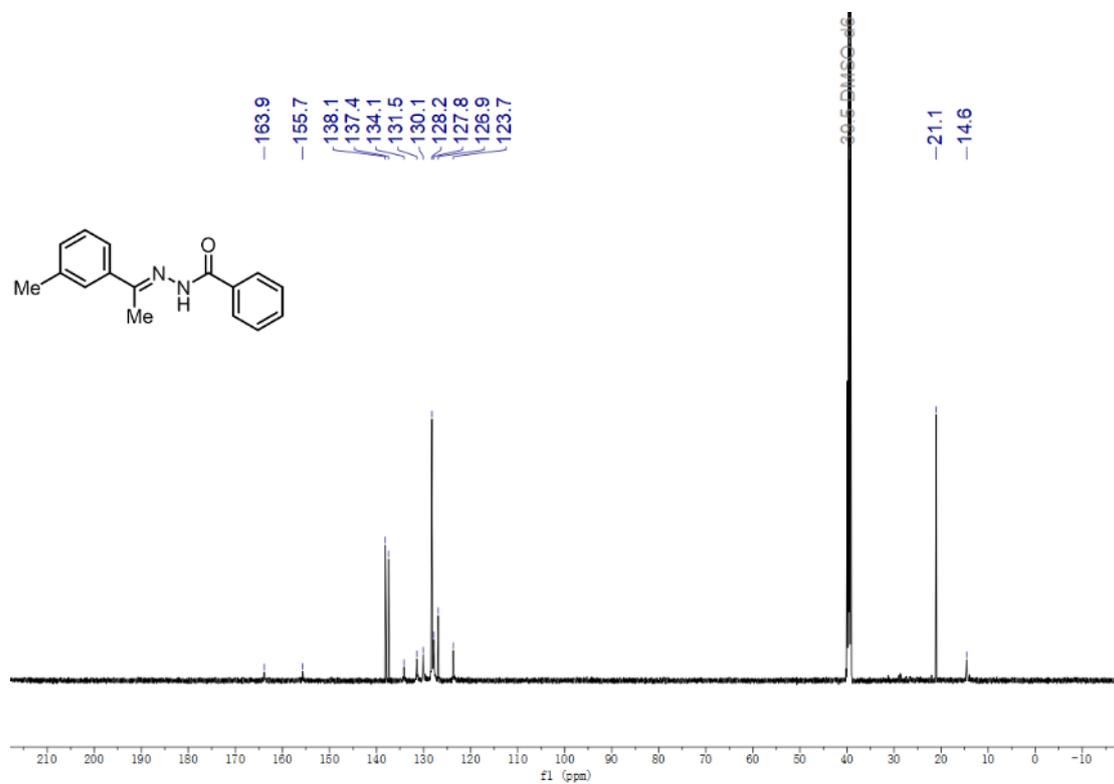


Figure S56. ¹³C NMR (151 MHz, DMSO) Spectrum of Compound **6ac**

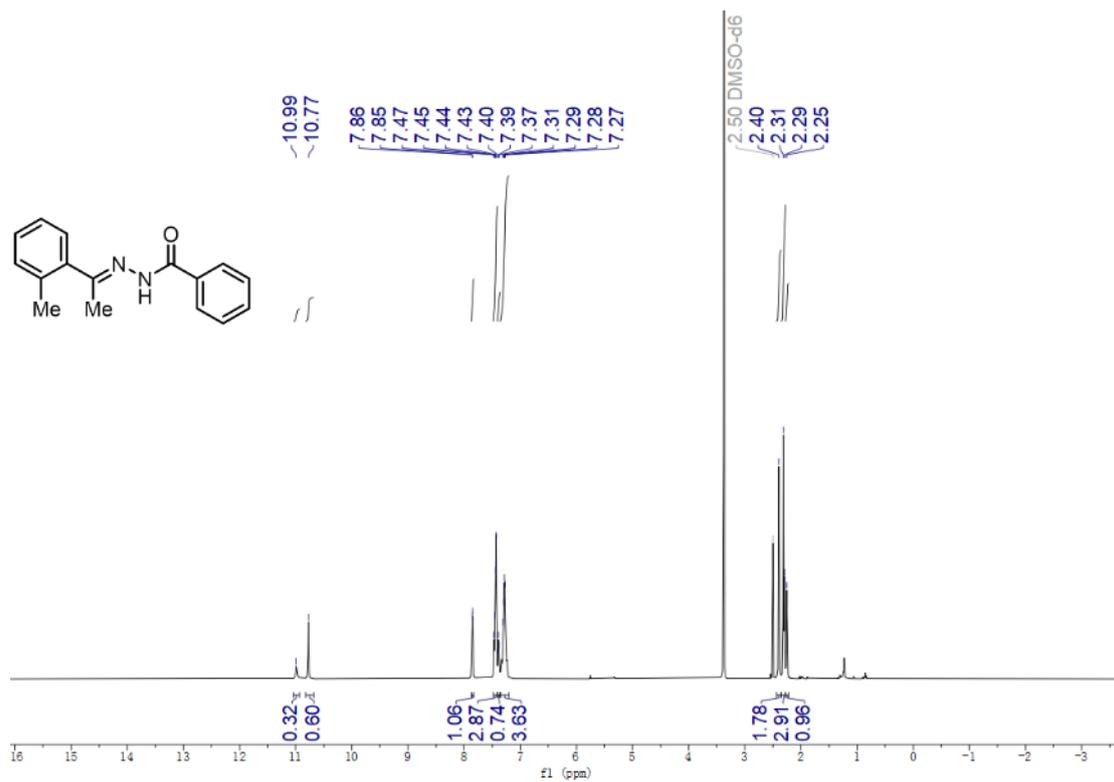


Figure S57. ¹H NMR (600 MHz, DMSO) Spectrum of Compound **6ad**

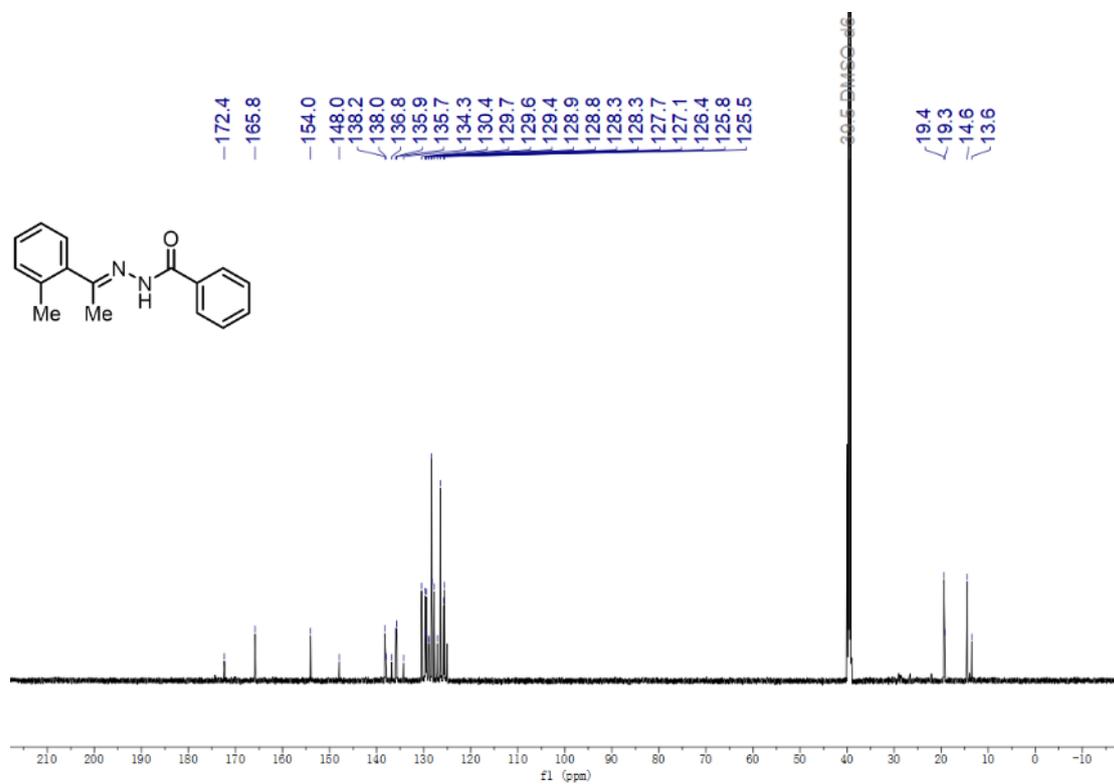


Figure S58. ¹³C NMR (151 MHz, DMSO) Spectrum of Compound **6ad**

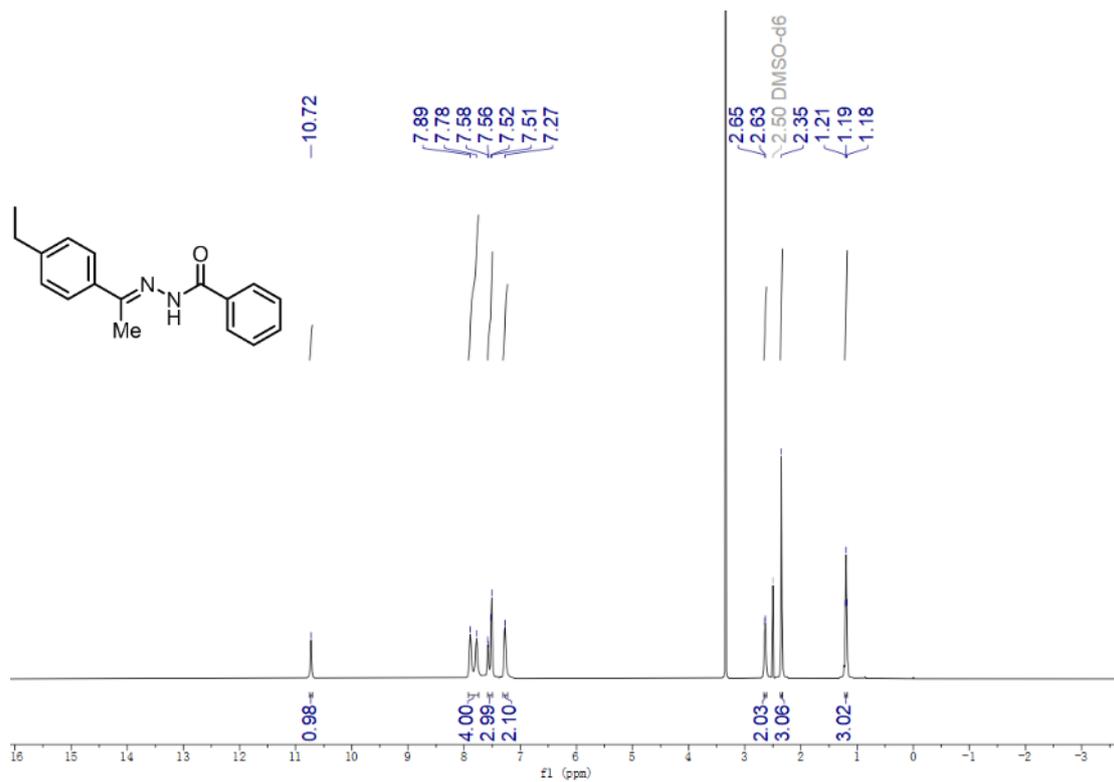


Figure S59. ¹H NMR (600 MHz, DMSO) Spectrum of Compound **6ae**

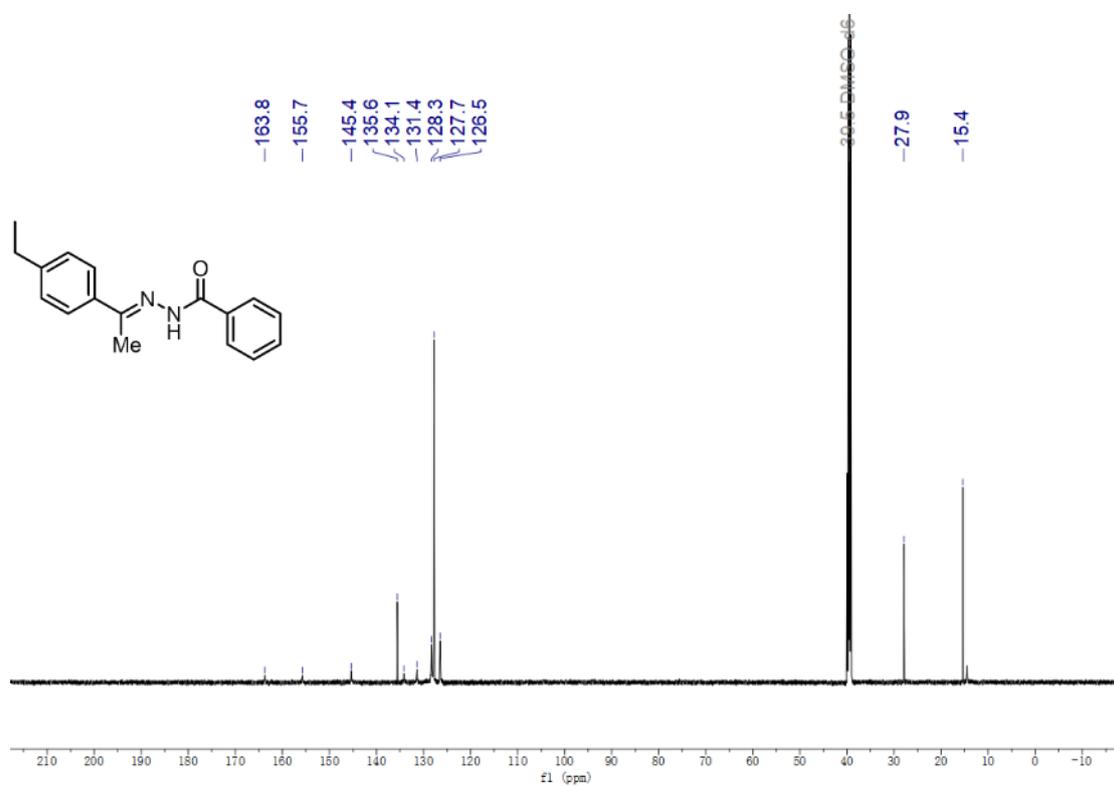


Figure S60. ¹³C NMR (151 MHz, DMSO) Spectrum of Compound **6ae**

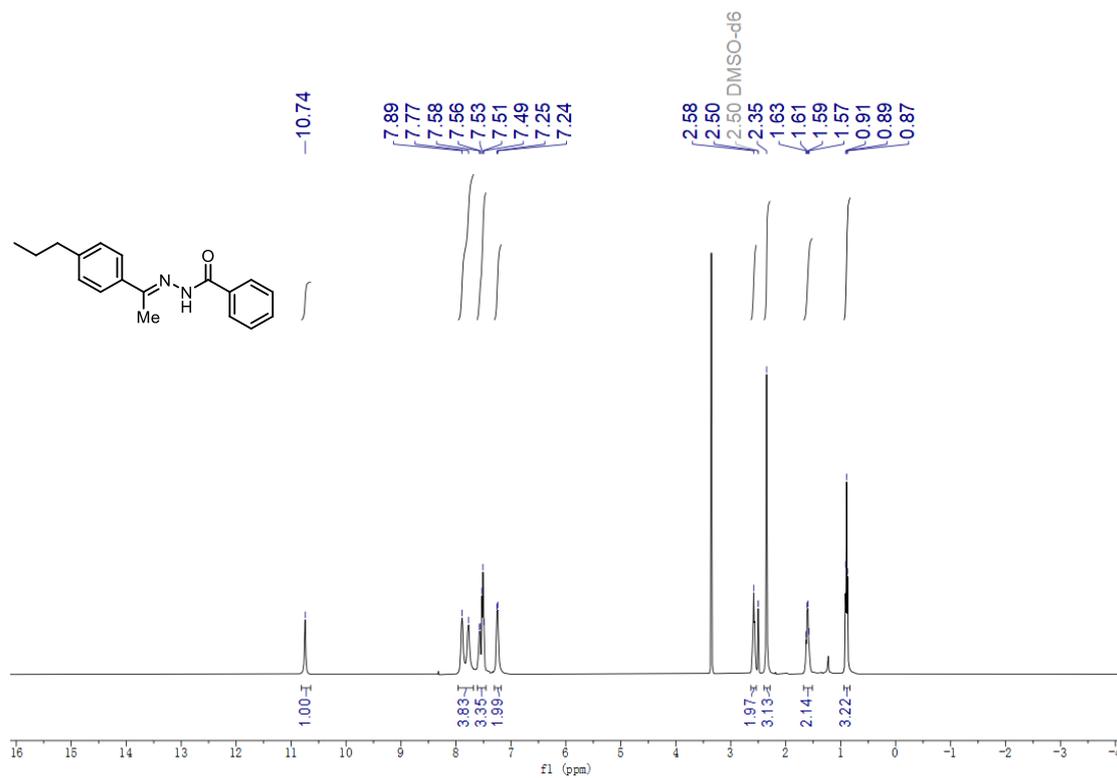


Figure S61. ¹H NMR (400 MHz, DMSO) Spectrum of Compound **6af**

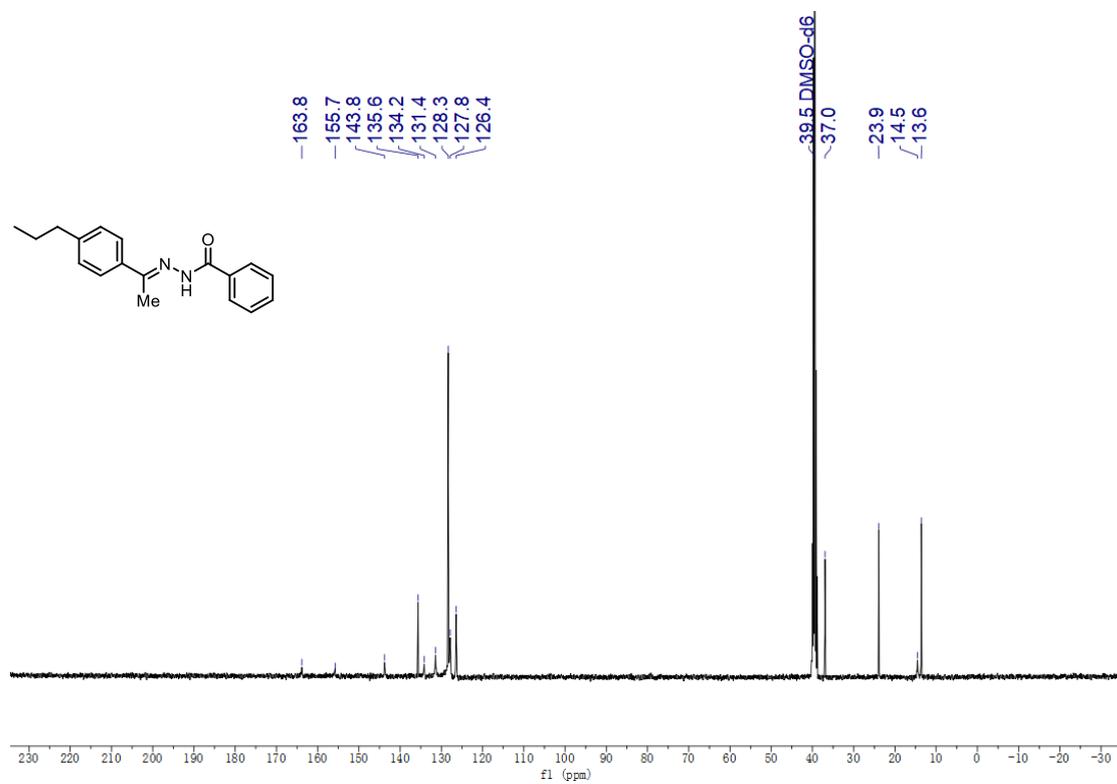


Figure S62. ¹³C NMR (101 MHz, DMSO) Spectrum of Compound **6af**

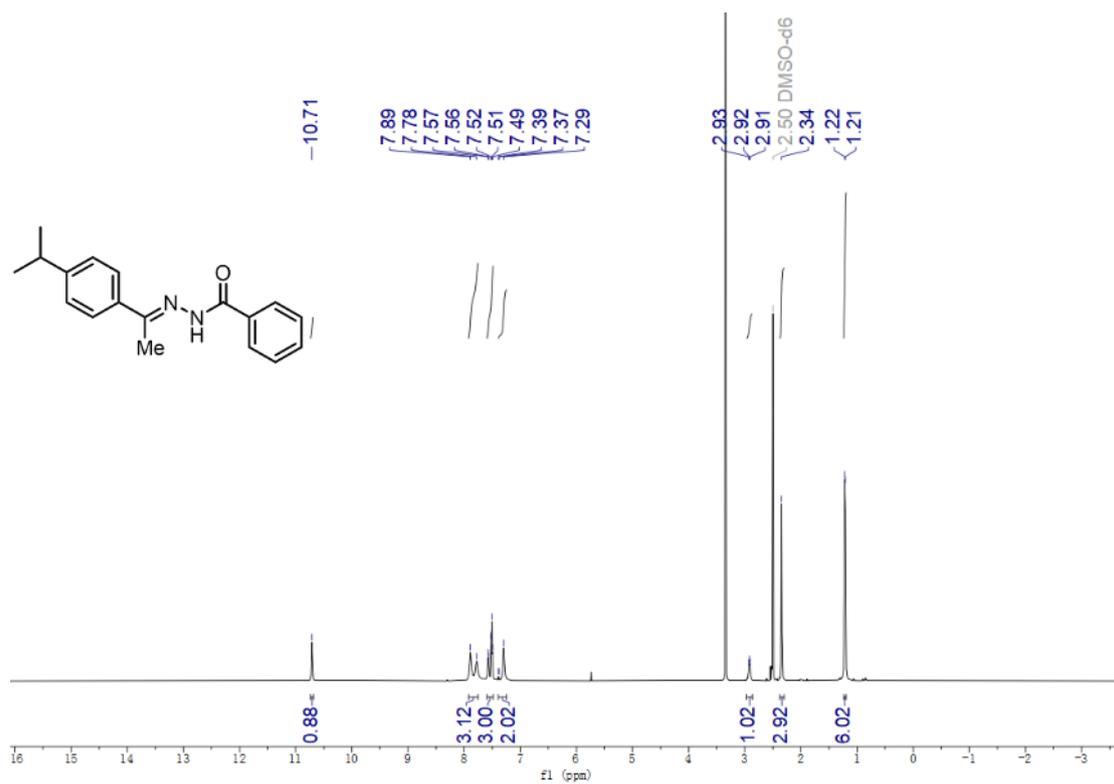


Figure S63. ¹H NMR (600 MHz, DMSO) Spectrum of Compound **6ag**

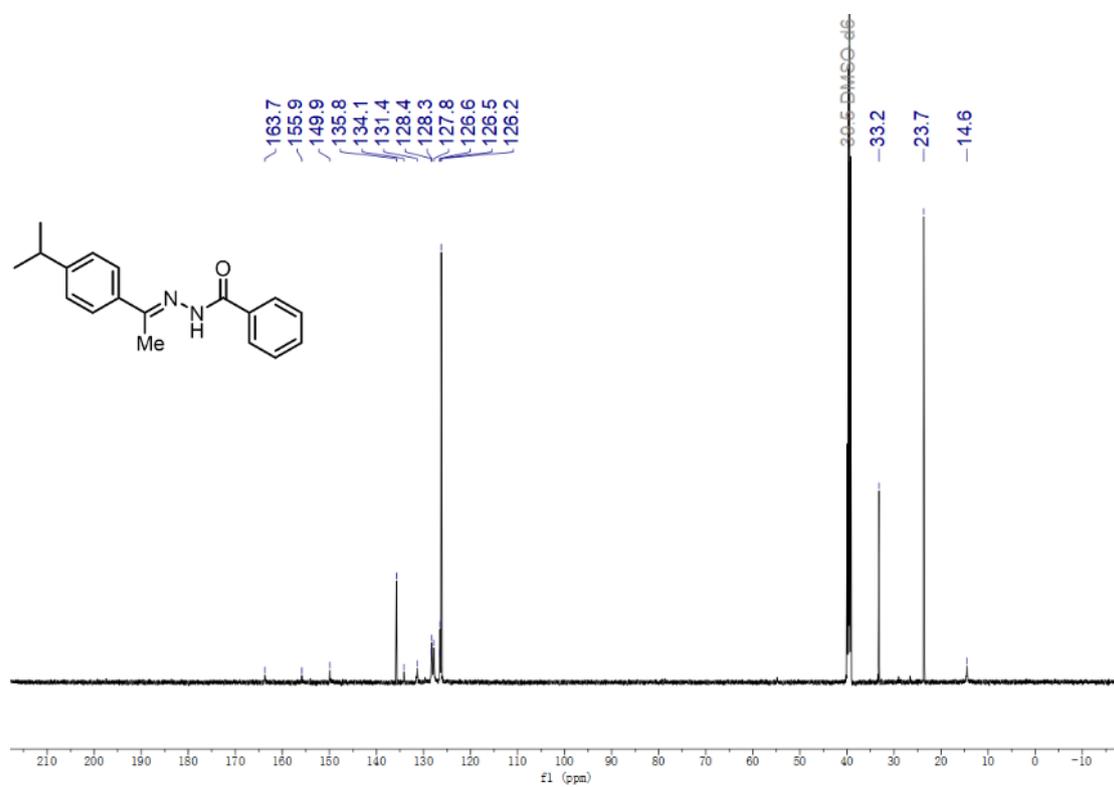


Figure S64. ¹³C NMR (151 MHz, DMSO) Spectrum of Compound **6ag**

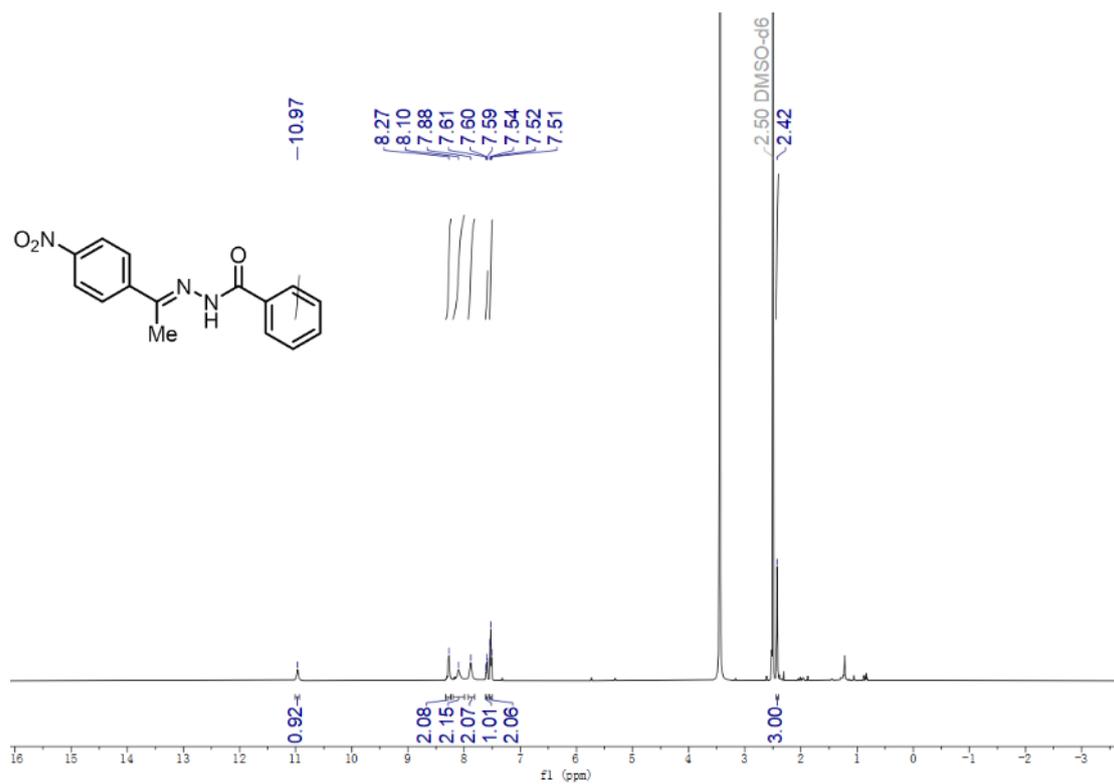


Figure S65. ¹H NMR (600 MHz, DMSO) Spectrum of Compound **6ah**

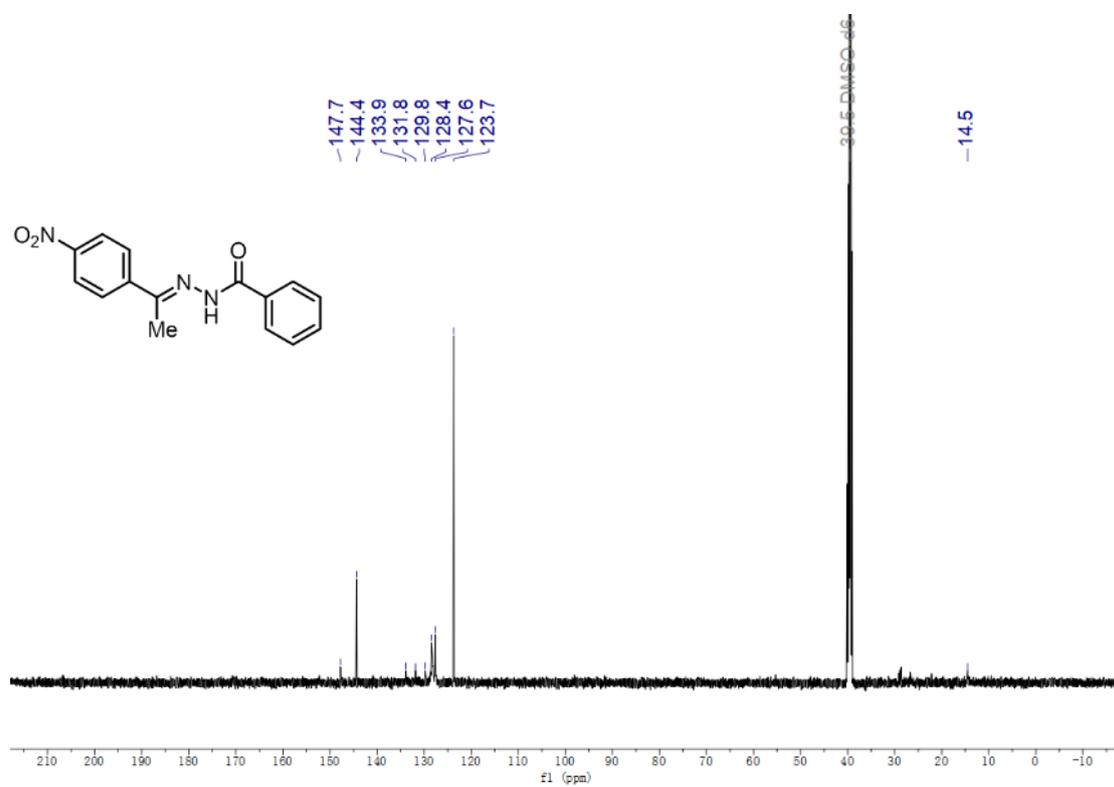


Figure S66. ¹³C NMR (151 MHz, DMSO) Spectrum of Compound **6ah**

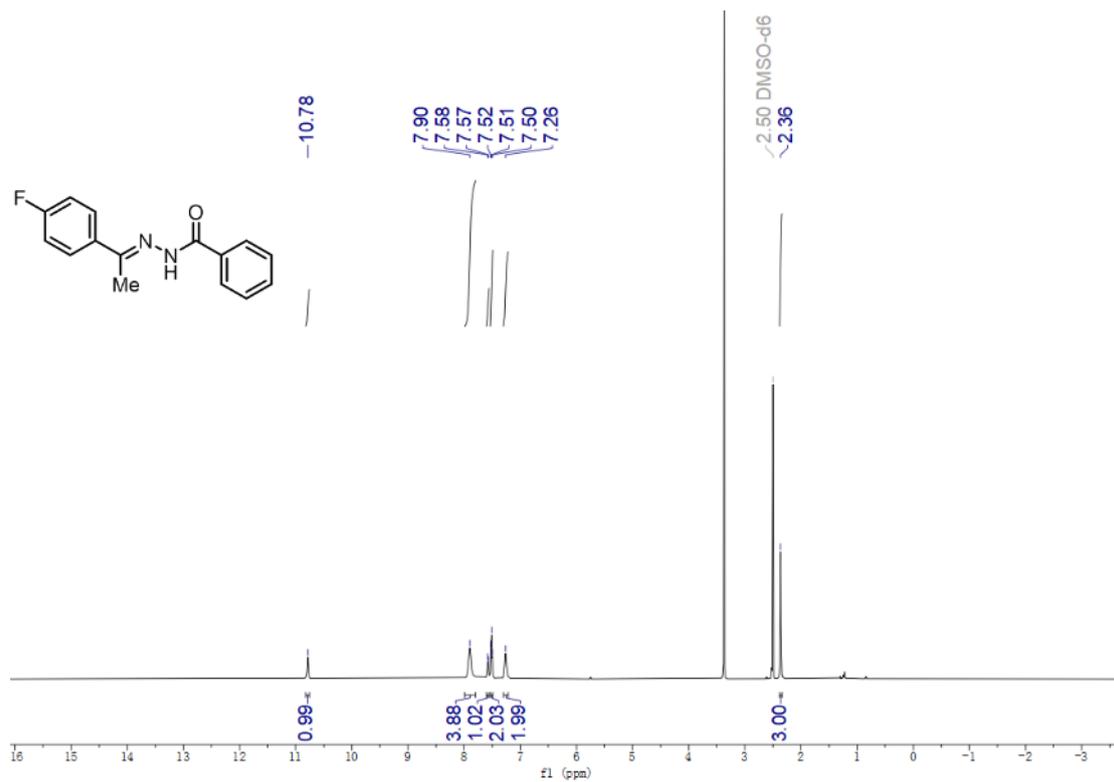


Figure S67. ¹H NMR (600 MHz, DMSO) Spectrum of Compound **6ai**

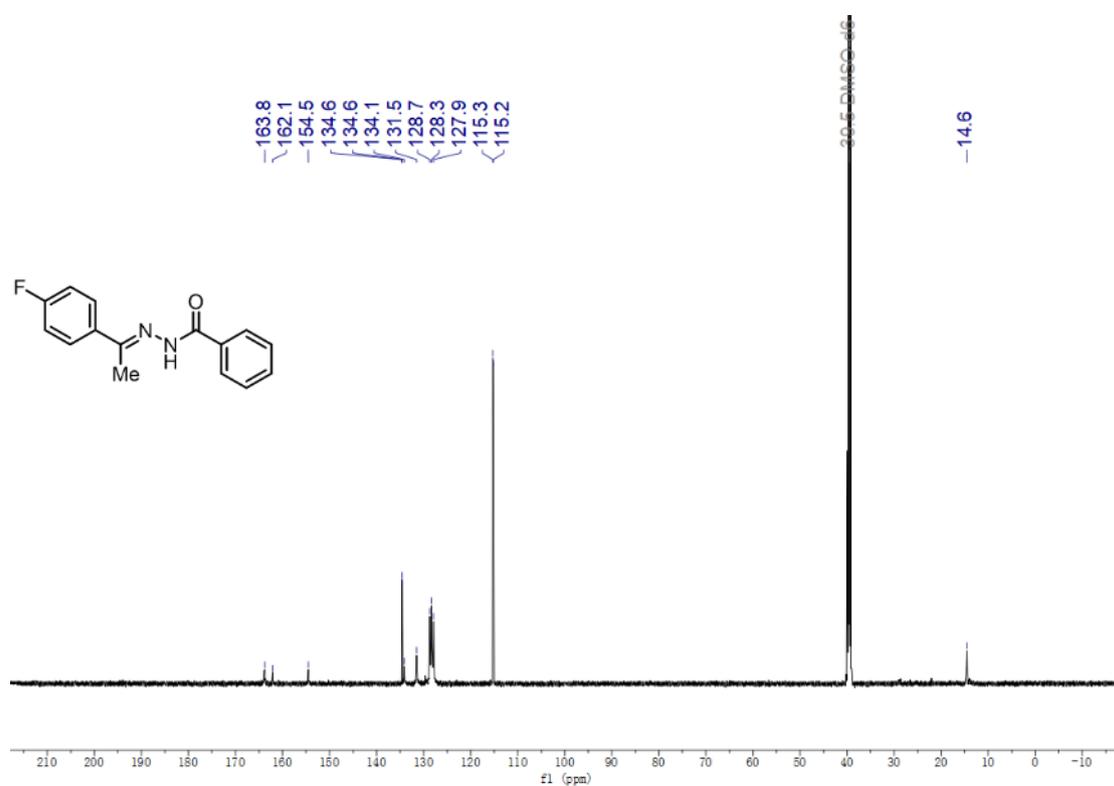


Figure S68. ¹³C NMR (151 MHz, DMSO) Spectrum of Compound **6ai**

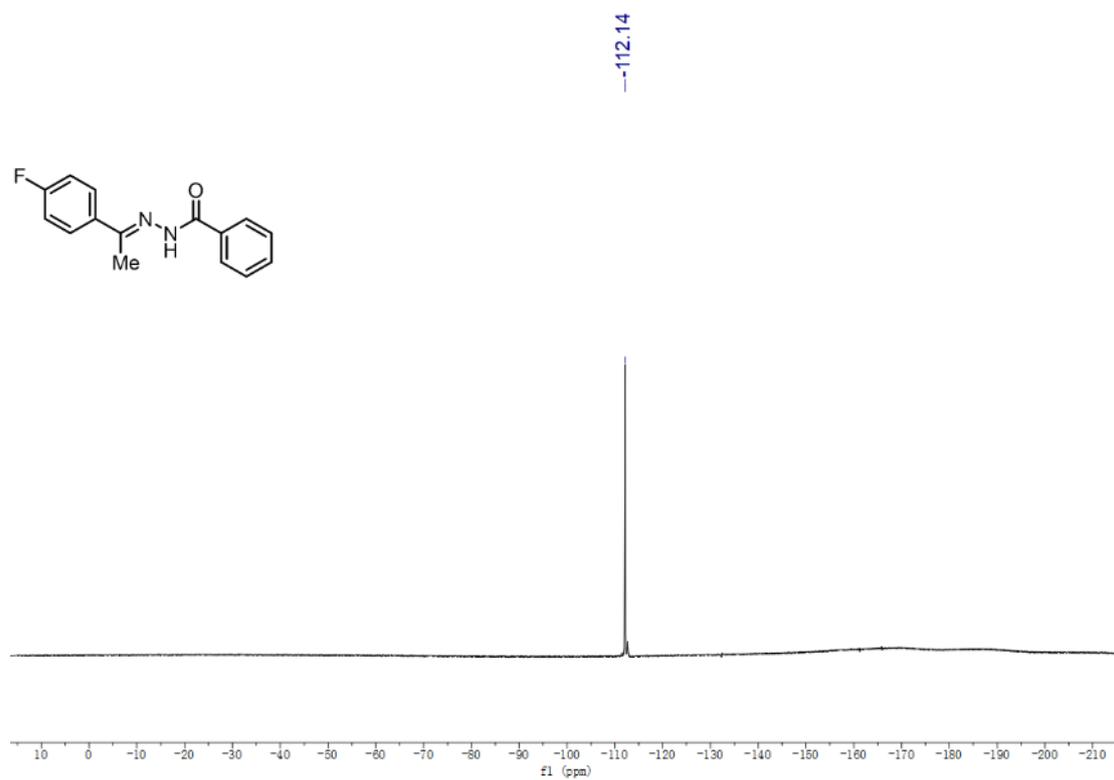


Figure S69. ^{19}F NMR (565 MHz, $\text{DMSO-}d_6$) Spectrum of Compound **6ai**

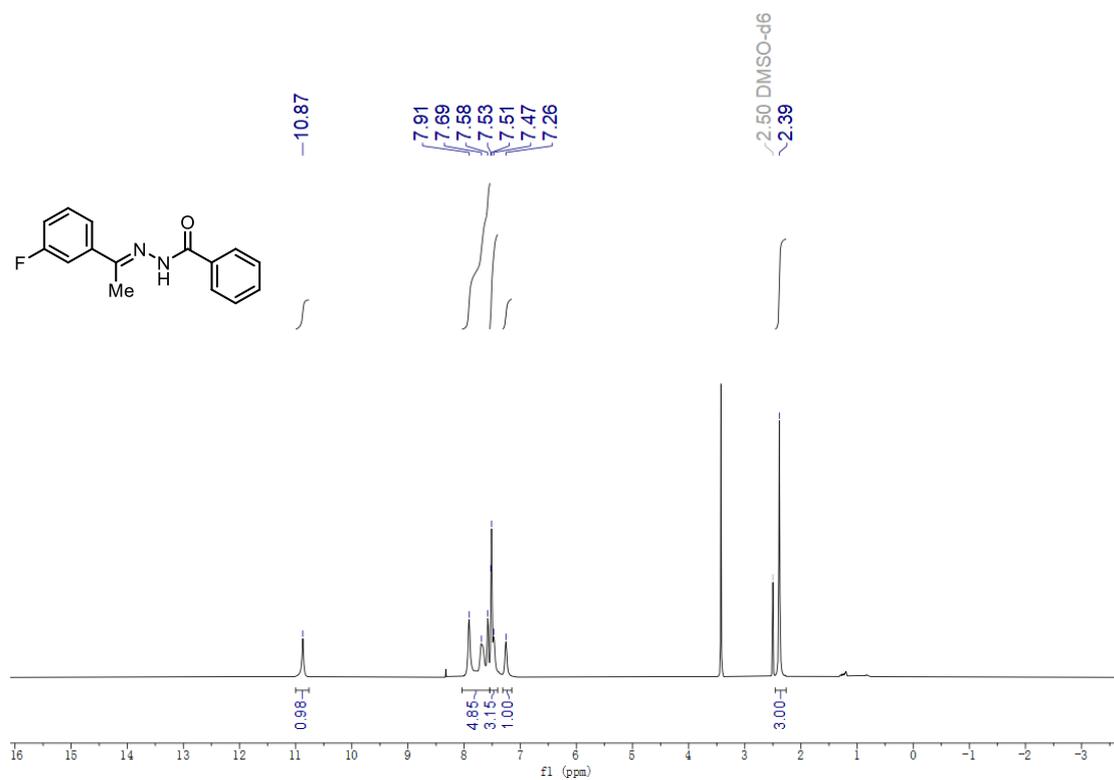


Figure S70. ^1H NMR (600 MHz, DMSO) Spectrum of Compound **6aj**

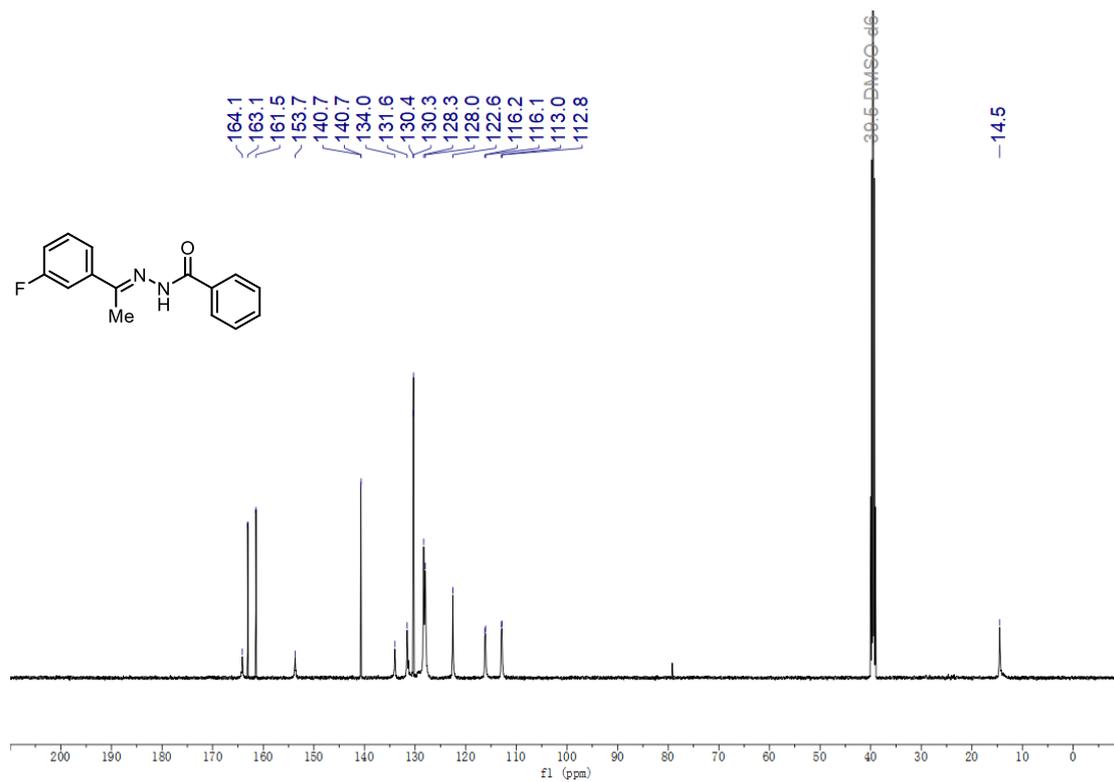


Figure S71. ¹³C NMR (151 MHz, DMSO) Spectrum of Compound **6aj**

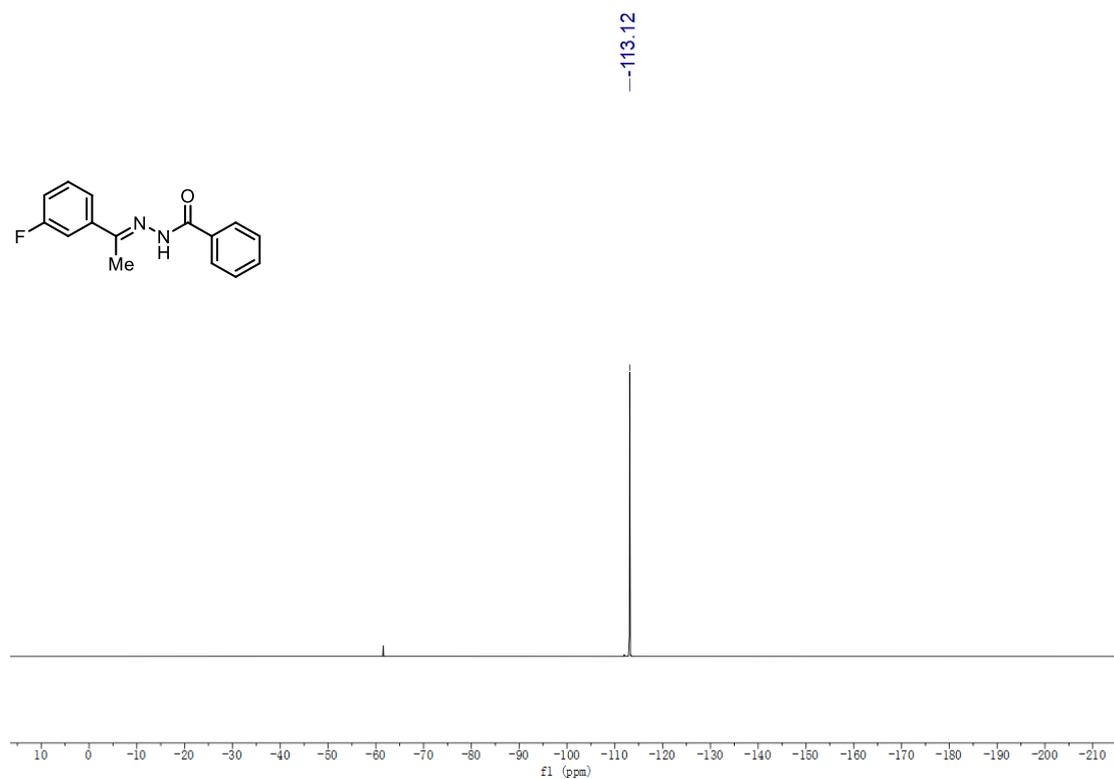


Figure S72. ¹⁹F NMR (565 MHz, DMSO-*d*₆) Spectrum of Compound **6aj**

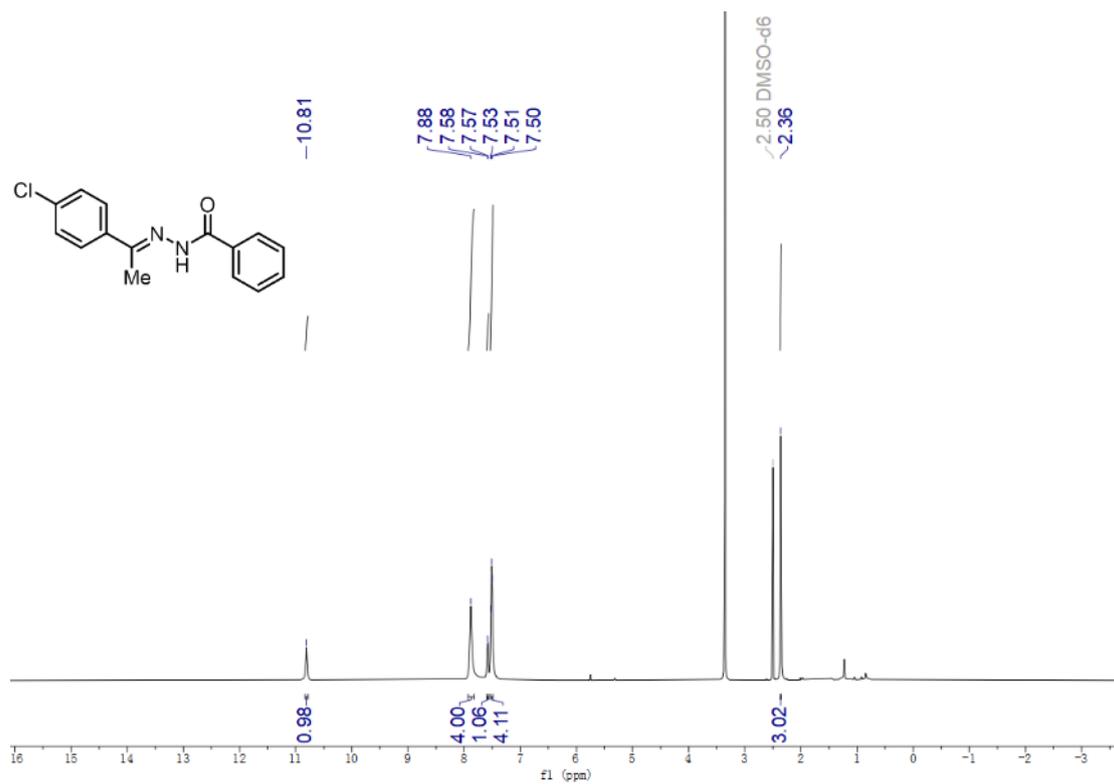


Figure S73. ¹H NMR (600 MHz, DMSO) Spectrum of Compound **6ak**

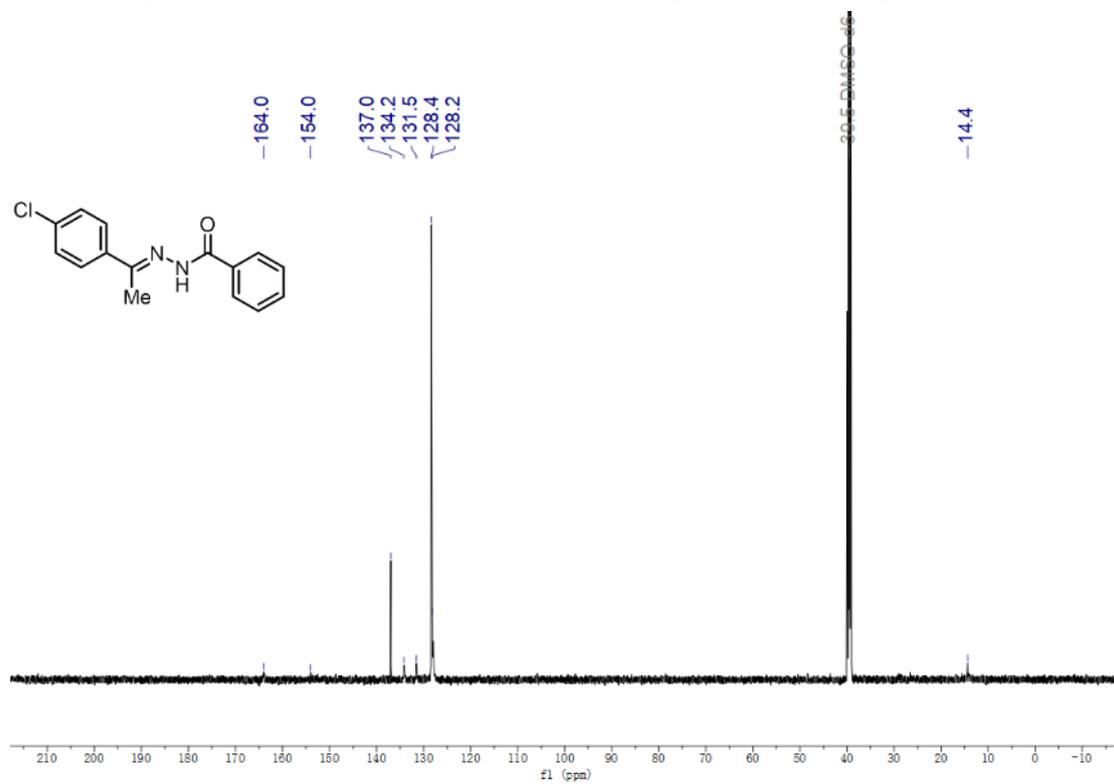


Figure S74. ¹³C NMR (151 MHz, DMSO) Spectrum of Compound **6ak**

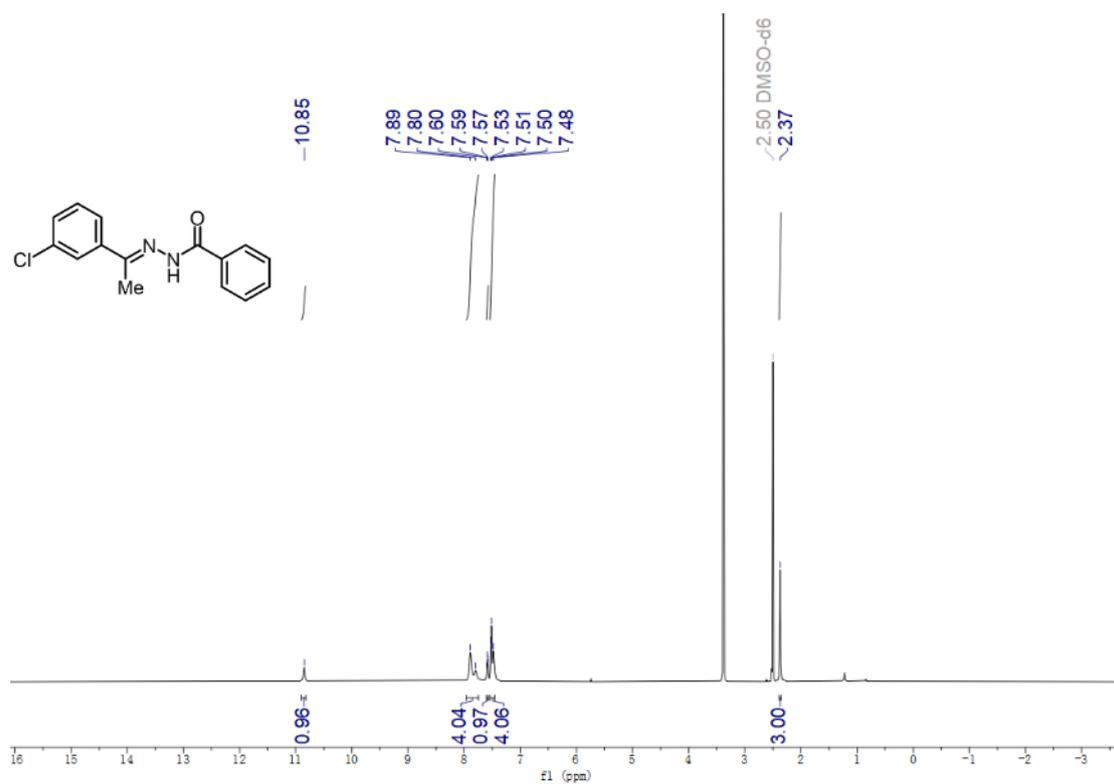


Figure S75. ¹H NMR (600 MHz, DMSO) Spectrum of Compound **6al**

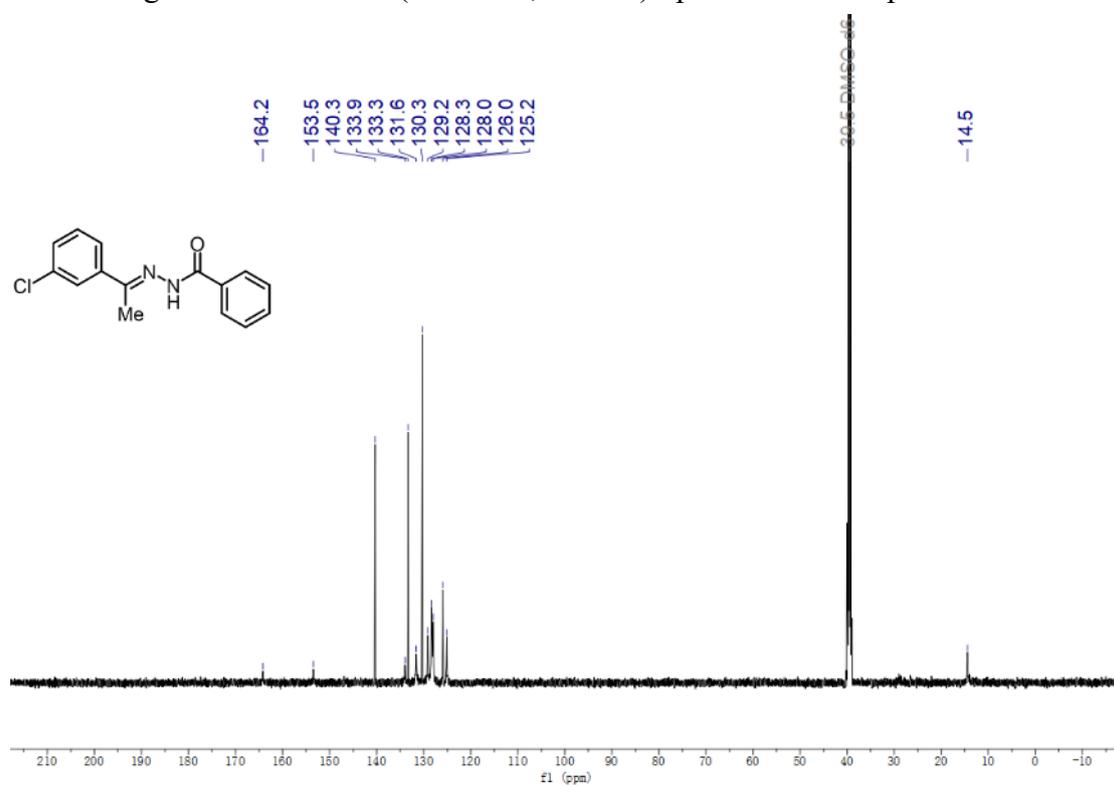


Figure S76. ¹³C NMR (151 MHz, DMSO) Spectrum of Compound **6al**

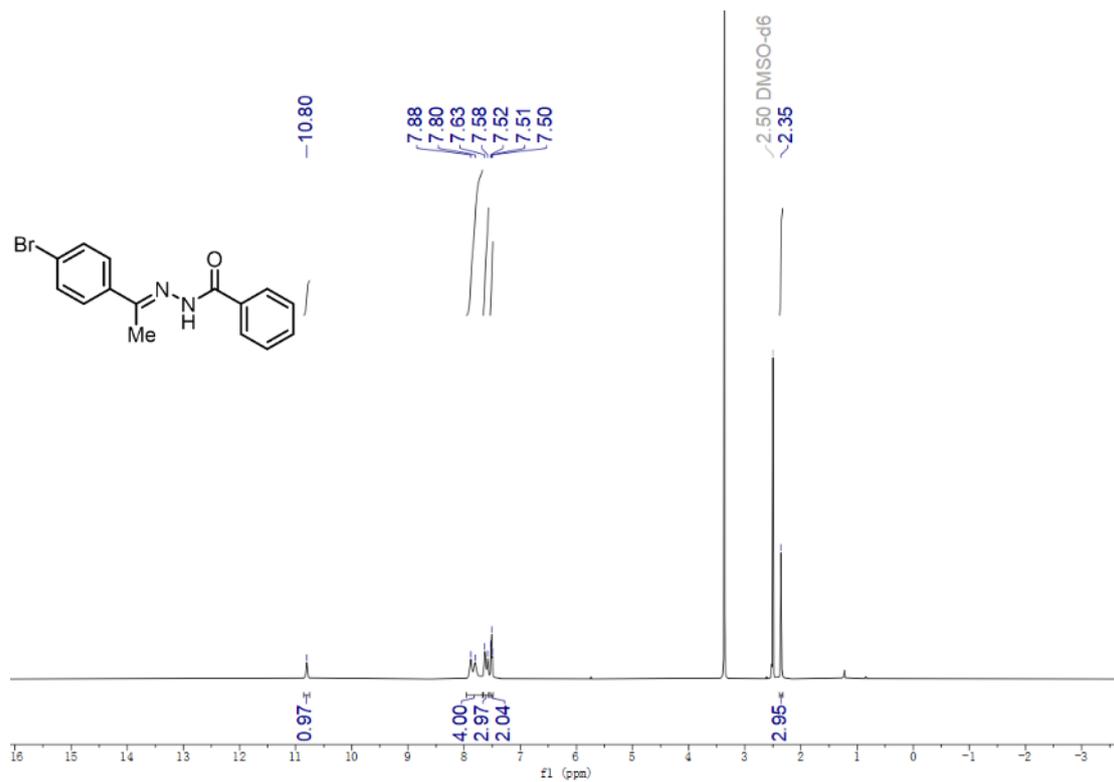


Figure S77. ¹H NMR (600 MHz, DMSO) Spectrum of Compound **6am**

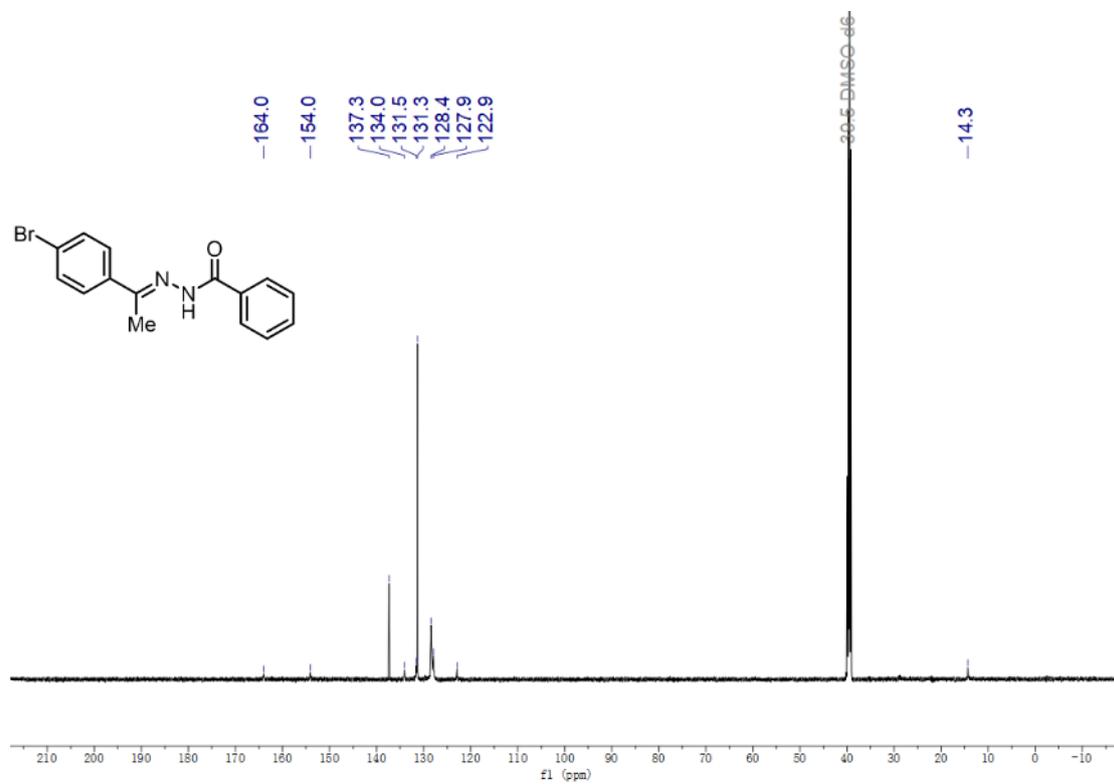


Figure S78. ¹³C NMR (151 MHz, DMSO) Spectrum of Compound **6am**

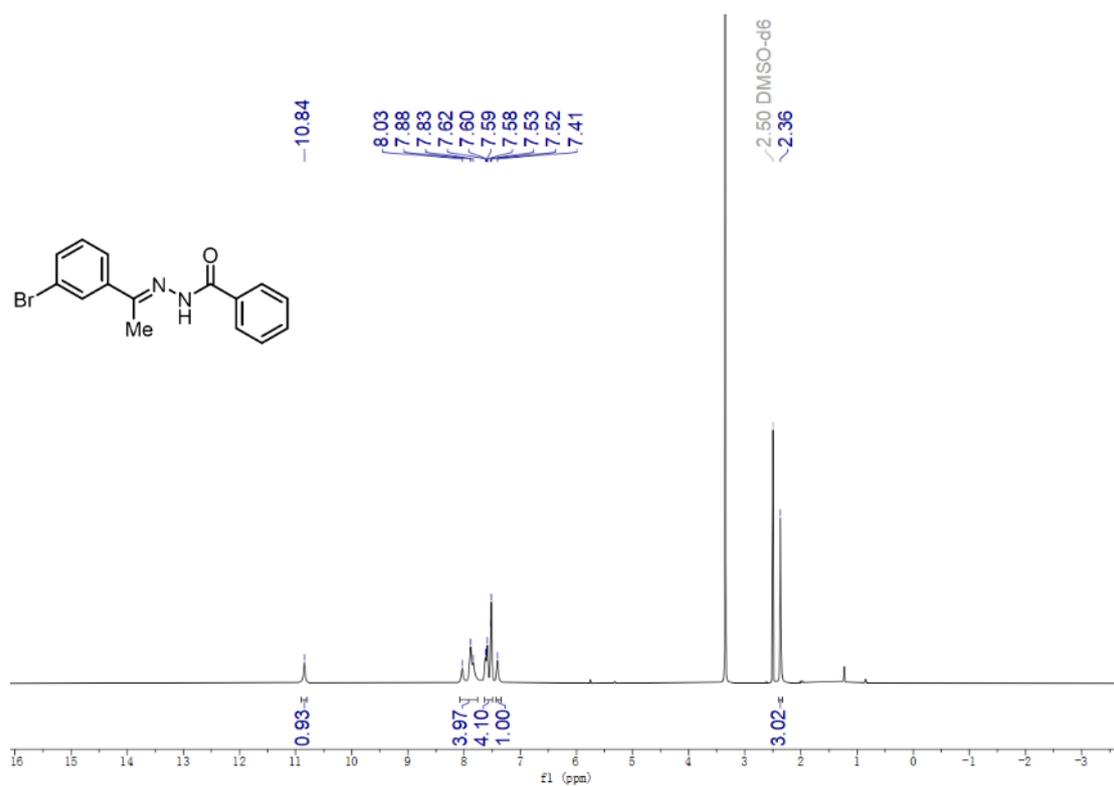


Figure S79. ¹H NMR (600 MHz, DMSO) Spectrum of Compound **6an**

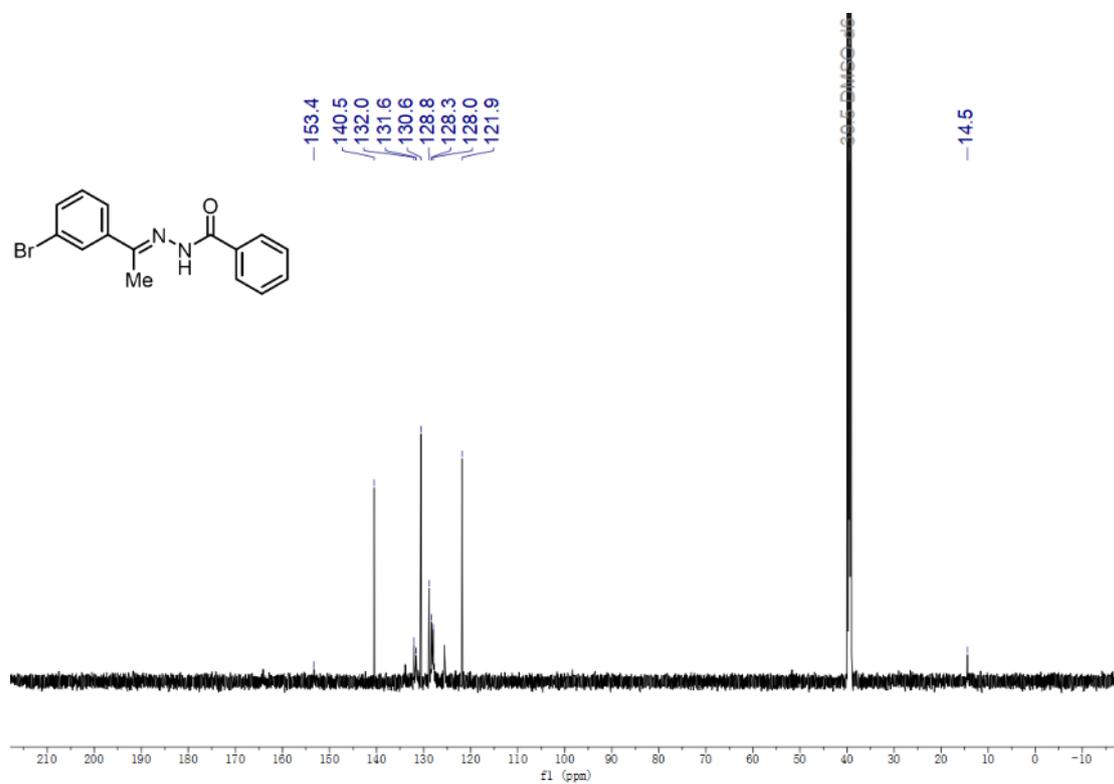


Figure S80. ¹³C NMR (151 MHz, DMSO) Spectrum of Compound **6an**

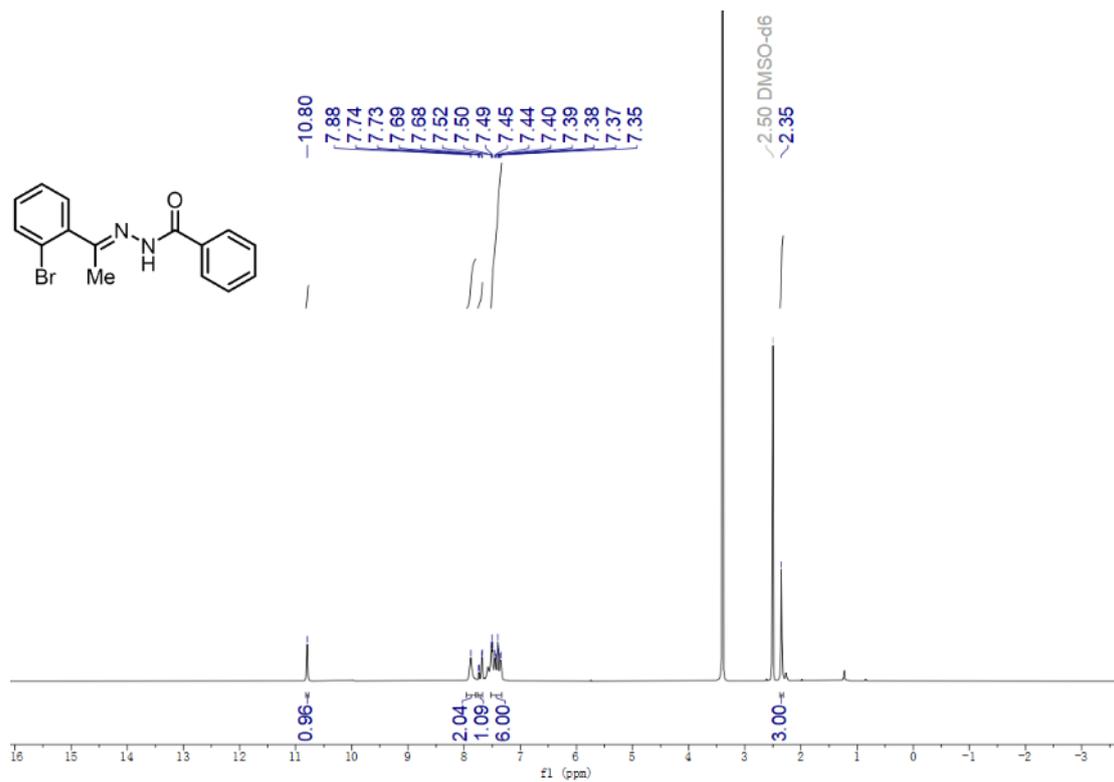


Figure S81. ¹H NMR (600 MHz, DMSO) Spectrum of Compound **6ao**

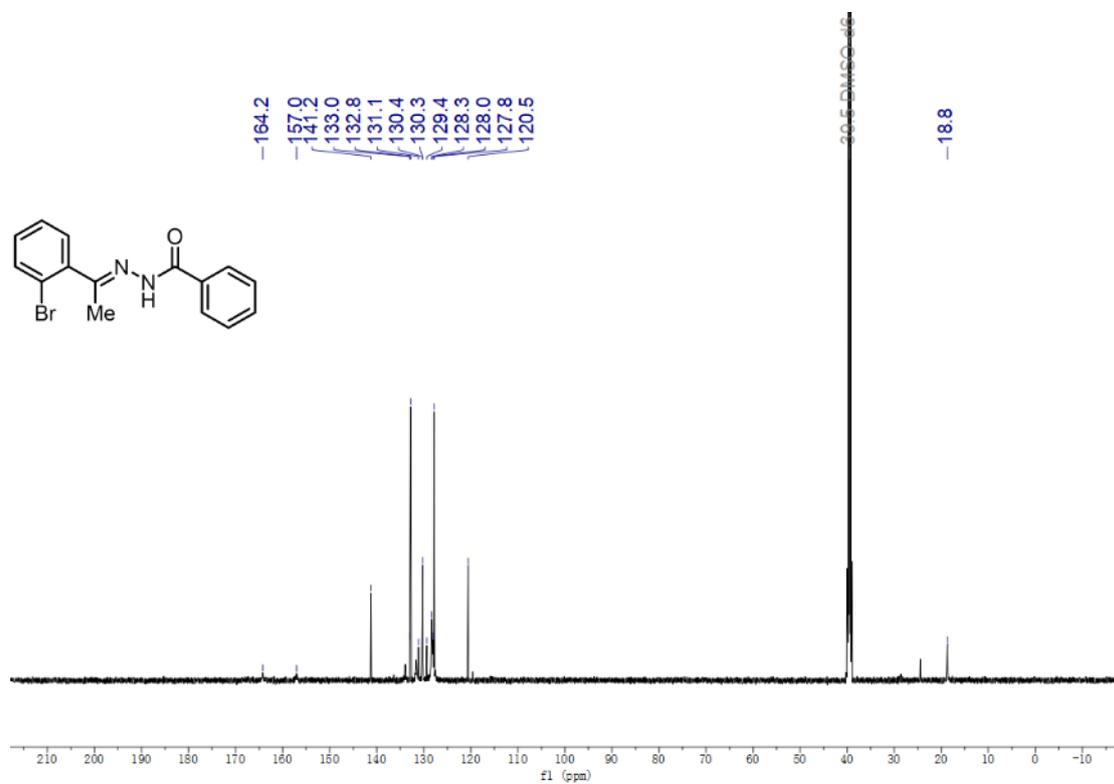


Figure S82. ¹³C NMR (151 MHz, DMSO) Spectrum of Compound **6ao**

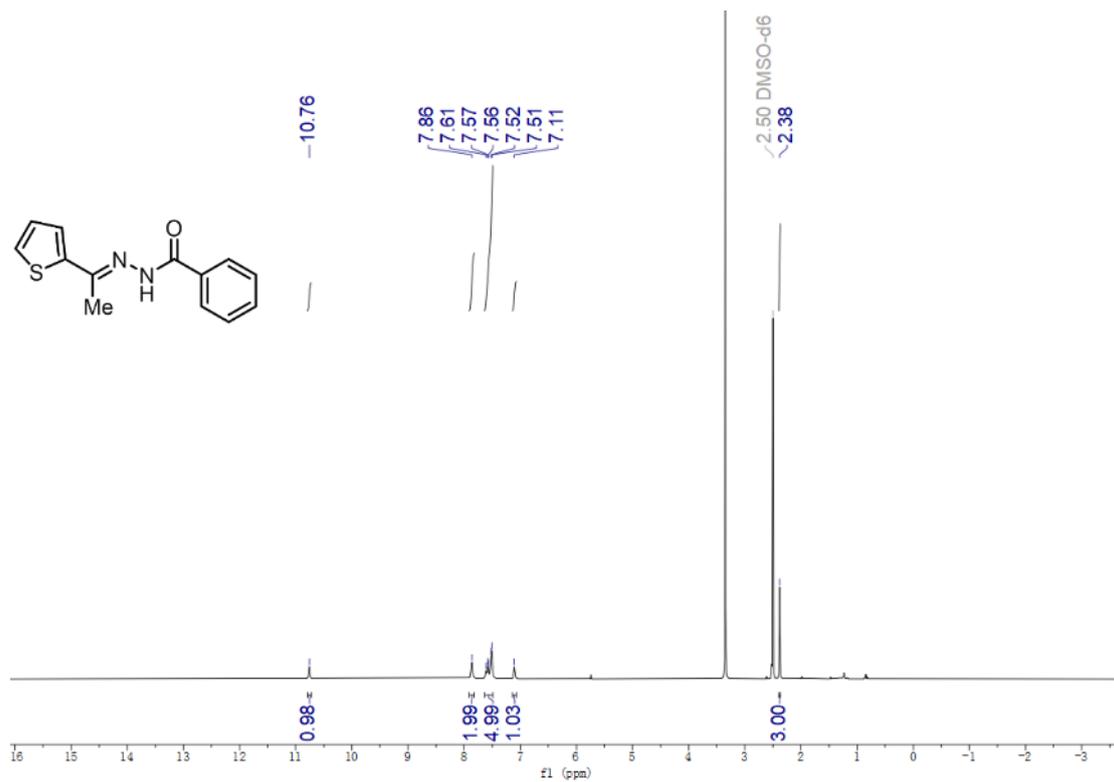


Figure S83. ¹H NMR (600 MHz, DMSO) Spectrum of Compound **6ap**

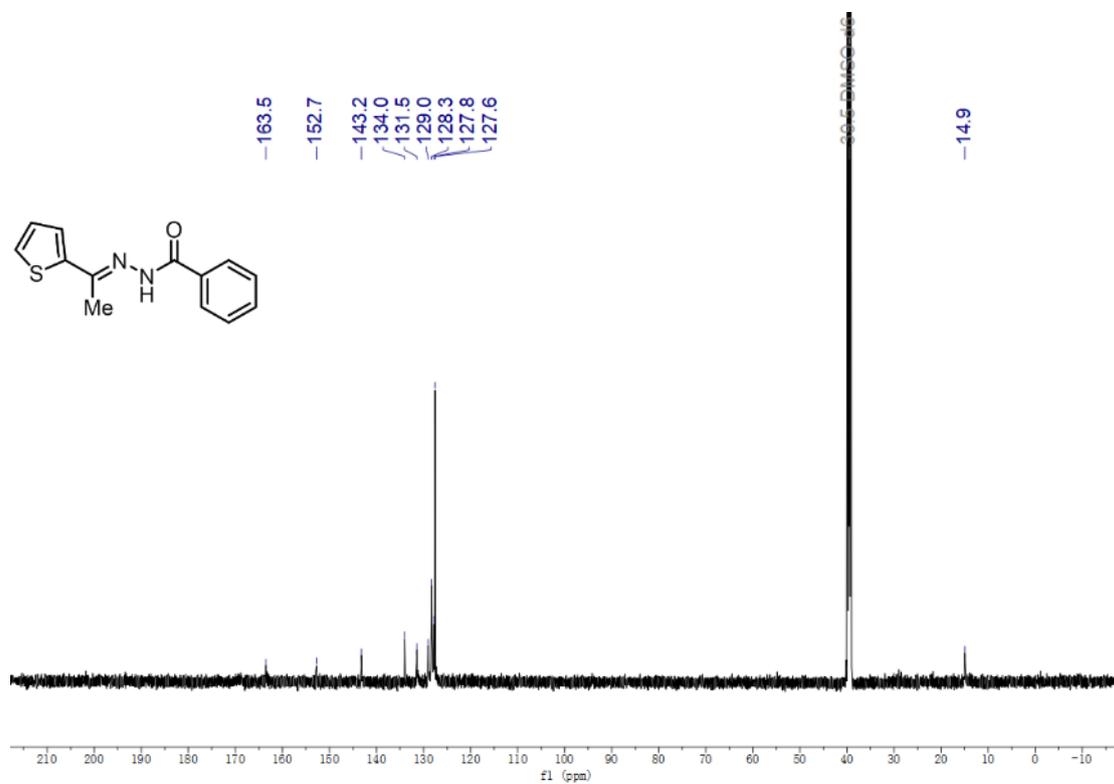


Figure S84. ¹³C NMR (151 MHz, DMSO) Spectrum of Compound **6ap**

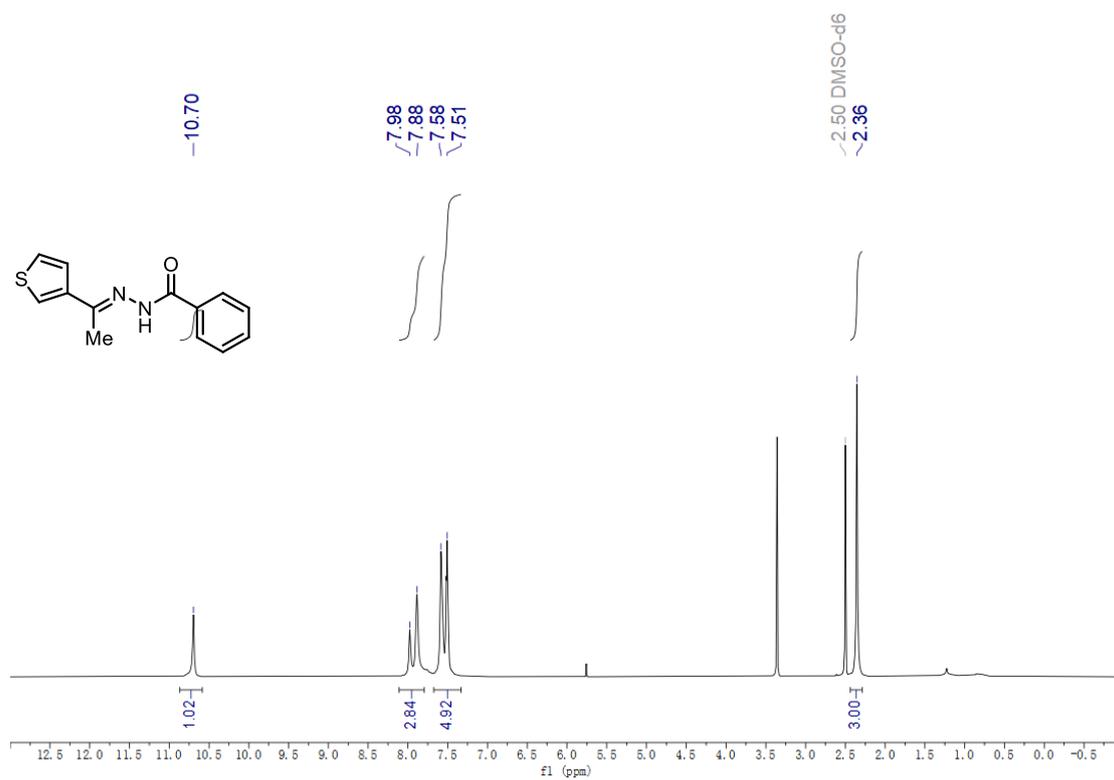


Figure S85. ¹H NMR (600 MHz, DMSO) Spectrum of Compound **6aq**

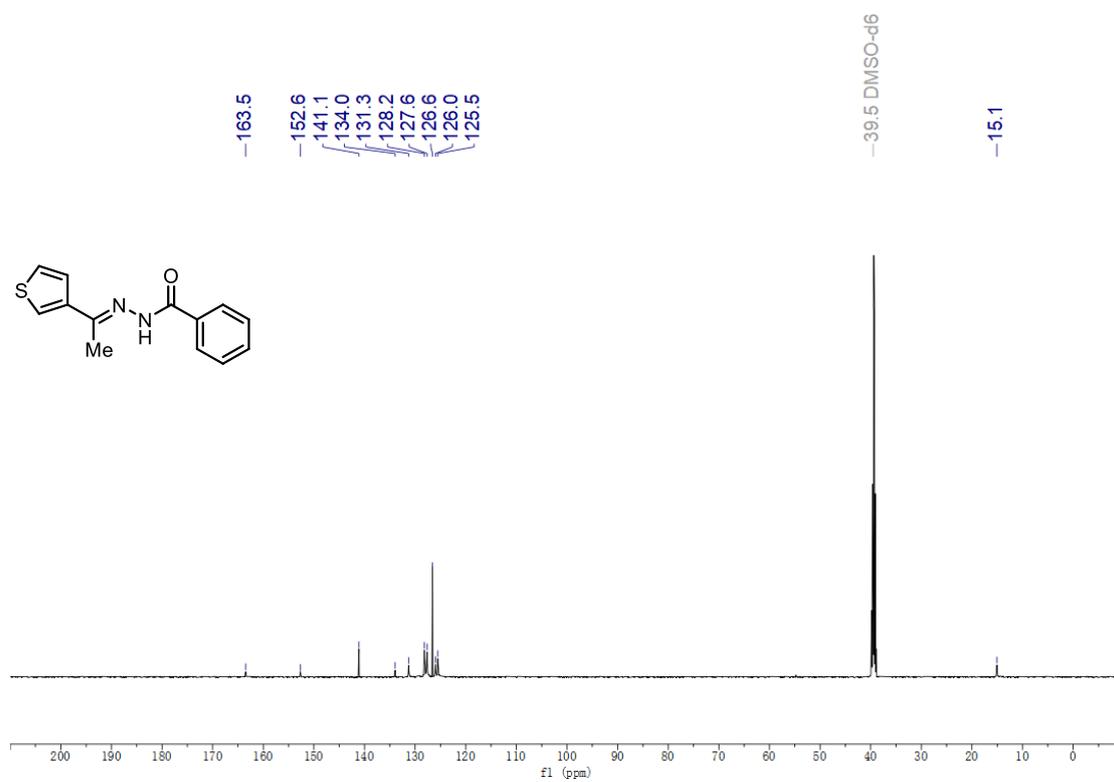


Figure S86. ¹³C NMR (151 MHz, DMSO) Spectrum of Compound **6aq**

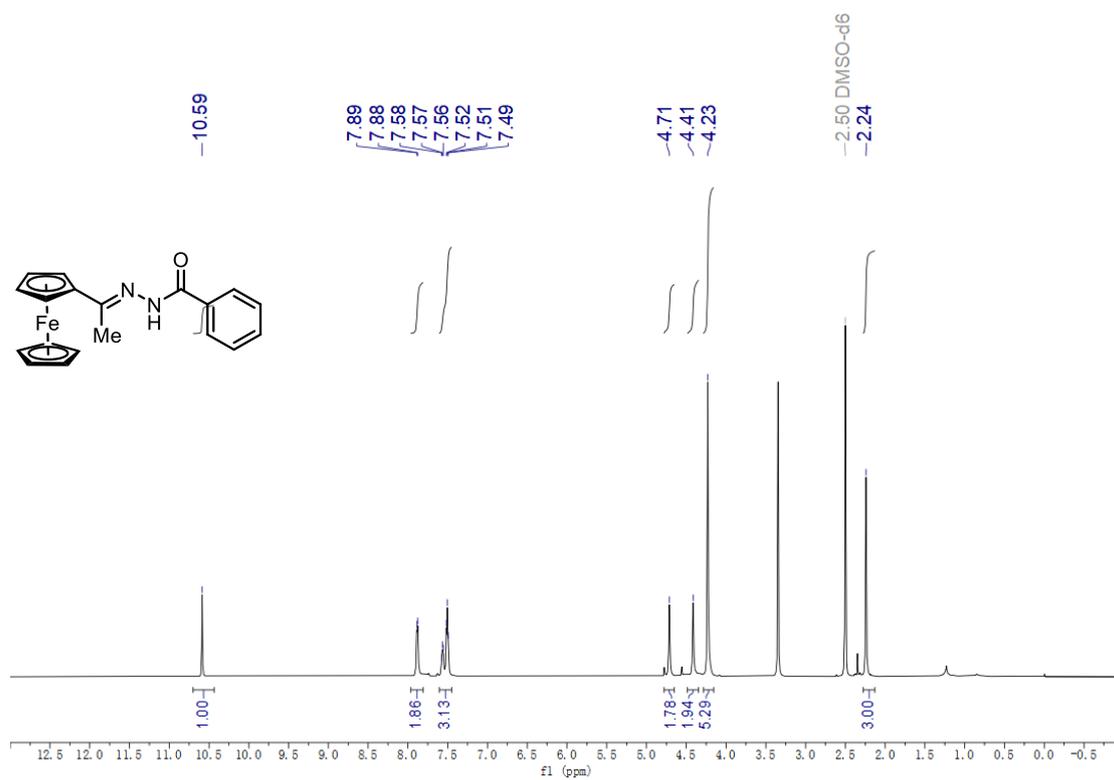


Figure S87. ^1H NMR (600 MHz, DMSO) Spectrum of Compound **6ar**

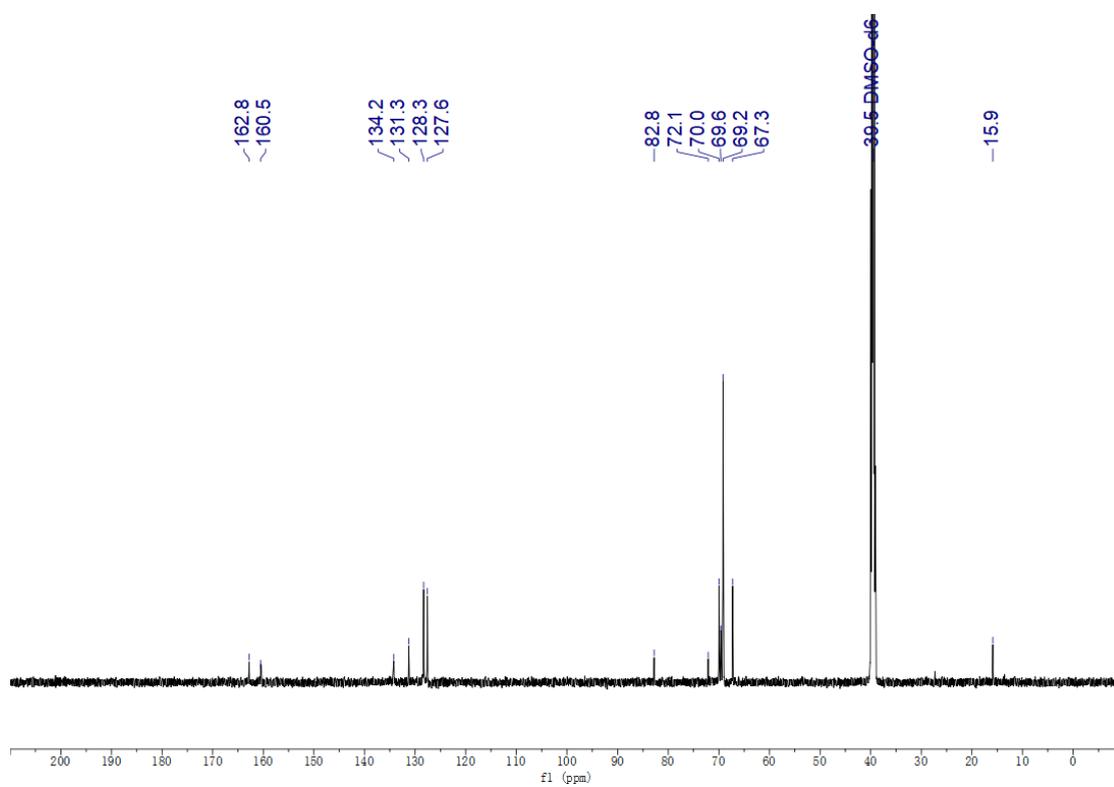


Figure S88. ^{13}C NMR (151 MHz, DMSO) Spectrum of Compound **6ar**

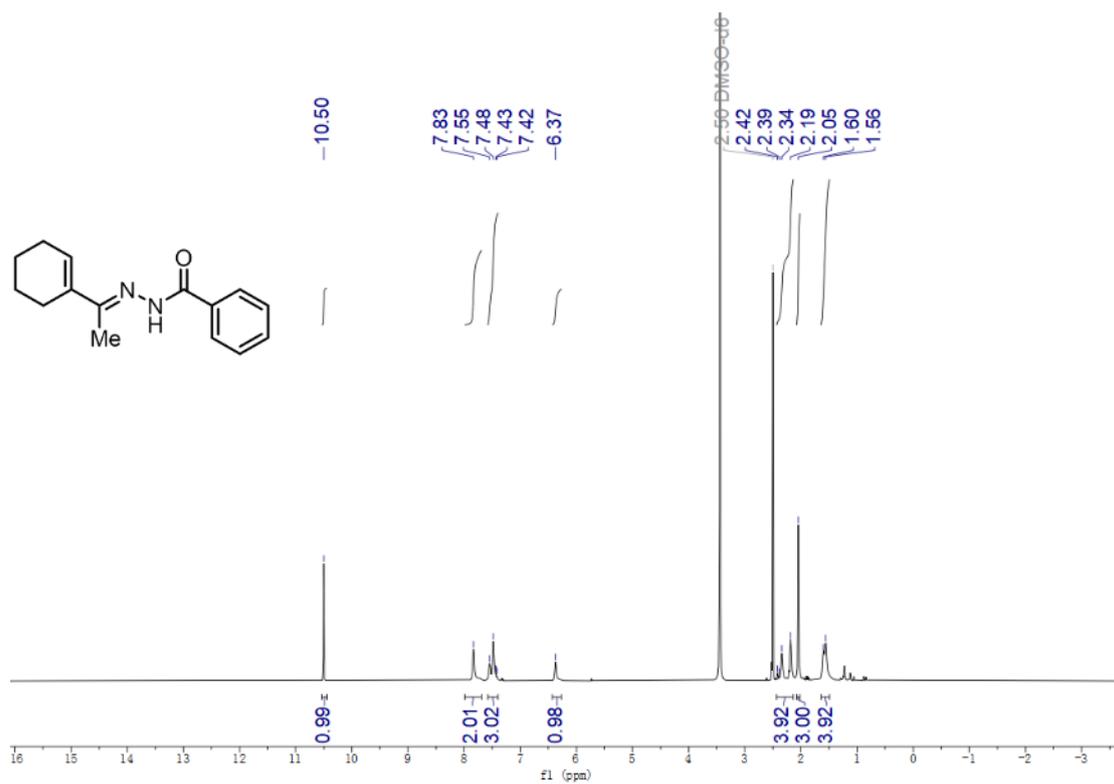


Figure S89. ¹H NMR (600 MHz, DMSO) Spectrum of Compound 6as

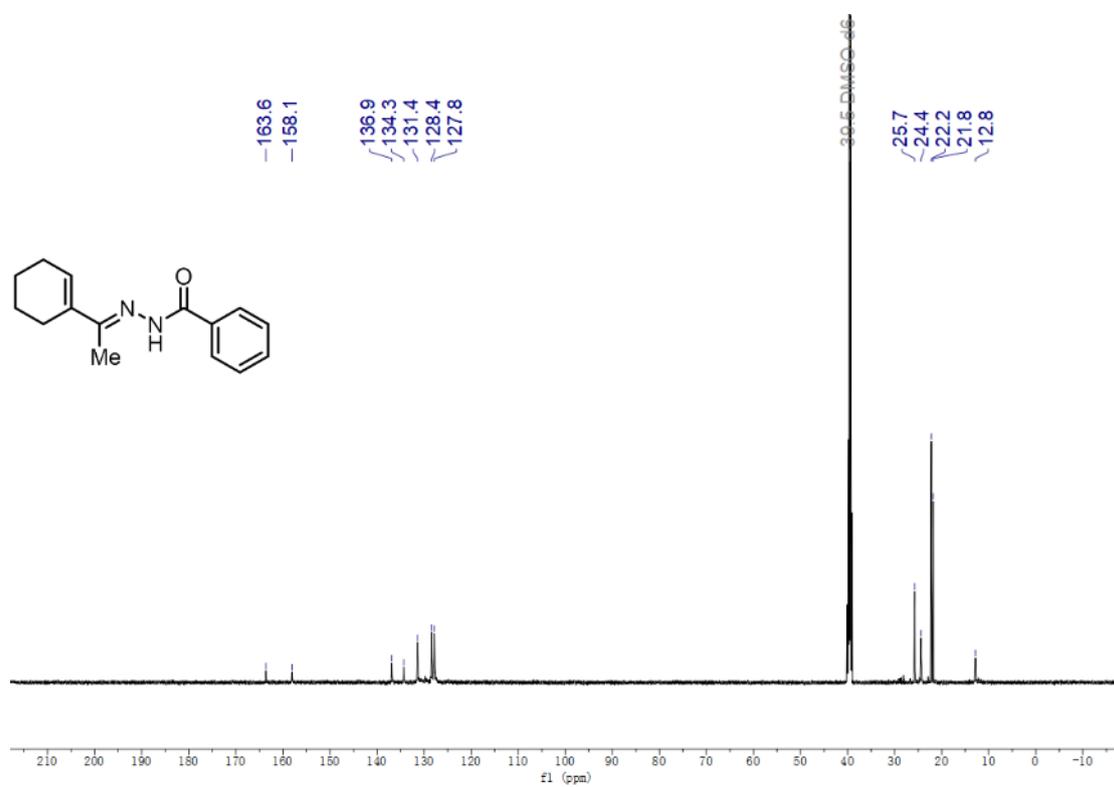


Figure S90. ¹³C NMR (151 MHz, DMSO) Spectrum of Compound 6as

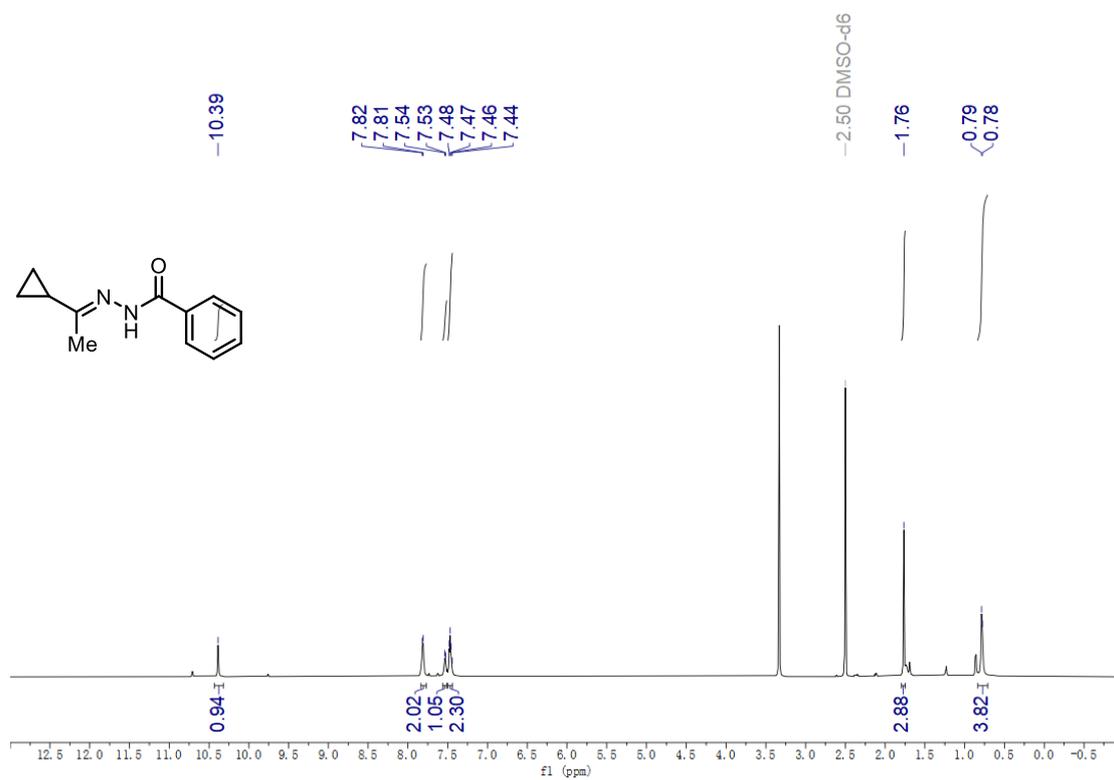


Figure S91. ¹H NMR (600 MHz, DMSO) Spectrum of Compound **6at**

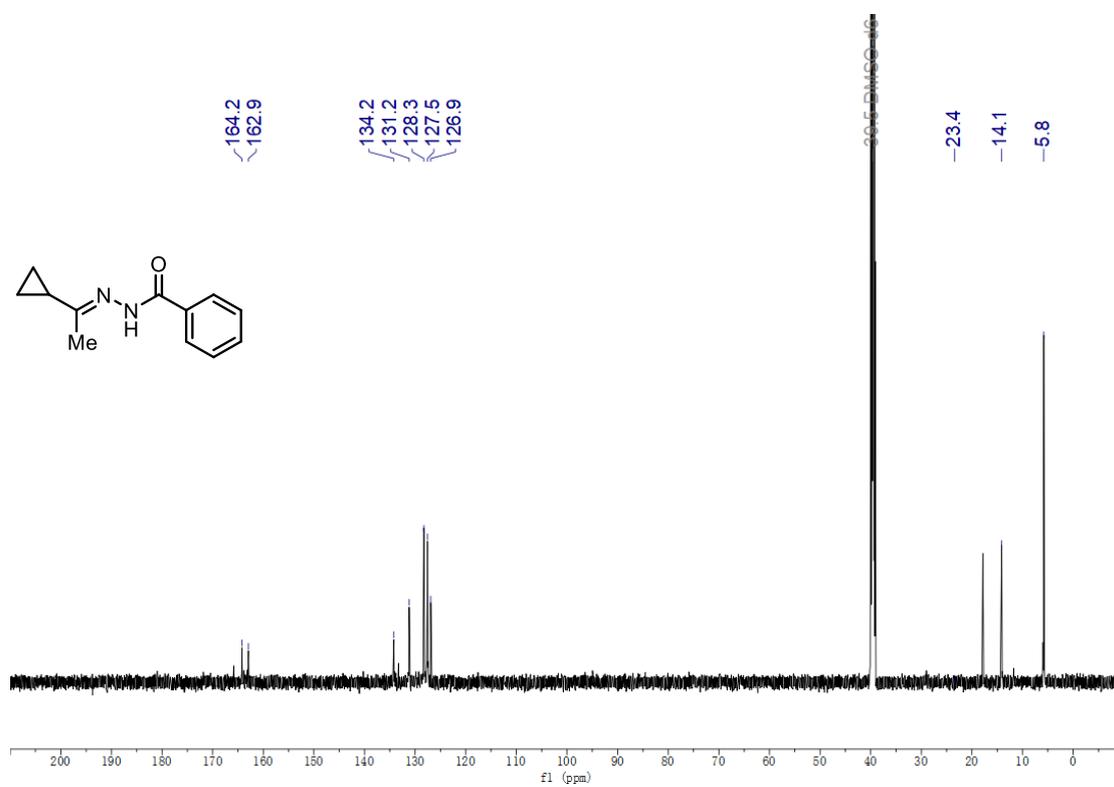


Figure S92. ¹³C NMR (151 MHz, DMSO) Spectrum of Compound **6at**

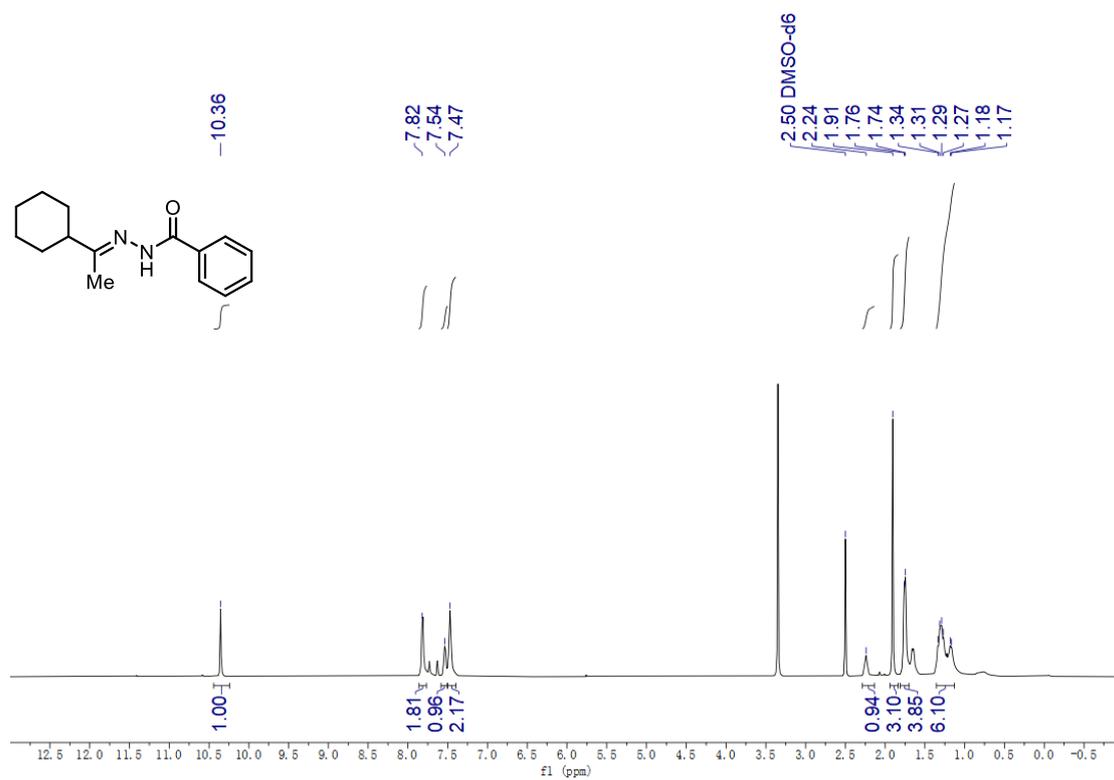


Figure S93. ¹H NMR (600 MHz, DMSO) Spectrum of Compound **6au**

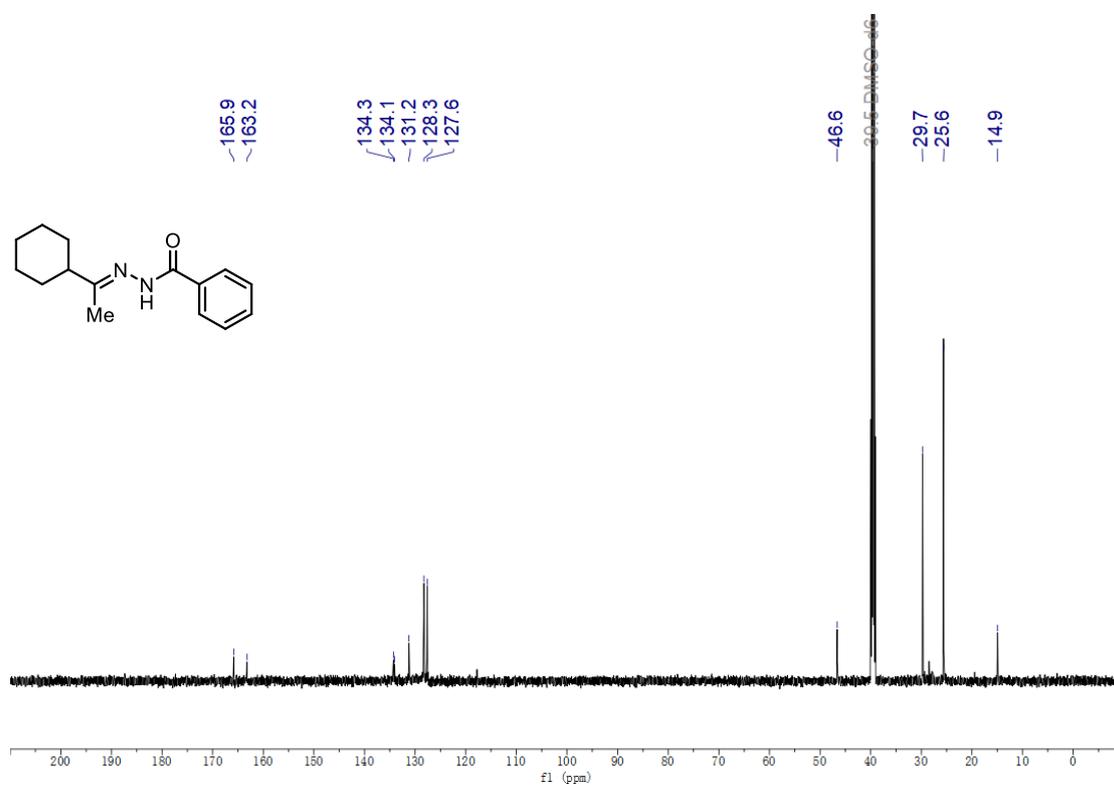


Figure S94. ¹³C NMR (151 MHz, DMSO) Spectrum of Compound **6au**

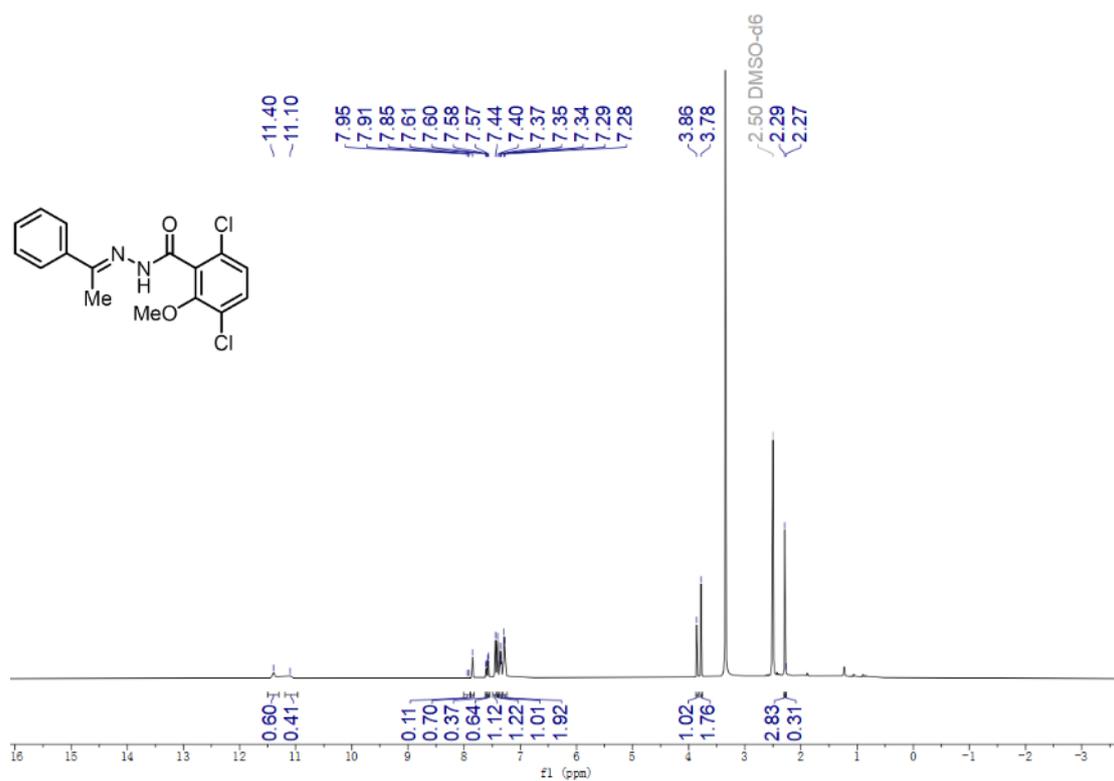


Figure S95. ¹H NMR (600 MHz, DMSO) Spectrum of Compound 6av

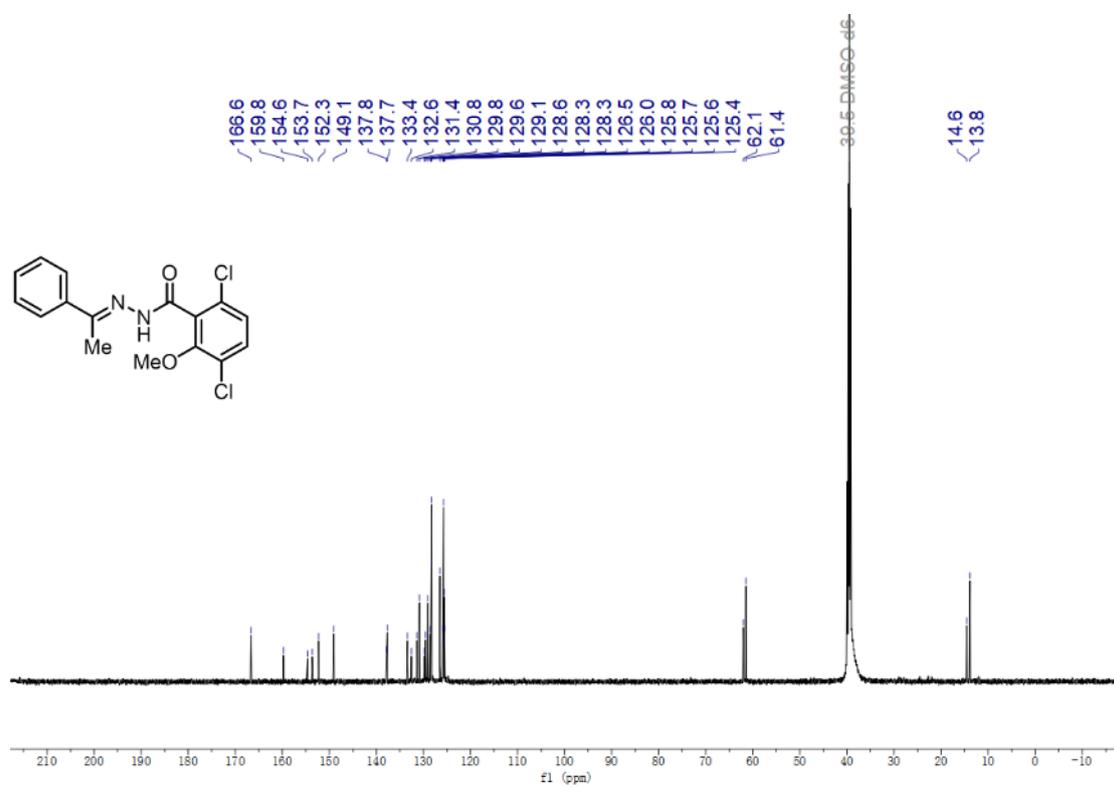


Figure S96. ¹³C NMR (151 MHz, DMSO) Spectrum of Compound 6av

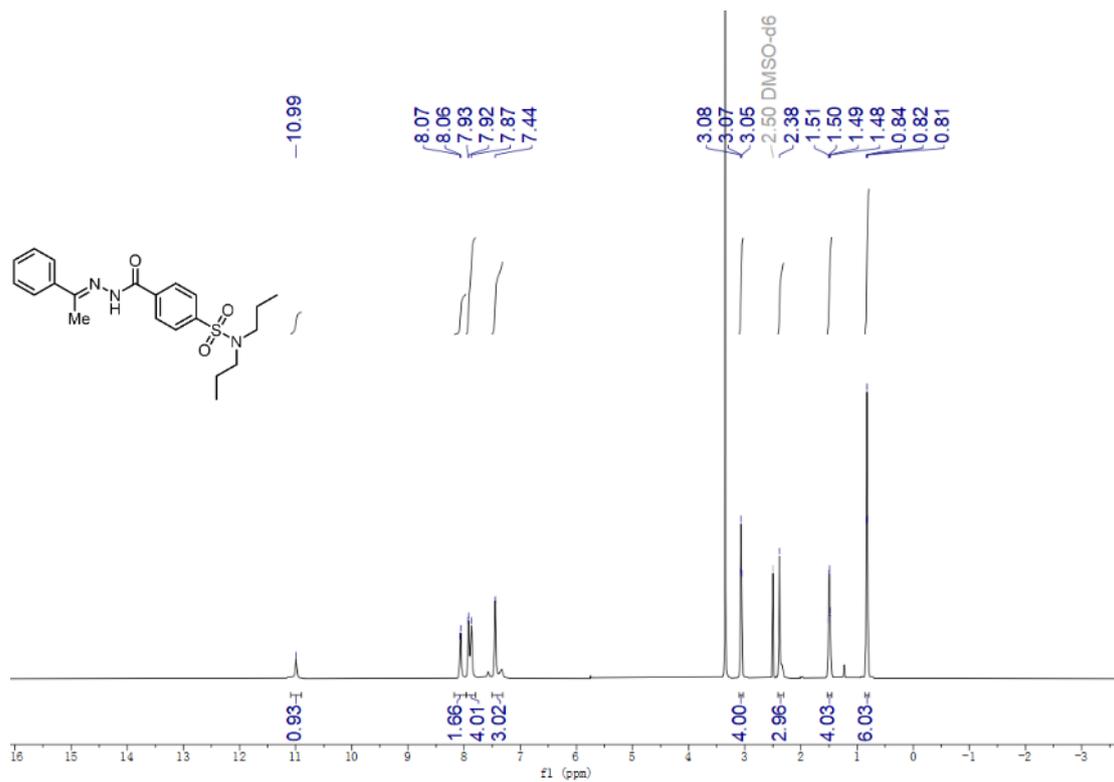


Figure S97. ^1H NMR (600 MHz, DMSO) Spectrum of Compound 6aw

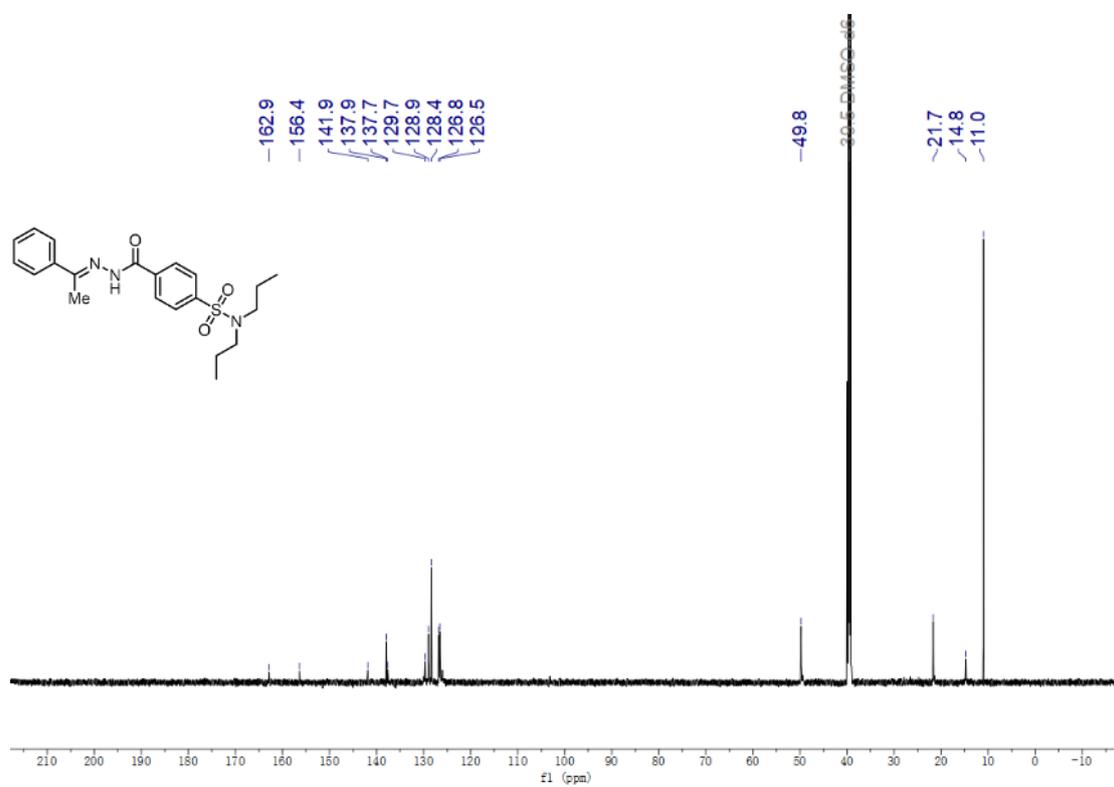


Figure S98. ^{13}C NMR (151 MHz, DMSO) Spectrum of Compound 6aw

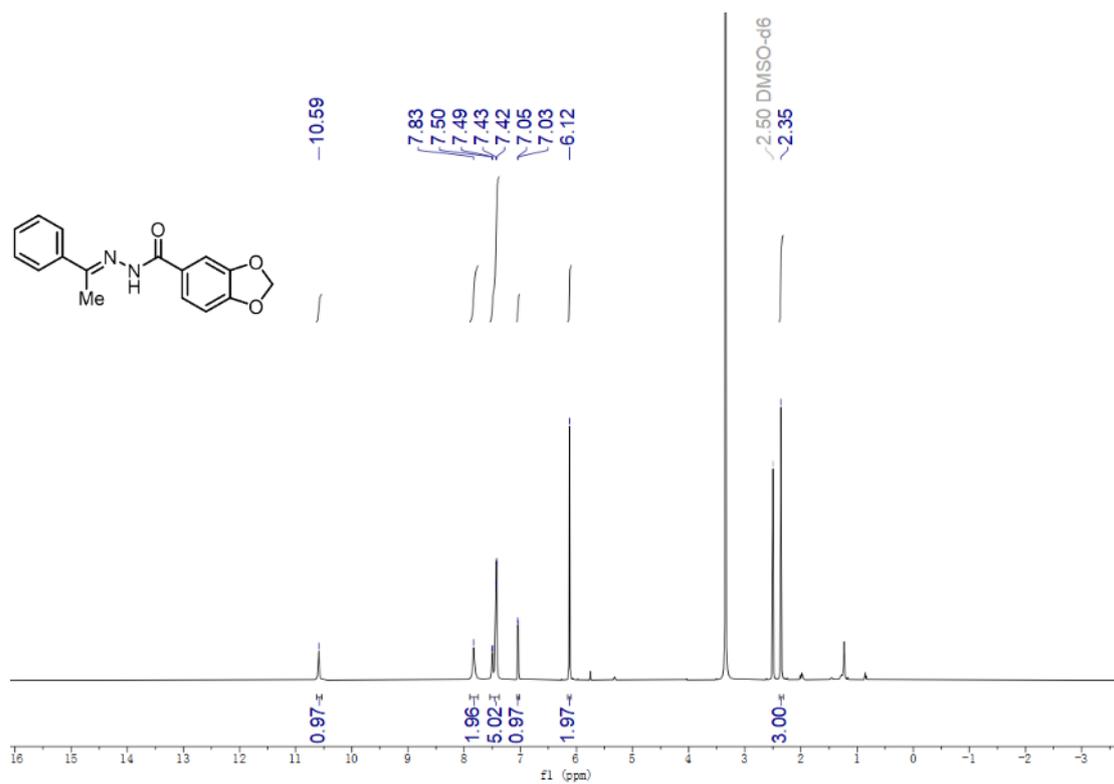


Figure S99. ¹H NMR (600 MHz, DMSO) Spectrum of Compound 6ax

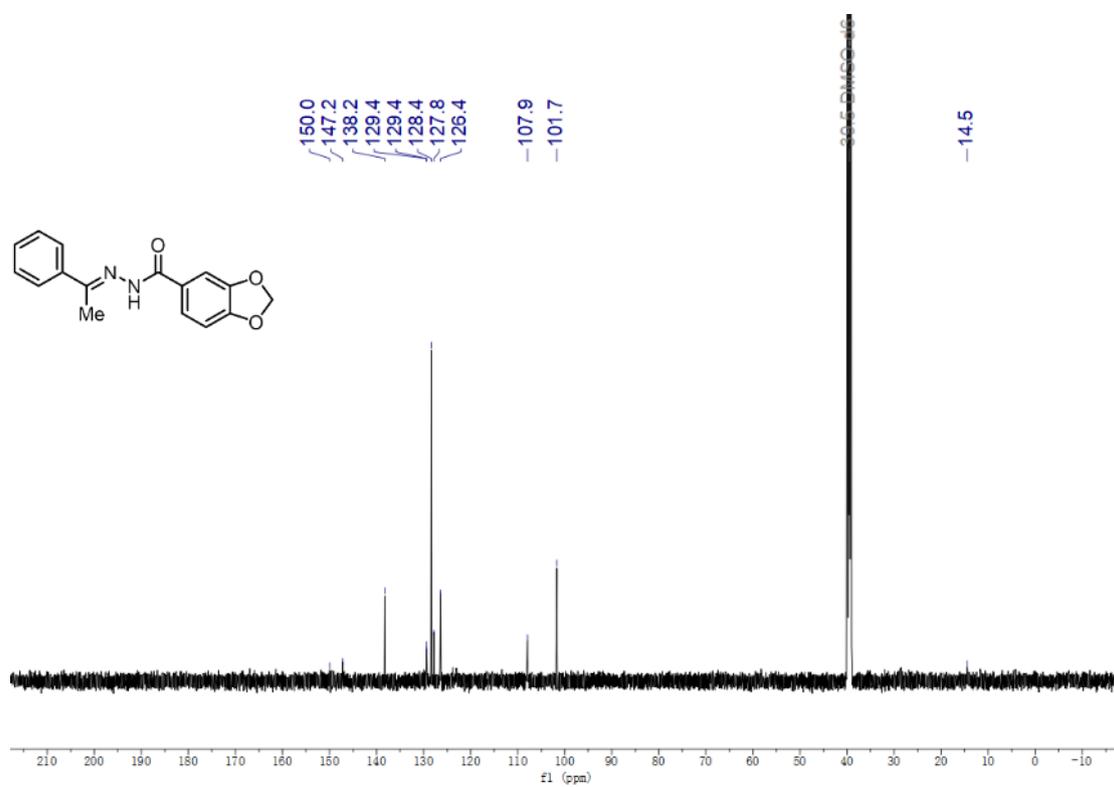


Figure S100. ¹³C NMR (151 MHz, DMSO) Spectrum of Compound 6ax

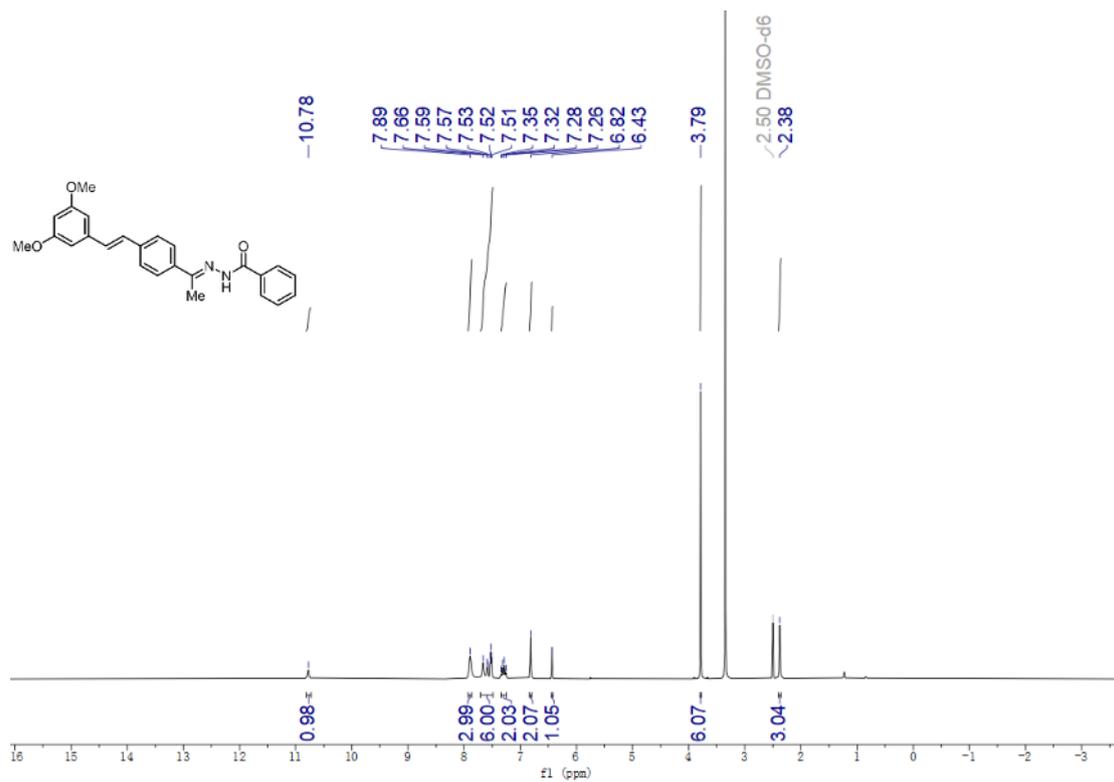


Figure S101. ¹H NMR (600 MHz, DMSO) Spectrum of Compound 6ay

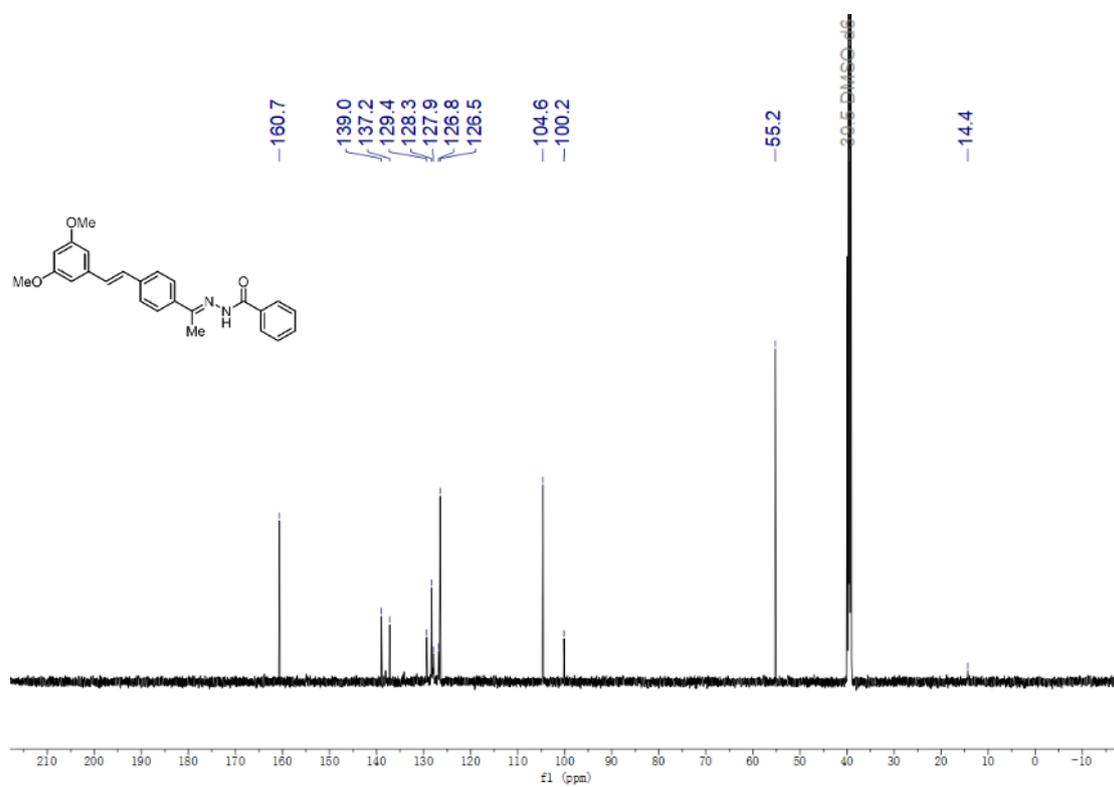


Figure S102. ¹³C NMR (151 MHz, DMSO) Spectrum of Compound 6ay

5. References

1. Zhang, J.; Li, X.; Li, T.; Zhang, G.; Wan, K.; Ma, Y.; Fang, R.; Szostak, R.; Szostak, M., Copper (I)–Thiazol-2-ylidenes: Highly Reactive N-Heterocyclic Carbenes for the Hydroboration of Terminal and Internal Alkynes. Ligand Development, Synthetic Utility, and Mechanistic Studies. *ACS Catal.* **2022**, *12*, 15323-15333.
2. Liu, S.; Li, J.; Hu, W.; Huang, B.; Cai, M., Recyclable gold (I)-catalyzed hydrohydrazidation of terminal alkynes towards keto-N-acylhydrazones. *J. Organomet. Chem.* **2022**, *975*, 122411.
3. Manikandan, T. S.; Saranya, S.; Ramesh, R., Synthesis and catalytic evaluation of ruthenium (II) benzhydrazone complex in transfer hydrogenation of ketones. *Tetrahedron Lett.* **2016**, *57*, 3764-3769.
4. Schuster, C. H.; Dropinski, J. F.; Shevlin, M.; Li, H.; Chen, S., Ruthenium-Catalyzed Enantioselective Hydrogenation of Hydrazones. *Org. Lett.* **2020**, *22*, 7562-7566.
5. Zimin, D. P.; Dar'in, D. V.; Rassadin, V. A.; Kukushkin, V. Y., Gold-catalyzed hydrohydrazidation of terminal alkynes. *Org. Lett.* **2018**, *20*, 4880-4884.
6. Wang, L.; Lin, J.; Xia, C.; Sun, W., Manganese-catalyzed asymmetric transfer hydrogenation of hydrazones. *J. Catal.* **2022**, *413*, 487-497.
7. Mondal, R.; Guin, A. K.; Chakraborty, S.; Paul, N. D., Iron-Catalyzed Metal–Ligand Cooperative Approach toward Sustainable Synthesis of Azines and N-Acylhydrazones in Air. *J. Org. Chem.* **2022**, *87*, 2921-2934.
8. Li, B.; Liu, D.; Hu, Y.; Chen, J.; Zhang, Z.; Zhang, W., Nickel-catalyzed asymmetric hydrogenation of hydrazones. *Eur. J. Org. Chem.* **2021**, *2021*, 3421-3425.
9. Layek, S.; Agrahari, B.; Dey, S.; Ganguly, R.; Pathak, D. D., Copper (II)-facilitated synthesis of substituted thioethers and 5-substituted 1H-tetrazoles: Experimental and theoretical studies. *J. Organomet. Chem.* **2019**, *896*, 194-206.
10. Hu, Y.; Zhang, Z.; Zhang, J.; Liu, Y.; Gridnev, I. D.; Zhang, W., Cobalt-Catalyzed Asymmetric Hydrogenation of C=N Bonds Enabled by Assisted Coordination and Nonbonding Interactions. *Angew. Chem., Int. Ed.* **2019**, *58*, 15767-15771.
11. Wang, Z.; Zhu, F.; Li, Y.; Wu, X. F., Palladium-Catalyzed Carbonylative Synthesis of 3-Methyleneisoindolin-1-ones from Ketimines with Hexacarbonylmolybdenum (0) as the Carbon Monoxide Source. *ChemCatChem* **2017**, *9*, 94-98.
12. Rahman, M. M.; Gao, P.; Zhao, Q.; Lalancette, R.; Szostak, R.; Szostak, M., [Au (Np#) Cl]: highly reactive and broadly applicable Au (I)–NHC catalysts for alkyne π -activation reactions. *Catal. Sci. Technol.* **2023**, *13*, 5131-5139.
13. Zhang, J.; Li, T.; Li, X.; Lv, A.; Li, X.; Wang, Z.; Wang, R.; Ma, Y.; Fang, R.; Szostak, R., Thiazol-2-ylidenes: Versatile N-Heterocyclic Carbene Ligands with Enhanced Electrophilicity for Transition-Metal-Catalysis. *Comm. Chem.* **2022**, *5*, 60.
14. Dilman, A. D.; Arkhipov, D. E.; Levin, V. V.; Belyakov, P. A.; Korlyukov, A. A.; Struchkova, M. I.; Tartakovsky, V. A., Trifluoromethylation of N-

benzoylhydrazones. *J. Org. Chem.* **2008**, *73*, 5643-5646.

6. Computational Details and Cartesian Coordinates

Computational Details

All density functional theory (DFT)¹ calculations were performed with the Gaussian 16, Revision A.03 software package² or ORCA 6.0.1 program package³⁻⁵ running on Linux systems.

Geometry optimizations and vibrational frequency analyses were conducted using the **PBE0**⁶ functional with Grimme's D3(BJ) empirical dispersion correction⁷ at gas phase and a mixed basis set: the **SDD**⁸ basis set for gold and **def2-SVP**^{9,10} for all other elements (via Gaussian 16 Revision A.03). Default convergence criteria in Gaussian 16 were employed, and vibrational frequencies were computed at standard conditions (1 atm, 298.15 K). All geometries were characterized as minima (no imaginary frequencies, NIMAG = 0) or transition states (the number of imaginary frequencies, NIMAG = 1). Intrinsic reaction coordinate (IRC)¹¹ calculations verified the connectivity between transition states and their associated reactant/product minima.

Single-point energy calculations were performed in ORCA 6.0.1 using the **PWPB95**¹² functional with Grimme's D4 dispersion correction⁷ and the **def2-TZVPP**^{9,10} basis set for all atoms. The **RIJCOSX** approximation¹³ was used together with the Coulomb-fitting auxiliary basis set **def2/J**¹⁴ to accelerate hybrid DFT calculations. Tight SCF convergence and increased integration grids (Grid5/NoFinalGrid) were applied throughout.

Solvent effects were incorporated by adding the single-point energy difference between solvated and gas-phase systems¹⁵ to the single-point energies calculated above. Solvation-free energies were computed via the **SMD model**¹⁶ at the **M05-2X**¹⁷ level with a mixed basis set **SDD**⁸ for gold, **6-31G(d)**¹⁸ for other atoms, using chloroform as the solvent elements (via Gaussian 16 Revision A.03).

Gibbs free energies were adjusted from the gas-phase standard state (1 atm) to solution (1 mol/L) by applying a correction term $RT\ln(c_s/c_g)$ (1.89 kcal/mol at 298.15 K), where $C_s = 1$ mol/L, $C_g = 0.0446$ mol/L, and $R = 8.31432$ J·K⁻¹·mol⁻¹. Thermochemical parameters (thermal corrections to Gibbs free energy, **TCG**) were calculated using **Shermo 2.6**¹⁹. Zero-point energies (ZPE) were scaled by a factor of 0.9817²⁰, and low-frequency modes (<100 cm⁻¹) were treated with the (modified rigid-rotor harmonic oscillator) (**mRRHO**) model²¹ (entropy/internal energy interpolations; Sherma keyword ilowfreq=3).

Optimized structures were visualized using the **CYLview**²² program.

Reference

1. Parr, R. G.; Yang, W. *Density-functional Theory of Atoms and Molecules*; Oxford University Press: New York, **1989**.
2. Gaussian 16, Revision A.03, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams-Young, D.; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2016.
3. Neese, F. *Wires.; Comput.Mol. Sci.* **2012**, *2*, 73-78.
4. Neese, F.; Wennmohs, F.; Becker, U.; Riplinger, C. *J. Chem. Phys.* **2020**, *152*.
5. Neese, F. *Wires Comput.Mol.Sci.* **2022**, *12*.
6. Adamo, C., & Barone, V. *J.Chem.Phys.* **1999**, *110*, 6158-6170.
7. (a) Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H. *J. Chem. Phys.* **2010**, *132*. (b) Caldeweyher, E.;

- Bannwarth, C.; Grimme, S. *J. Chem. Phys.* **2017**, *147*.
8. Andrae, D.; Häußermann, U.; Dolg, M.; Stoll, H.; Preuß, H. *Theor. Chem. Acc.* **1990**, *77*, 123-141.
9. Weigend, F.; & Ahlrichs, R. *PCCP*. **2005**, *7*, 3297-3305.14.
10. Weigend, F. *PCCP*. **2006**, *8*, 1057-1065.
11. Fukui, K. *Acc. Chem. Res.* **1981**, *14*, 363-368.
12. Goerigk, L.; Grimme, S. *J. Chem. Theory Comput.* **2011**, *7*, 291-309.
13. Kossmann, S.; Neese, F. *Chem. Phys. Lett.* **2009**, *481*, 240-243.
14. Weigend, F.; Ahlrichs, R. *Phys.Chem.Chem.Phys.* **2005**, *7*, 3297-3305.
15. Ho, J. M.; Klamt, A.; Coote, M. L. *J. Phys. Chem. A*. **2010**, *114*, 13442-13444.
16. Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. *J. Phys.Chem. B*. **2009**, *113*, 6378-6396.
17. Zhao, Y.; Schultz, N. E.; Truhlar, D. G. *J. Chem. Theory Comput.* **2006**, *2*, 364-382.
18. Wiberg, K. B. *J. Comput. Chem.* **1986**, *7*, 379-379.
19. Lu, T.; Chen, Q. *Comput. Theor. Chem.* **2021**, *1200*, 113249.
20. Kesharwani, M. K.; Brauer, B.; Martin, J. M. L. *J. Phys. Chem. A*. **2015**, *119*, 1701-1714.
21. Otyotov, A. A.; Minenkov, Y. *J. Comput. Chem.* **2023**, *44*, 1807-1816.
22. CYLview20; Legault, C. Y., Université de Sherbrooke, **2020**. (<http://www.cylview.org>)

Table S9. Calculated Energies and Imaginary Frequencies

Compounds	SPE+solvation free energy +1.89/627.509 (a.u.)	TcG (a.u.)	Gibbs free energy (a.u.)	Imaginary frequencies (cm ⁻¹)
IPr_Au_Cation	-1295.1208507877	0.4882430000	-1294.6326077877	
Acetylene	-308.2821921432	0.0742210000	-308.2079711432	
IPr_INT1	-1603.4611221466	0.5866030000	-1602.8745191466	
Bnezoimidazole	-456.1482701660	0.1039290000	-456.0443411660	
IPr_INT1_2	-1751.3316505538	0.6190310000	-1750.7126195538	
IPr_TS1	-2059.6112642971	0.7183600000	-2058.8929042971	-75.65
IPr_INT2	-2059.6177679415	0.7143450000	-2058.9034229415	
IPr_TS2	-2059.5992092163	0.7172850000	-2058.8819242163	-272.93
IPr_INT3	-2059.6380245768	0.7221970000	-2058.9158275768	
IPr_INT4	-2515.8026020868	0.8545940000	-2514.9480080868	
IPr_TS3	-2515.7970445562	0.8518290000	-2514.9452155562	-111.21

IPr_INT5	-2515.8065342382	0.8510100000	-2514.9555242382	
IPr_INT6	-2515.8137691584	0.8538240000	-2514.9599451584	
IPr_TS4	-2515.8035906421	0.8499060000	-2514.9536846421	-458.43
IPr_INT7	-2059.6675949718	0.7243740000	-2058.9432209718	
IPr_TS5	-2367.9503145839	0.8218390000	-2367.1284755839	-58.54
IPr_TS5_2	-2515.8261732299	0.8547710000	-2514.9714022299	-26.92
N'-(1-phenylvinyl)benzo hydrazide	-764.4867094738	0.2048850000	-764.2818244738	

Compounds	SPE+solvation free energy +1.89/627.509 (a.u.)	TcG (a.u.)	Gibbs free energy (a.u.)	Imaginary frequencies (cm ⁻¹)
Thiazol_Au_Cation	-1249.7715013318	0.29403900	-1249.4774623318	
Acetylene	-308.2821921432	0.0742210000	-308.2079711432	
Thiazol_INT1	-1558.0998586268	0.3956500000	-1557.7042086268	
Benzohydrazide	-456.1482701660	0.1039290000	-456.0443411660	
Thiazol_INT1_2	-1705.9732769853	0.4258390000	-1705.5474379853	
Thiazol_TS1	-2014.2573348715	0.5228840000	-2013.7344508715	-71.68
Thiazol_INT2	-2014.2735357888	0.5202850000	-2013.7532507888	
Thiazol_TS2	-2014.2490041649	0.5237600000	-2013.7252441649	-253.09
Thiazol_INT3	-2014.2866700757	0.5270310000	-2013.7596390757	
Thiazol_INT4	-2470.4583268938	0.6571610000	-2469.8011658938	
Thiazol_TS3	-2470.4475403641	0.6545560000	-2469.7929843641	-121.85
Thiazol_INT5	-2470.4597711883	0.6581970000	-2469.8015741883	
Thiazol_INT6	-2470.4588841878	0.6579060000	-2469.8009781878	
Thiazol_TS4	-2470.4505113418	0.6538340000	-2469.7966773418	-641.51
Thiazol_INT7	-2014.3175963805	0.5272050000	-2013.7903913805	
Thiazol_TS5	-2322.5959125408	0.6257560000	-2321.9701565408	-52.58
Thiazol_TS5_2	-2470.4735521670	0.6610340000	-2469.8125181670	-68.77
N'-(1-phenylvinyl)benzohydrazide	-764.4867094738	0.2048850000	-764.2818244738	

Cartesian Coordinates of all the Structures

IPr_Au_Cation

1 1

N	1.07971700	0.00011600	1.16960400
N	-1.07962200	0.00018600	1.16962500
C	0.68110500	0.00028500	2.48992500
H	1.40177900	0.00036200	3.30299500
C	-3.05985100	-1.23864100	0.47646400
C	0.00004000	0.00005300	0.37080200
C	-0.68099100	0.00033100	2.48993800
H	-1.40165000	0.00044900	3.30302200
C	3.05987600	-1.23873600	0.47627900
C	2.43780500	0.00005600	0.70114800
C	-2.43770600	0.00014400	0.70116500
C	-4.37325500	-1.20810300	0.00006200
H	-4.89752300	-2.14695300	-0.19052900
C	4.37341500	1.20816600	-0.00001900
H	4.89772500	2.14697700	-0.19068400
C	4.37329200	-1.20821100	-0.00008600
H	4.89751100	-2.14706400	-0.19079400
C	3.06000100	1.23879800	0.47634600
C	-3.05981300	1.23889200	0.47614800
C	5.02194200	-0.00004900	-0.23483400
H	6.04922500	-0.00009100	-0.60589100
C	-5.02182300	0.00006500	-0.23487800
H	-6.04909800	0.00003400	-0.60595800
C	-4.37322100	1.20827400	-0.00023100
H	-4.89746600	2.14709200	-0.19104100
C	-2.34888600	-2.55905700	0.69909600
H	-1.38187400	-2.34816800	1.18311200
C	2.34905500	2.55925800	0.69878300
H	1.38216500	2.34847500	1.18309200
C	3.13023000	3.47811300	1.63688600
H	2.55857300	4.39670900	1.83667500
H	4.09411300	3.78074700	1.20030100
H	3.33822800	2.98869100	2.59985500
C	-3.12987800	-3.47761000	1.63765000
H	-2.55823400	-4.39619400	1.83753600
H	-4.09390000	-3.78028300	1.20139900
H	-3.33758900	-2.98791500	2.60054200
C	2.04787400	3.24207900	-0.63630400
H	1.48597400	4.17513300	-0.47865700

H	2.97430200	3.49374800	-1.17505200
H	1.44726600	2.59087400	-1.29212600
C	-2.04804600	-3.24226700	-0.63586700
H	-2.97460200	-3.49403900	-1.17434500
H	-1.44754700	-2.59127400	-1.29200200
H	-1.48615900	-4.17530700	-0.47808900
C	2.34881800	-2.55914100	0.69869500
H	1.38191800	-2.34827800	1.18294800
C	2.04766400	-3.24198000	-0.63638700
H	1.44714200	-2.59074800	-1.29226700
H	2.97409900	-3.49373700	-1.17508000
H	1.48568100	-4.17498600	-0.47874500
C	3.12988000	-3.47802700	1.63686300
H	3.33784500	-2.98860100	2.59983600
H	2.55815800	-4.39658800	1.83663100
H	4.09377500	-3.78072000	1.20034300
C	-2.34882600	2.55934500	0.69848800
H	-1.38181800	2.34855300	1.18255700
C	-3.12984000	3.47808600	1.63684200
H	-2.55821000	4.39671700	1.83655300
H	-4.09385700	3.78065100	1.20050200
H	-3.33756800	2.98858900	2.59983200
C	-2.04796800	3.24229900	-0.63660100
H	-1.44749900	2.59118500	-1.29263200
H	-2.97451800	3.49402700	-1.17511000
H	-1.48605300	4.17534800	-0.47897900
Au	-0.00008000	-0.00025400	-1.60028600

Acetylene

0 1

C	2.21047400	0.00000400	0.00001200
C	1.51125700	1.20692800	-0.00000900
C	0.12046300	1.21147300	-0.00000500
C	-0.59182900	-0.00000300	-0.00002600
C	0.12047000	-1.21147800	-0.00001400
C	1.51126600	-1.20692400	0.00001300
H	3.30300400	0.00000900	0.00002000
H	2.05502500	2.15453300	0.00003600
H	-0.43174400	2.15319100	0.00000000
H	-0.43173000	-2.15320000	-0.00003500
H	2.05503700	-2.15452700	0.00002700
C	-2.02112400	-0.00000300	-0.00000800
C	-3.23446800	0.00000000	0.00002000

H	-4.30865400	0.00000300	0.00004400
IPr_INT1			
1 1			
N	-0.03871100	-1.24843200	1.48835300
N	-1.97274500	-0.36985400	1.17037100
C	-0.82742300	-1.63768200	2.55157900
H	-0.44670400	-2.26973000	3.34888100
C	-3.90917100	-0.28280800	-0.30610100
C	-0.73967300	-0.47068700	0.63950600
C	-2.05280300	-1.08022500	2.35007000
H	-2.96827700	-1.12441500	2.93322000
C	1.62818200	-2.72132400	0.49227400
C	1.33684700	-1.60661400	1.29509300
C	-3.03581500	0.38344700	0.56962300
C	-4.91766800	0.48058800	-0.89959500
H	-5.61863500	0.00402300	-1.58785100
C	3.65393200	-1.18830300	1.70628200
H	4.45062600	-0.60136500	2.16735600
C	2.97749600	-3.04608600	0.31905500
H	3.24726600	-3.91006400	-0.29245500
C	2.32291600	-0.81451500	1.90745500
C	-3.12881000	1.75278700	0.86500500
C	3.97773800	-2.29367100	0.92542600
H	5.02485500	-2.57470500	0.78902700
C	-5.04090600	1.83962800	-0.62682100
H	-5.83836600	2.41705200	-1.09988400
C	-4.15690900	2.46776900	0.24388500
H	-4.26670300	3.53554400	0.44585100
C	-3.74342600	-1.75150600	-0.64531100
H	-3.05382900	-2.19264100	0.09183900
C	1.97898400	0.42821100	2.70515500
H	0.90226900	0.39495000	2.93493400
C	2.72127000	0.49374900	4.03768700
H	2.37305400	1.35674300	4.62447400
H	3.80625900	0.61485100	3.89734500
H	2.55897600	-0.41430600	4.63705400
C	-5.05629400	-2.52549400	-0.55081300
H	-4.87836800	-3.59888400	-0.71412700
H	-5.78102400	-2.19757400	-1.31142400
H	-5.52669800	-2.40346700	0.43603400
C	2.22511400	1.68192600	1.86257500
H	1.94492800	2.58719000	2.42247300

H	3.28602800	1.76982000	1.58116500
H	1.63750000	1.66144100	0.93199000
C	-3.09677600	-1.91031500	-2.02320200
H	-3.73883300	-1.48788800	-2.81188000
H	-2.12339900	-1.39551100	-2.07014100
H	-2.93002700	-2.97318700	-2.25602600
C	0.54915900	-3.54761800	-0.17870800
H	-0.42759500	-3.13471100	0.11733000
C	0.64369300	-3.43621300	-1.70058500
H	0.58660800	-2.38546700	-2.02668300
H	1.58958500	-3.85502700	-2.07758300
H	-0.17918100	-3.98653100	-2.18122700
C	0.58605100	-5.00324900	0.28569000
H	0.49434000	-5.07928400	1.37938500
H	-0.24040100	-5.57190700	-0.16654000
H	1.52533200	-5.49787900	-0.00583300
C	-2.15396200	2.45418800	1.79020500
H	-1.47753700	1.69365900	2.21081000
C	-2.86849900	3.12279400	2.96383700
H	-2.13765900	3.57131900	3.65355400
H	-3.53860900	3.92780500	2.62531200
H	-3.47452100	2.40047900	3.53067400
C	-1.28909600	3.44864100	1.01441200
H	-0.75474200	2.95158800	0.18922300
H	-1.89866100	4.25615700	0.58025100
H	-0.54155000	3.91134800	1.67659300
Au	-0.06580200	0.35387800	-1.06496500
C	4.82482300	0.77634200	-1.01550400
C	3.57210400	0.50498800	-1.55012800
C	2.73519300	1.57069300	-1.92553000
C	3.15424900	2.90071600	-1.74410700
C	4.40978200	3.15562800	-1.20703600
C	5.24460300	2.09649900	-0.84588400
H	5.47803600	-0.04921700	-0.72784100
H	3.23097000	-0.52524600	-1.67245400
H	2.49271600	3.72005800	-2.03125900
H	4.74193500	4.18676300	-1.07107200
H	6.23254700	2.30327400	-0.42810700
C	1.44576400	1.31115600	-2.48428000
C	0.34817200	1.14852600	-3.04208400
H	-0.39700000	1.12476800	-3.82592700

Benzohydrazide

0 1

C	2.99770000	-0.23260200	0.06450800
C	2.44128300	1.04082700	0.19032800
C	1.06167900	1.20706400	0.12789100
C	0.22462700	0.10050200	-0.04602100
C	0.78838900	-1.17287600	-0.18686900
C	2.17047900	-1.33777800	-0.13044200
H	4.08157800	-0.36339500	0.10964100
H	3.08887800	1.90895200	0.33383100
H	0.59923800	2.19301800	0.20793800
H	0.15222500	-2.04141500	-0.37460100
H	2.60445000	-2.33326800	-0.24928100
C	-1.24875000	0.35656900	-0.10427500
O	-1.71572900	1.44918400	-0.37076600
N	-2.04932300	-0.71147000	0.17741400
H	-1.66876000	-1.52911100	0.63571100
N	-3.42656200	-0.58005700	0.22811600
H	-3.64071800	0.30224300	0.69832500
H	-3.77230600	-0.46005000	-0.72486500

IPr_INT1_2

1 1

N	2.11002500	-0.75348100	1.05258000
N	1.57771000	1.32175600	1.20590300
C	2.84661600	-0.23399100	2.09697700
H	3.53957500	-0.84359400	2.66950500
C	-0.31146200	2.81799000	1.56402100
C	1.33026400	0.19807500	0.50179500
C	2.50870900	1.08013800	2.19564500
H	2.84208800	1.86051300	2.87365100
C	1.24805300	-3.02115300	1.25071300
C	2.12389100	-2.12104900	0.62125600
C	0.93068400	2.57629000	0.95491600
C	-0.93614500	4.03429200	1.27277200
H	-1.90312500	4.26282500	1.72643700
C	2.97123000	-3.81979300	-0.82953300
H	3.63172900	-4.14566600	-1.63615600
C	1.27138900	-4.34497000	0.80450400
H	0.60997700	-5.07918600	1.26879900
C	2.99335900	-2.48388800	-0.41930600
C	1.55969900	3.48748100	0.09061500
C	2.12212100	-4.73972400	-0.22312900
H	2.12364500	-5.78020200	-0.55583500

C	-0.34251200	4.95790700	0.41895300
H	-0.84596100	5.90435700	0.20871700
C	0.89171100	4.68795500	-0.16453300
H	1.34524400	5.42483000	-0.83064400
C	-0.97796800	1.81159800	2.48188800
H	-0.26931400	0.98556000	2.64931200
C	3.90320300	-1.48164700	-1.10200700
H	3.83439000	-0.53145000	-0.54953500
C	5.36593500	-1.92113400	-1.06554400
H	6.01119900	-1.14533000	-1.50469500
H	5.52746000	-2.84622400	-1.63987600
H	5.70508000	-2.10448600	-0.03519500
C	-1.29766200	2.41488600	3.84872500
H	-1.71234000	1.64643500	4.51837500
H	-2.04297000	3.22154800	3.77356200
H	-0.39862600	2.83380000	4.32472600
C	3.43175300	-1.20803900	-2.53081900
H	4.06047700	-0.44095000	-3.00836700
H	3.48138300	-2.11805800	-3.14881200
H	2.38971200	-0.84980000	-2.53766700
C	-2.22109500	1.21134500	1.82391900
H	-2.98229100	1.98177100	1.62436300
H	-1.96614200	0.72748300	0.86871000
H	-2.67576400	0.44765500	2.47300700
C	0.34012700	-2.60045400	2.38959800
H	0.32361600	-1.49942400	2.41601700
C	-1.10218600	-3.05981700	2.18810300
H	-1.50876100	-2.70348900	1.23096800
H	-1.18762000	-4.15719100	2.21523900
H	-1.73598200	-2.66753700	2.99841700
C	0.90502900	-3.08418000	3.72690300
H	1.92736900	-2.71352500	3.89632100
H	0.27544700	-2.74033100	4.56176600
H	0.94201800	-4.18416000	3.76395600
C	2.88032900	3.17370400	-0.58531400
H	3.32157800	2.30367400	-0.07412400
C	3.88270000	4.31968300	-0.47002900
H	4.85445600	4.01946600	-0.88974200
H	3.55187000	5.21158500	-1.02380600
H	4.04010100	4.61452700	0.57804500
C	2.65033100	2.77167600	-2.04375400
H	1.96931400	1.90849900	-2.11188900
H	2.20776700	3.60205300	-2.61635400

H	3.60069900	2.49657900	-2.52654500
Au	0.03532900	-0.00642300	-0.98543200
C	-7.22785000	-0.53140300	-0.11964100
C	-6.48311700	-1.67300200	0.17986600
C	-5.14731800	-1.75028000	-0.19715000
C	-4.55320300	-0.68697200	-0.88756200
C	-5.30014300	0.46360700	-1.17580100
C	-6.63549200	0.53786600	-0.79180200
H	-8.27681400	-0.47117400	0.17927000
H	-6.94831200	-2.50593200	0.71112700
H	-4.54418000	-2.63086100	0.03242400
H	-4.83385100	1.32145200	-1.66650400
H	-7.21491500	1.43782900	-1.00791300
C	-3.12388500	-0.82236400	-1.25157600
O	-2.35076400	-1.58913500	-0.71056800
N	-2.68690100	0.00963600	-2.26647300
H	-3.34381800	0.27961600	-2.99200900
N	-1.34435200	-0.09518700	-2.64509400
H	-1.17146600	-0.95498400	-3.17936200
H	-1.11680100	0.69916700	-3.24442500

IPr_INT2

I 1

Au	0.12080600	0.03484000	-0.47236300
C	-1.63617000	-0.66287000	-1.57176600
H	-2.52776200	-0.01323800	-1.47344700
C	-0.82561800	-1.58404800	-1.75410800
C	0.01689700	-2.70338300	-2.05871800
C	0.49949400	-3.52606000	-1.02679100
C	0.37336600	-2.96450800	-3.39211200
C	1.31815100	-4.60570900	-1.33439900
H	0.23573500	-3.30592700	0.00994600
C	1.19436900	-4.04717900	-3.68575800
H	0.00033200	-2.31522100	-4.18623600
C	1.66528600	-4.86808500	-2.66010300
H	1.68986700	-5.24551000	-0.53197700
H	1.46834400	-4.25351600	-4.72243800
N	1.68459500	2.31274000	0.75097700
N	2.39348400	0.41774400	1.46936200
C	2.70852100	2.58547100	1.63469000
H	3.02059900	3.60202400	1.85630700
C	3.41620900	-1.69920000	0.82523400
C	1.48723800	0.98437700	0.64732900

C	3.15938000	1.38443300	2.08901600
H	3.94953300	1.13043800	2.78974200
C	1.40879600	3.68536300	-1.24121400
C	0.92888200	3.28628800	0.01672900
C	2.52633700	-0.99771400	1.65519700
C	3.52613600	-3.07709700	1.03049100
H	4.20802700	-3.65835200	0.40639000
C	-0.99487200	4.69008900	-0.17507100
H	-1.93332700	5.08345700	0.22110000
C	0.64244000	4.61540700	-1.94834400
H	0.97811300	4.95138900	-2.93175900
C	-0.26703300	3.76372300	0.57623300
C	1.74323900	-1.61505600	2.64406100
C	-0.54446800	5.11327700	-1.42094700
H	-1.12870800	5.83881300	-1.99134500
C	2.77621200	-3.71773500	2.01132100
H	2.88354300	-4.79481600	2.16080500
C	1.88863700	-2.99634900	2.80331100
H	1.30155900	-3.51416500	3.56516100
C	4.19464100	-1.02168800	-0.28496500
H	4.07192300	0.06651700	-0.16848800
C	-0.79080500	3.27096700	1.91068900
H	0.00161500	2.66954000	2.38378500
C	-1.11423600	4.41933000	2.86427100
H	-1.42072000	4.02703900	3.84572200
H	-1.94125100	5.04069500	2.48802600
H	-0.24435700	5.07570600	3.01522100
C	5.69063400	-1.31877400	-0.20532600
H	6.23375300	-0.75202800	-0.97637500
H	5.90440300	-2.38539200	-0.37386100
H	6.10587900	-1.04463800	0.77592500
C	-1.99589200	2.35276800	1.70122600
H	-2.34952600	1.94764500	2.66211400
H	-2.83167500	2.88801700	1.22567600
H	-1.74174600	1.50887000	1.04114600
C	3.61465500	-1.40020300	-1.64923300
H	3.69700400	-2.48259000	-1.83358600
H	2.54858300	-1.13566400	-1.71760400
H	4.14945800	-0.87641900	-2.45605400
C	2.67030600	3.10370800	-1.84816200
H	3.17647100	2.50812800	-1.07225200
C	2.31996800	2.15142800	-2.99327300
H	1.63878600	1.35519300	-2.65432800

H	1.82397300	2.68730200	-3.81744300
H	3.22799600	1.67757800	-3.39663100
C	3.64955400	4.18746900	-2.29440800
H	3.90536800	4.86564400	-1.46672100
H	4.58102600	3.73294000	-2.66413100
H	3.23717900	4.79807000	-3.11218800
C	0.75045600	-0.84404800	3.49093200
H	0.85732200	0.22467700	3.24941800
C	1.02827300	-1.00252000	4.98463500
H	0.33239800	-0.38490100	5.57224200
H	0.90065000	-2.04534600	5.31354200
H	2.05397600	-0.69576000	5.23784600
C	-0.68121800	-1.24571000	3.13420200
H	-0.87462300	-1.10503400	2.05903600
H	-0.86809800	-2.30386400	3.37631300
H	-1.40866300	-0.63942100	3.69545700
C	-4.77691500	-3.39702600	1.04340500
C	-3.86962100	-2.39845300	1.39514700
C	-3.96668100	-1.13703900	0.81627200
C	-4.98898000	-0.85447600	-0.09847100
C	-5.90130100	-1.85858200	-0.44249000
C	-5.78590700	-3.12683400	0.11953000
H	-4.69882800	-4.39058400	1.49092500
H	-3.08107300	-2.60418200	2.12173200
H	-3.25502800	-0.35128800	1.07716800
H	-6.69805800	-1.65077200	-1.15561900
H	-6.49283800	-3.90994600	-0.16291700
C	-4.97361100	0.49262500	-0.73792700
O	-3.91119500	1.03281500	-1.04990700
N	-6.13617700	1.14288200	-0.98518600
H	-6.00633600	2.05424000	-1.42519800
N	-7.36845500	0.73851300	-0.52953300
H	-7.72411800	1.36267000	0.19234000
H	-8.04111400	0.68492200	-1.29092900
H	2.30776200	-5.71920800	-2.89701600

IPr_INT3

1 1

Au	-0.44918900	0.45276800	-0.28626300
C	1.33359800	1.04633800	-1.05147700
H	1.51186500	2.12390000	-1.18970000
C	2.31493000	0.24303600	-1.48488600
C	2.43719600	-1.22532300	-1.39003100

C	2.91327400	-1.99578100	-2.46341500
C	2.08332300	-1.87654900	-0.19886800
C	3.01581200	-3.38062500	-2.35441400
H	3.17953000	-1.52690400	-3.41644900
C	2.19018600	-3.25885500	-0.09130400
H	1.72366400	-1.28276400	0.64399700
C	2.65316800	-4.01511200	-1.16747100
H	3.37325500	-3.96608900	-3.20430100
H	1.90841300	-3.74586100	0.84308600
N	-2.72193400	-1.28034100	0.85823200
N	-3.38305500	0.70576000	0.40655400
C	-4.06895700	-1.23342000	1.16527100
H	-4.59889400	-2.09738100	1.55578400
C	-3.68275200	2.32935600	-1.38322900
C	-2.28976300	-0.08893900	0.38815300
C	-4.48705900	0.02774900	0.88043000
H	-5.46063600	0.50121200	0.96839300
C	-1.76027200	-3.31933600	-0.07455500
C	-1.92022900	-2.45672900	1.02124800
C	-3.38000200	2.06830600	-0.03686400
C	-3.65133900	3.66349700	-1.79729500
H	-3.87865900	3.90919200	-2.83689800
C	-0.68735700	-3.92243900	2.45717100
H	-0.26307200	-4.16943000	3.43213800
C	-1.06034000	-4.50967700	0.14522200
H	-0.92167800	-5.20951200	-0.68168000
C	-1.37804100	-2.71896800	2.29167500
C	-3.05271800	3.07179500	0.88839500
C	-0.54573400	-4.81628100	1.39937200
H	-0.01940900	-5.76131500	1.55474400
C	-3.33229700	4.68221600	-0.90505300
H	-3.31506800	5.71899100	-1.24883000
C	-3.03579700	4.38920900	0.42184400
H	-2.78440100	5.19947700	1.10982000
C	-3.98470200	1.21937800	-2.37112800
H	-4.12246300	0.28847200	-1.79929900
C	-1.47992900	-1.71127300	3.41995900
H	-2.33580500	-1.05242300	3.20382000
C	-1.73693100	-2.35269800	4.78004600
H	-1.91289700	-1.57492900	5.53797500
H	-0.87713600	-2.94763200	5.12464300
H	-2.61718800	-3.01227600	4.75799800
C	-5.27804500	1.46851400	-3.14403700

H	-5.50784500	0.60928900	-3.79215200
H	-5.20252400	2.35494000	-3.79242100
H	-6.13041300	1.62200400	-2.46548700
C	-0.22595600	-0.83254900	3.44271900
H	-0.30367300	-0.06176800	4.22493900
H	0.67031700	-1.43854500	3.65141700
H	-0.07645000	-0.32373800	2.47712100
C	-2.79735900	1.00026600	-3.31073200
H	-2.60819000	1.89534900	-3.92413800
H	-1.87906300	0.77889800	-2.74353500
H	-2.99278500	0.15822700	-3.99288000
C	-2.28216000	-2.98257500	-1.45650000
H	-2.89270800	-2.07035700	-1.37337600
C	-1.11740800	-2.66330000	-2.39607700
H	-0.50726900	-1.83554900	-2.00159400
H	-0.45617100	-3.53483300	-2.52397700
H	-1.49157800	-2.37130700	-3.38939000
C	-3.18103500	-4.08193300	-2.01849300
H	-4.02053900	-4.30167800	-1.34206500
H	-3.59738100	-3.77590400	-2.99017600
H	-2.62728800	-5.01959200	-2.18071400
C	-2.69142700	2.75842800	2.32670200
H	-2.87760900	1.68620600	2.49440300
C	-3.56242100	3.52980300	3.31660900
H	-3.32486400	3.23251900	4.34932900
H	-3.39893600	4.61597800	3.24256600
H	-4.63254300	3.34064100	3.14440400
C	-1.20168700	3.00216800	2.57239500
H	-0.58486600	2.41244600	1.87576200
H	-0.94426300	4.06415500	2.43509900
H	-0.92656500	2.71945100	3.60026400
C	8.54947300	1.23175800	1.79066000
C	7.81176500	2.41636400	1.78473700
C	6.73478100	2.55887500	0.91841500
C	6.38772300	1.50759600	0.05966300
C	7.13681200	0.32198400	0.06027400
C	8.21546200	0.18767000	0.92687600
H	9.39801300	1.12272000	2.46995000
H	8.08092300	3.23273600	2.45792500
H	6.14466400	3.47684600	0.89180000
H	6.90843200	-0.48900800	-0.63566000
H	8.80566700	-0.73078400	0.92297300
C	5.23168300	1.71239900	-0.82522600

O	4.68437200	2.78054700	-1.03438600
N	4.74032700	0.58866000	-1.49587700
H	4.76618000	-0.33392600	-1.06510300
N	3.51131200	0.86437600	-2.12364200
H	3.46167400	1.91305300	-2.02644000
H	3.58125100	0.62924000	-3.12155100
H	2.73660500	-5.10070200	-1.08023600

IPr_INT4

1 1

Au	0.91231200	0.46442900	0.13772500
C	-0.97462500	0.69456500	0.83753600
H	-1.13159600	1.27054900	1.76330500
C	-2.07605600	0.12436000	0.33237500
C	-2.18181700	-0.78250600	-0.83438600
C	-1.40440800	-1.94992200	-0.85732700
C	-3.07527800	-0.54610400	-1.89062400
C	-1.54049000	-2.87072700	-1.89184100
H	-0.70281900	-2.14343900	-0.04358900
C	-3.20271600	-1.46571600	-2.93058100
H	-3.66585300	0.37141300	-1.91798900
C	-2.44262000	-2.63471400	-2.92894200
H	-0.93335400	-3.77657300	-1.88153300
H	-3.89808300	-1.26327000	-3.74823200
N	3.38040600	-0.77868000	-1.21624600
N	3.86147800	1.05587300	-0.22217500
C	4.73291000	-0.56782400	-1.40946000
H	5.34638700	-1.26268600	-1.97559100
C	3.86496900	2.19386400	1.93207600
C	2.83328600	0.21897500	-0.48687400
C	5.03815500	0.59537300	-0.77698600
H	5.97535200	1.13420800	-0.67205900
C	2.68744300	-3.10569000	-0.99480300
C	2.68216800	-1.91502300	-1.74227600
C	3.72442800	2.26265400	0.53698900
C	3.70784700	3.38283300	2.64973000
H	3.81070200	3.37169900	3.73718900
C	1.50498200	-2.95856800	-3.54424300
H	1.03300200	-2.91336800	-4.52791500
C	2.09487900	-4.22929900	-1.57774100
H	2.08610600	-5.17501500	-1.03301200
C	2.07773700	-1.80335600	-3.00472800
C	3.43342600	3.45235800	-0.15000700

C	1.52977400	-4.16137500	-2.84757000
H	1.09307300	-5.05769500	-3.29509100
C	3.42254000	4.57870500	1.99922000
H	3.30647900	5.49763500	2.57848700
C	3.28518100	4.61214300	0.61516100
H	3.05709200	5.55790700	0.11895600
C	4.13418500	0.88817000	2.65385600
H	4.32695200	0.11595500	1.89328400
C	1.98996200	-0.48414800	-3.74482100
H	2.65068400	0.23362100	-3.23433500
C	2.46654700	-0.58950300	-5.19140800
H	2.46057900	0.40241400	-5.66803300
H	1.81402000	-1.24218900	-5.79161200
H	3.48932200	-0.99059100	-5.25181800
C	5.37265900	0.96808200	3.54409600
H	5.58086500	-0.01127800	4.00100500
H	5.23989200	1.69101000	4.36377600
H	6.26083600	1.27292600	2.97082900
C	0.56473400	0.06700100	-3.65478200
H	0.49738700	1.04904600	-4.14793400
H	-0.15473200	-0.61028600	-4.14129300
H	0.25115900	0.18607700	-2.60549300
C	2.89811000	0.44606400	3.43890400
H	2.65465400	1.16949100	4.23355900
H	2.02443200	0.36200300	2.77294900
H	3.06755000	-0.53305700	3.91317500
C	3.25479800	-3.16182400	0.41001000
H	3.96988200	-2.32993200	0.51382500
C	2.13561800	-2.93226400	1.42968600
H	1.63639700	-1.96604100	1.25161100
H	1.36861000	-3.72047800	1.37666200
H	2.53957300	-2.92383700	2.45416800
C	4.01662700	-4.45130300	0.70071200
H	4.79517000	-4.64288400	-0.05279100
H	4.50297900	-4.38855700	1.68554000
H	3.34843200	-5.32549400	0.72936600
C	3.23133800	3.48329800	-1.65221600
H	3.57970900	2.52054200	-2.05748100
C	4.05188900	4.57990000	-2.32729500
H	3.94408900	4.51906500	-3.42079500
H	3.72114600	5.58490000	-2.02312500
H	5.12131000	4.49136400	-2.08437800
C	1.74315100	3.60252700	-1.98734700

H	1.16643100	2.78326300	-1.52903200
H	1.33092100	4.55449400	-1.61682500
H	1.58694000	3.56697300	-3.07675400
C	-7.97786700	3.51564700	-1.98187100
C	-8.52910100	2.41256700	-1.32925000
C	-7.70614700	1.53166300	-0.63726300
C	-6.32530900	1.75619300	-0.58291200
C	-5.77497700	2.86061200	-1.24800000
C	-6.60110000	3.73597400	-1.94593000
H	-8.62457900	4.20612300	-2.52794600
H	-9.60656500	2.23848700	-1.36286800
H	-8.11307900	0.65705300	-0.12648000
H	-4.69641400	3.04104000	-1.26054200
H	-6.16830500	4.59057100	-2.46981600
C	-5.51506700	0.76568800	0.16744200
O	-5.90576700	-0.34651700	0.46367800
N	-4.25896300	1.18369100	0.54362300
H	-3.85674100	2.07633800	0.28576700
N	-3.35560100	0.26007400	1.07738100
H	-3.13956700	0.49726000	2.05623900
H	-2.54924200	-3.35860100	-3.74016800
C	-2.02333700	0.25679800	4.82059200
C	-0.86026800	-0.26083200	4.24788800
C	-0.93045400	-1.36905400	3.40949400
C	-2.16575000	-1.95736900	3.11772100
C	-3.32630300	-1.45928100	3.72421700
C	-3.25512100	-0.35231900	4.57002600
H	-1.96842200	1.12329600	5.48383200
H	0.10648000	0.20220700	4.45531900
H	-0.03098200	-1.78921800	2.95712400
H	-4.28885300	-1.94432800	3.55305000
H	-4.16102800	0.02332300	5.05148200
C	-2.16057700	-3.15672200	2.22394900
O	-1.22687400	-3.93122200	2.19678500
N	-3.27789600	-3.39449500	1.45552200
H	-3.20379600	-4.24643300	0.90429600
N	-4.12443500	-2.39597200	0.98965500
H	-4.10704600	-2.36974400	-0.03290800
H	-5.09372300	-2.55058000	1.27020200
H	-3.81600300	-0.73149500	1.12293900

IPr_INT5

1 1

Au	-1.47995100	0.09760000	-0.53963500
C	0.29021000	0.75753500	-1.27728800
H	0.35686400	1.03565500	-2.34236600
C	1.43655000	0.91551700	-0.59253100
C	1.63341400	0.53706700	0.83341500
C	1.41373600	-0.79417400	1.22313600
C	2.14408500	1.43291800	1.78548900
C	1.74364800	-1.22730000	2.50536000
H	1.00408700	-1.49581700	0.49318900
C	2.46940600	1.00186300	3.07205800
H	2.28072600	2.48404100	1.52592400
C	2.28697700	-0.33418500	3.43179300
H	1.57345500	-2.26944900	2.78012800
H	2.86431200	1.71629700	3.79833200
N	-3.56232100	-1.30753800	1.23637600
N	-4.49800900	-0.17301900	-0.31776400
C	-4.92592600	-1.46664400	1.40032600
H	-5.34176600	-2.07437300	2.19863000
C	-4.72706600	0.08788400	-2.72885900
C	-3.28598900	-0.51112000	0.17867500
C	-5.51921300	-0.74596500	0.41332200
H	-6.56476700	-0.58854800	0.16498900
C	-2.12883300	-3.20858000	1.74987800
C	-2.58689600	-1.92376700	2.08428100
C	-4.68041500	0.67729100	-1.45555600
C	-4.89090300	0.94153600	-3.82311200
H	-4.92935200	0.52188600	-4.83077500
C	-1.27841700	-1.89338100	4.08701900
H	-0.93197500	-1.39048600	4.99220600
C	-1.23955900	-3.82308300	2.63670000
H	-0.86874700	-4.82626700	2.41584100
C	-2.16430700	-1.23292400	3.23179400
C	-4.78443500	2.06140700	-1.24422900
C	-0.83323100	-3.17971100	3.80109700
H	-0.15437600	-3.68577400	4.49219000
C	-5.00174100	2.31685000	-3.64725600
H	-5.13113500	2.96647700	-4.51601000
C	-4.94750900	2.87008700	-2.37211800
H	-5.03065200	3.95231600	-2.24986300
C	-4.55944500	-1.40477000	-2.93220400
H	-4.58890600	-1.88368700	-1.94117700
C	-2.59383500	0.19246200	3.51387800
H	-3.43829400	0.42635100	2.84711100

C	-3.07996800	0.38879700	4.94746900
H	-3.46049700	1.41239900	5.08340100
H	-2.26971100	0.24469900	5.67888700
H	-3.88950400	-0.31220900	5.20038300
C	-5.69456900	-2.00541300	-3.75878800
H	-5.58252400	-3.09826000	-3.82593100
H	-5.70141300	-1.61416200	-4.78785000
H	-6.67686700	-1.78955000	-3.31239100
C	-1.45710300	1.15538300	3.16295600
H	-1.77126100	2.19911000	3.31912200
H	-0.57126700	0.96684400	3.78977200
H	-1.15081400	1.04140900	2.11110800
C	-3.19006200	-1.71046600	-3.54143700
H	-3.09618400	-1.26922700	-4.54626700
H	-2.37985400	-1.30337500	-2.91597900
H	-3.04107100	-2.79738900	-3.63519200
C	-2.53195700	-3.89240500	0.45878000
H	-3.38874300	-3.34119700	0.04130800
C	-1.39400200	-3.79774100	-0.56020300
H	-1.11648300	-2.74791100	-0.74677900
H	-0.49843600	-4.33021500	-0.20181100
H	-1.69272800	-4.24692100	-1.51988000
C	-2.98219200	-5.33543700	0.67142200
H	-3.79399400	-5.40094100	1.41125400
H	-3.34739400	-5.76324900	-0.27436900
H	-2.15747800	-5.97638400	1.01956400
C	-4.67732200	2.67561300	0.13748600
H	-4.69406300	1.85527600	0.87162500
C	-5.85763600	3.59122200	0.45503900
H	-5.78684200	3.96338900	1.48845500
H	-5.88249100	4.46986600	-0.20794900
H	-6.81741800	3.06408300	0.34705700
C	-3.33841500	3.39768400	0.29903600
H	-2.49666800	2.71572800	0.09896800
H	-3.26060200	4.24657300	-0.39872000
H	-3.23072800	3.78988100	1.32241400
C	5.02168400	7.08282700	0.28587500
C	6.05525300	6.14806700	0.22225300
C	5.76699400	4.80573000	0.00325200
C	4.44174700	4.39056100	-0.17250400
C	3.40574400	5.33183600	-0.09624500
C	3.69748200	6.67281000	0.13395000
H	5.24834800	8.13667700	0.46252100

H	7.09164400	6.46871400	0.34714000
H	6.56028200	4.05763600	-0.03916400
H	2.35858900	5.02840900	-0.17967100
H	2.88628700	7.40042400	0.20304200
C	4.19987500	2.94296100	-0.39942500
O	5.03299100	2.10262400	-0.03126500
N	3.05313700	2.61622500	-1.02077100
H	2.41203000	3.35558100	-1.30027200
N	2.67407800	1.30165900	-1.24118400
H	2.59562500	1.14617400	-2.24540000
H	2.54855800	-0.67407100	4.43665600
C	8.62317000	-4.61836400	-1.97394900
C	7.50475600	-4.46827700	-2.79488100
C	6.44675800	-3.66415000	-2.38746000
C	6.51019200	-2.99661700	-1.15825900
C	7.62902800	-3.15930900	-0.32992100
C	8.68292500	-3.96910900	-0.74054700
H	9.45264400	-5.25308200	-2.29400000
H	7.45829000	-4.98375600	-3.75637200
H	5.55826400	-3.53598500	-3.00868100
H	7.66927100	-2.68739600	0.65493900
H	9.55067600	-4.10377900	-0.09163500
C	5.35892500	-2.14947800	-0.78589700
O	4.25817900	-2.20695000	-1.29725300
N	5.57796700	-1.22783200	0.23429200
H	6.49796800	-0.82411100	0.37287600
N	4.50866700	-0.36022800	0.44732600
H	4.09185000	-0.47241100	1.38215000
H	4.73463600	0.69758200	0.24110700
H	3.78305000	-0.62540800	-0.25082800

IPr_INT6

1 1

Au	-0.96058000	-0.30560400	-0.43172200
C	1.03173600	-0.34268000	-0.83877200
H	1.35586700	-0.00198200	-1.83565100
C	2.04700300	-0.56986200	0.02380100
C	1.88018000	-1.08073600	1.40277700
C	1.05501700	-2.18802000	1.64144800
C	2.53275500	-0.48321600	2.49488000
C	0.87709200	-2.67627800	2.93331400
H	0.57667500	-2.67625200	0.79032100
C	2.34184400	-0.96330100	3.78915800

H	3.20106000	0.36845100	2.33362800
C	1.51442500	-2.06414900	4.01166600
H	0.24008400	-3.54838400	3.09723700
H	2.85122400	-0.48281700	4.62799600
C	8.11823100	-4.42427600	0.07547800
C	7.84613700	-4.10301000	-1.25497600
C	6.77708000	-3.26916900	-1.56460000
C	5.98202200	-2.74056200	-0.54229100
C	6.24798400	-3.07713300	0.79095700
C	7.31554000	-3.91682000	1.09690100
H	8.95575000	-5.08267400	0.31753400
H	8.46968000	-4.50946500	-2.05427900
H	6.53476900	-3.01264800	-2.59790300
H	5.59852100	-2.71697300	1.59318400
H	7.51558600	-4.18699700	2.13606700
C	4.85233500	-1.85593000	-0.93416700
O	4.35025500	-1.84206500	-2.04084700
N	4.39862000	-1.00186600	0.04580100
H	4.99182700	-0.74918700	0.82500100
N	3.37528200	-0.12675000	-0.27904900
H	3.44113700	0.06083200	-1.28513300
H	1.37669600	-2.45012600	5.02410500
C	5.90675300	4.73176400	-1.87709300
C	4.79160400	5.56867400	-1.92836200
C	3.61375600	5.19478500	-1.29250500
C	3.54508900	3.97750800	-0.60320000
C	4.66986000	3.14196100	-0.54799600
C	5.84553000	3.52075800	-1.18675000
H	6.83242400	5.02564000	-2.37717600
H	4.84257800	6.51695200	-2.46724400
H	2.72778500	5.83176000	-1.31741300
H	4.64160500	2.19268400	-0.00872500
H	6.72124300	2.86994900	-1.14423800
C	2.25724500	3.64267800	0.03686300
O	1.29114300	4.38661300	0.07525200
N	2.16389000	2.40012400	0.64092900
H	2.74360400	1.59058700	0.35973300
N	0.87080200	2.08784300	1.06009400
H	0.45221900	1.30123400	0.48143600
H	0.83715000	1.80297900	2.04646900
H	0.31034300	2.96611600	0.93110700
N	-3.51974200	0.99439600	0.59061000
N	-3.98869900	-0.80671000	-0.46771500

C	-4.89872200	0.89497500	0.58075800
H	-5.53571900	1.63962600	1.04932900
C	-3.82956900	-3.23805000	-0.52103200
C	-2.95044100	-0.04941100	-0.05569500
C	-5.19469200	-0.24733500	-0.09386700
H	-6.14591200	-0.70999200	-0.34133000
C	-2.40918800	1.93048800	2.54678800
C	-2.78120000	2.05902900	1.19717000
C	-3.83100400	-2.01799400	-1.21895200
C	-3.64137900	-4.40068000	-1.27118000
H	-3.63109300	-5.36999200	-0.76970300
C	-1.74730800	4.21623300	1.04352200
H	-1.46672200	5.10112800	0.47009900
C	-1.70002800	2.99015500	3.12457100
H	-1.40684800	2.92920900	4.17542500
C	-2.45838200	3.18459800	0.41888800
C	-3.66163900	-1.92344800	-2.60875600
C	-1.37894900	4.12488600	2.38386200
H	-0.83088000	4.94686400	2.85034600
C	-3.46307200	-4.34126800	-2.65057800
H	-3.31523300	-5.26288900	-3.21790100
C	-3.47432000	-3.11832600	-3.31054100
H	-3.33555800	-3.08857700	-4.39352400
C	-3.96075300	-3.28927500	0.98935000
H	-4.46525000	-2.36431800	1.31232300
C	-2.81632400	3.28730500	-1.04970200
H	-3.45975400	2.42990500	-1.29932100
C	-3.60771500	4.55812400	-1.35364300
H	-3.92045100	4.56810600	-2.40840900
H	-3.00615800	5.46388100	-1.18172900
H	-4.51102000	4.63074400	-0.72973300
C	-4.81216000	-4.45771200	1.47686300
H	-4.97267000	-4.38267000	2.56279700
H	-4.32535700	-5.42715200	1.29029100
H	-5.79687700	-4.47471200	0.98673000
C	-1.55880300	3.18074200	-1.91505200
H	-1.82047700	3.23856000	-2.98235500
H	-0.84773100	3.99223600	-1.69437600
H	-1.04696700	2.21861800	-1.74902100
C	-2.57502100	-3.29878700	1.63898800
H	-2.01642800	-4.20316700	1.34915300
H	-1.98087100	-2.42560200	1.33034800
H	-2.65877800	-3.28646300	2.73706800

C	-2.71234400	0.68472300	3.35270500
H	-3.35311000	0.03428500	2.73853400
C	-1.42296700	-0.08680800	3.63120900
H	-0.90492500	-0.35450500	2.69700600
H	-0.73007600	0.49737700	4.25831300
H	-1.63555700	-1.02410800	4.16625100
C	-3.47685200	1.00181500	4.63628100
H	-4.40752600	1.54991200	4.42714200
H	-3.74032800	0.07200700	5.16223200
H	-2.87751300	1.61154300	5.33004700
C	-3.66919100	-0.59738300	-3.34330500
H	-3.86733800	0.19624600	-2.60619000
C	-4.78957500	-0.54031700	-4.38138600
H	-4.81916700	0.44962900	-4.86161500
H	-4.64314600	-1.28807800	-5.17597000
H	-5.77256900	-0.72809000	-3.92402300
C	-2.30421900	-0.30450300	-3.96618700
H	-1.50970100	-0.31655400	-3.20307500
H	-2.04330000	-1.04973900	-4.73330800
H	-2.30369500	0.68558900	-4.44744000

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C	4.32119000	-4.12393200	0.33838600
C	4.85295200	-3.05611900	1.06352800
C	4.93544500	-1.79455200	0.48475900
C	4.47163000	-1.58778200	-0.82023400
C	3.94592400	-2.66374400	-1.54560100
C	3.87196500	-3.92828700	-0.96689300
H	4.26883000	-5.11751100	0.78919800
H	5.22392500	-3.21598200	2.07845000
H	5.38390900	-0.95419100	1.01843800
H	3.65379200	-2.53766200	-2.59101800
H	3.48146500	-4.76913000	-1.54390200
C	4.72327400	-0.25511900	-1.42963300
O	5.64495200	0.45314000	-1.10430600
N	3.90755800	0.15155900	-2.49277900
H	4.19862300	1.05084700	-2.87210800
N	2.55767300	-0.07754500	-2.56596300
H	2.26943300	-0.93066100	-3.03713700
C	1.63040600	0.86897900	-2.37032300
C	2.06685800	2.15224300	-1.77918100
C	1.75234600	3.35232100	-2.43105400

C	2.78797500	2.18153200	-0.57669400
C	2.18253900	4.56566000	-1.90132100
H	1.19296700	3.33397000	-3.36900700
C	3.21107800	3.39721800	-0.05379600
H	2.98990500	1.25849300	-0.02993900
C	2.91859600	4.58834900	-0.71779700
H	1.94851200	5.49678000	-2.42130800
H	3.77525200	3.41145500	0.88014000
H	3.26373700	5.54052800	-0.30879300
C	0.28479800	0.65259800	-2.75120900
H	-0.26448100	1.57290800	-2.98510200
H	0.10256000	-0.16365400	-3.46134600
N	-1.13224900	-0.12066100	2.10940100
N	-2.88596300	-0.63006100	0.98550300
C	-2.10108400	-0.46943300	3.03032100
H	-1.91207600	-0.45126500	4.09992800
C	-3.75248300	-2.09626900	-0.75837500
C	-1.60996600	-0.21445200	0.85050200
C	-3.21130900	-0.79705700	2.31703500
H	-4.19687700	-1.12885900	2.63096800
C	1.18793800	-0.65018300	2.63096200
C	0.19277800	0.32184200	2.42782600
C	-3.77428100	-0.84723000	-0.11838800
C	-4.61647100	-2.27225300	-1.84310100
H	-4.63169900	-3.23011800	-2.36801200
C	1.73228500	2.10536000	2.82829400
H	1.95373700	3.17099300	2.91846600
C	2.47457000	-0.19158700	2.92419300
H	3.27729000	-0.91192600	3.08703500
C	0.43022100	1.70200300	2.51572500
C	-4.60814100	0.21080000	-0.51733100
C	2.74253700	1.17148100	3.02665000
H	3.75306800	1.50682100	3.27301100
C	-5.45605000	-1.24635900	-2.26272200
H	-6.12458200	-1.40501500	-3.11189700
C	-5.45070000	-0.01864000	-1.60793200
H	-6.11317100	0.77800500	-1.95245800
C	-2.82489800	-3.21429700	-0.32591900
H	-2.27627900	-2.87336500	0.56577200
C	-0.65750900	2.73175100	2.28403100
H	-1.59161200	2.19260600	2.06454400
C	-0.90311000	3.57508600	3.53476800
H	-1.73315500	4.27815700	3.36771900

H	-0.01556900	4.16913500	3.80262200
H	-1.15757900	2.94657000	4.40122100
C	-3.59957400	-4.47035900	0.07041400
H	-2.91181000	-5.24765400	0.43669600
H	-4.15101800	-4.89318600	-0.78346700
H	-4.32914900	-4.25803800	0.86601500
C	-0.34368000	3.60183800	1.06739600
H	-1.17673600	4.29100500	0.86223500
H	0.56081700	4.20831100	1.22622700
H	-0.17664200	2.98767800	0.16868000
C	-1.78699900	-3.50780100	-1.40956800
H	-2.26308200	-3.87800300	-2.33086500
H	-1.21807800	-2.59961800	-1.66527000
H	-1.07504900	-4.27433700	-1.06734500
C	0.88499600	-2.12989700	2.49205400
H	-0.17924900	-2.27378100	2.73981500
C	1.08503900	-2.57978200	1.04335000
H	0.43157200	-2.02623900	0.35293100
H	2.12384900	-2.41285000	0.72650100
H	0.86492700	-3.65288500	0.93467500
C	1.69116700	-2.99896100	3.45204400
H	1.59716400	-2.65456700	4.49259700
H	1.33759200	-4.03956300	3.40432000
H	2.75996600	-3.01126700	3.19066500
C	-4.56514400	1.56728400	0.15918400
H	-4.02577000	1.45144900	1.11247100
C	-5.95650500	2.10011000	0.49268600
H	-5.87860800	3.03803200	1.06273100
H	-6.54012500	2.31982200	-0.41435300
H	-6.53084500	1.38104900	1.09546200
C	-3.77140900	2.56055500	-0.69227500
H	-2.74951600	2.19542100	-0.88121700
H	-4.25793400	2.72056300	-1.66722100
H	-3.69839100	3.53558300	-0.18617300
Au	-0.63111000	0.19531000	-0.87277000

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N	0.46284600	2.13381300	-0.77878500
N	-1.66629500	1.87803800	-0.86773400
C	-0.04501900	3.27363500	-1.37102600
H	0.59499300	4.09056600	-1.69213800
C	-3.72947200	1.65566900	0.40698300

C	-0.53097200	1.27334100	-0.46157000
C	-1.39290900	3.10801200	-1.43391200
H	-2.17894300	3.74739400	-1.82537900
C	2.35055100	2.11664000	0.76353400
C	1.84859900	1.87463800	-0.52590200
C	-2.97435300	1.31158300	-0.72636000
C	-5.00618100	1.09997400	0.51367400
H	-5.62801300	1.34392900	1.37753700
C	3.98297900	1.11990800	-1.30044800
H	4.63077800	0.72852800	-2.08629100
C	3.70318800	1.83420100	0.98769700
H	4.13363400	2.01274300	1.97583800
C	2.63793000	1.37475700	-1.57779600
C	-3.43480300	0.44023700	-1.72556500
C	4.51162100	1.34813700	-0.03361900
H	5.56502800	1.13480100	0.15948900
C	-5.49494600	0.23752800	-0.46223400
H	-6.49642800	-0.18498900	-0.35997000
C	-4.71581800	-0.09502400	-1.56391800
H	-5.11156000	-0.77951400	-2.31718400
C	-3.17618300	2.54552600	1.50256100
H	-2.26644300	3.03056900	1.11532900
C	2.04912400	1.05955300	-2.93952400
H	1.14624600	1.67821400	-3.06550400
C	2.99149800	1.39824900	-4.09065200
H	2.47218100	1.27276400	-5.05216000
H	3.86925200	0.73450000	-4.11206300
H	3.35169300	2.43595700	-4.03040400
C	-4.14448700	3.65668700	1.90040400
H	-3.67419500	4.32840000	2.63414200
H	-5.05818700	3.25666000	2.36603400
H	-4.44745800	4.25910300	1.03116800
C	1.60747700	-0.40546300	-2.99636100
H	1.15986500	-0.63777800	-3.97479700
H	2.46115700	-1.08453100	-2.84337500
H	0.85711200	-0.62026300	-2.22029200
C	-2.75862200	1.70095700	2.70828300
H	-3.62977900	1.19616900	3.15522800
H	-2.03170200	0.92712100	2.41838900
H	-2.30177900	2.33195100	3.48638200
C	1.49172700	2.67220000	1.88253700
H	0.48018000	2.84025900	1.48260000
C	1.35956100	1.66975500	3.02832400

H	0.91811300	0.72526400	2.66997100
H	2.33587500	1.44395100	3.48525300
H	0.70421200	2.06579000	3.81870500
C	2.01924900	4.02130500	2.37070800
H	2.09206200	4.74541300	1.54579400
H	1.34986500	4.44203200	3.13620500
H	3.01949700	3.92664000	2.82070800
C	-2.59103600	0.06594900	-2.92820100
H	-1.67692300	0.67930400	-2.90518400
C	-3.30629200	0.36956000	-4.24365700
H	-2.64621600	0.15559900	-5.09783200
H	-4.21160800	-0.24458300	-4.36626100
H	-3.60890900	1.42559600	-4.30209200
C	-2.15444800	-1.39662400	-2.84831600
H	-1.59430000	-1.58603400	-1.91886400
H	-3.02252600	-2.07380900	-2.86026700
H	-1.50760700	-1.65814100	-3.69941300
Au	-0.29138100	-0.49760300	0.44102700
C	7.54872400	-1.00014200	0.98333000
C	7.27443000	-1.40234300	-0.32558200
C	6.00120200	-1.84884700	-0.66305700
C	4.99027200	-1.87350700	0.30344000
C	5.27208300	-1.48787700	1.61908400
C	6.55078100	-1.05314900	1.95694800
H	8.55129200	-0.65719400	1.24928100
H	8.06168000	-1.37481200	-1.08208300
H	5.76465400	-2.18077800	-1.67610600
H	4.49819000	-1.54955500	2.38729500
H	6.77450000	-0.76386500	2.98606300
C	3.64155600	-2.32332500	-0.11825600
O	3.42713800	-3.02140500	-1.09085000
N	2.59100100	-1.89286600	0.67401400
H	2.66017200	-0.95921600	1.07156300
N	1.31236800	-2.25173600	0.24204100
H	1.40601800	-2.51156500	-0.74953100
H	1.02973300	-3.10745600	0.72545900
C	-5.68385100	-3.26827800	0.38070300
C	-4.53186400	-3.63197900	-0.31816500
C	-3.28186800	-3.25412800	0.15483800
C	-3.17865300	-2.49429100	1.33344500
C	-4.34361900	-2.11569400	2.02400100
C	-5.58745400	-2.51201600	1.54880300
H	-6.66415600	-3.58008400	0.01307200

H	-4.60910200	-4.22609200	-1.23121500
H	-2.37603300	-3.55020500	-0.37689000
H	-4.25749400	-1.52448900	2.93717200
H	-6.49018600	-2.22934600	2.09444900
C	-1.90451500	-2.15206200	1.86817900
C	-0.81872600	-1.85424900	2.36137300
H	0.02534100	-1.81782300	3.03273600

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Au	-0.28369500	-0.15758200	-0.67445000
C	1.18552200	-0.91484000	-1.94207400
H	1.36513200	-0.44999300	-2.91037600
C	1.79354600	-1.78388000	-1.24771300
C	2.07517400	-2.66990000	-0.16632100
C	1.62562000	-4.00224900	-0.20604900
C	2.76923900	-2.19383500	0.96052800
C	1.87222100	-4.84568400	0.86997900
H	1.07220600	-4.35754200	-1.07783800
C	2.99940200	-3.04371400	2.03475700
H	3.10617200	-1.15705800	0.98392500
C	2.55580700	-4.36691800	1.98966000
H	1.52243500	-5.87971900	0.84267100
H	3.52965300	-2.67203500	2.91403900
N	-1.67016100	1.87464900	1.11456000
N	-2.97386600	0.23937300	0.63776700
C	-2.88218300	2.14732100	1.71845200
H	-3.04324000	3.04976200	2.30127100
C	-3.22051000	-2.17759100	0.81411200
C	-1.72175400	0.70340800	0.44614300
C	-3.70701600	1.10809200	1.41976900
H	-4.74067400	0.90915200	1.68781100
C	0.29035200	2.63460100	2.34263000
C	-0.51500400	2.72006400	1.19280700
C	-3.45160000	-0.99656400	0.09131400
C	-3.67558900	-3.37092100	0.24602000
H	-3.51853600	-4.31245700	0.77721800
C	0.86624300	4.43177800	0.25411500
H	1.10668100	5.12929100	-0.55123000
C	1.37796100	3.50676000	2.42503100
H	2.01635200	3.48755600	3.31043400
C	-0.25195000	3.59963800	0.13134900
C	-4.10028200	-0.96616100	-1.15413300

C	1.66283700	4.39692200	1.39223600
H	2.51981900	5.06928400	1.47533700
C	-4.32569200	-3.37615700	-0.98345400
H	-4.67614400	-4.31955200	-1.40836000
C	-4.53378900	-2.18749500	-1.67622900
H	-5.04130200	-2.20910800	-2.64280800
C	-2.48854700	-2.18909300	2.14182900
H	-2.27160800	-1.14565000	2.41836200
C	-1.11841900	3.66549600	-1.11024900
H	-1.94350700	2.94741600	-0.98605100
C	-1.74303100	5.04957300	-1.28418900
H	-2.41411800	5.06095100	-2.15636800
H	-0.97613100	5.82232700	-1.44756500
H	-2.32828900	5.34134100	-0.39932500
C	-3.34811100	-2.78451100	3.25603300
H	-2.82146100	-2.72687700	4.22077600
H	-3.57758100	-3.84482100	3.06843000
H	-4.30425200	-2.24963000	3.35669100
C	-0.33044500	3.23918700	-2.34909400
H	-0.98196000	3.22582300	-3.23595800
H	0.50384600	3.92654800	-2.55723600
H	0.09308200	2.23016000	-2.22210800
C	-1.14637400	-2.90974000	2.01506400
H	-1.28366500	-3.97039100	1.75335400
H	-0.52048800	-2.45147300	1.23409000
H	-0.59023900	-2.86895800	2.96407000
C	0.04221600	1.58436100	3.40850600
H	-1.01946200	1.29541500	3.35548500
C	0.86824800	0.33136300	3.10065000
H	0.65937000	-0.05222500	2.09002900
H	1.94614100	0.55125100	3.15595700
H	0.64671100	-0.46964800	3.82281000
C	0.30065800	2.08664200	4.82525400
H	-0.26249000	3.00706000	5.03936000
H	-0.00180600	1.32407300	5.55823300
H	1.36743500	2.29450200	5.00057300
C	-4.27695400	0.32014100	-1.93727200
H	-4.06406600	1.16024100	-1.25762800
C	-5.70538600	0.50370500	-2.44461000
H	-5.81417300	1.48512100	-2.93006500
H	-5.97643800	-0.25901400	-3.19052200
H	-6.43613300	0.44562200	-1.62425300
C	-3.26015600	0.39220900	-3.07868700

H	-2.22925800	0.30084600	-2.70045500
H	-3.42361100	-0.41926100	-3.80505800
H	-3.34501800	1.34957400	-3.61562700
C	5.03796400	0.71208000	1.41137300
C	3.96631600	1.43221200	0.87869300
C	3.59486600	1.25373400	-0.45022300
C	4.27891000	0.33056000	-1.24860800
C	5.35502400	-0.38531400	-0.71306800
C	5.73849600	-0.19061700	0.61232600
H	5.33649600	0.86570100	2.45111800
H	3.41736800	2.14517100	1.49525400
H	2.77241700	1.82957000	-0.88020600
H	5.93082400	-1.06455600	-1.34749200
H	6.59284100	-0.73652400	1.01831900
C	3.90564700	0.21472300	-2.68793900
O	3.61110300	1.16958300	-3.37259700
N	3.98440200	-1.05070000	-3.24903300
H	3.79742500	-1.06477500	-4.24746600
N	3.68020600	-2.20465200	-2.53185900
H	3.27192500	-2.89376700	-3.16011000
H	4.51121300	-2.62146000	-2.10764800
H	2.74226700	-5.03197100	2.83610400

IPr_TS3

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Au	1.19174400	-0.02514300	-0.46148900
C	-0.72100500	-0.29871800	-1.07617900
H	-0.95073800	-0.24158600	-2.15251500
C	-1.77827700	-0.58139100	-0.29758200
C	-1.77793000	-0.62535600	1.18812800
C	-1.31385900	0.49202900	1.90212400
C	-2.29544200	-1.71041100	1.91249000
C	-1.38211100	0.52992000	3.29247400
H	-0.90326800	1.33757600	1.34566800
C	-2.35909800	-1.67300900	3.30541300
H	-2.63085900	-2.60749300	1.38987400
C	-1.90966800	-0.55113500	3.99972500
H	-1.01287200	1.40839500	3.82418300
H	-2.75729500	-2.53230400	3.85005100
N	3.65220200	0.51735400	1.31056300
N	4.21626300	-0.02461900	-0.68138500
C	5.03448100	0.51557900	1.27965200
H	5.62880600	0.75774500	2.15585900

C	4.05785200	0.58510300	-3.03505900
C	3.13635700	0.18468500	0.10554700
C	5.39169200	0.17237000	0.01462300
H	6.36519900	0.04997300	-0.45115700
C	2.59754200	2.18046100	2.74351700
C	2.89130400	0.83146800	2.48255600
C	4.13164900	-0.41801100	-2.05593900
C	3.96064700	0.17260800	-4.36681300
H	3.89864300	0.92273800	-5.15830700
C	1.85589800	0.13102600	4.52205400
H	1.55190900	-0.65556800	5.21584400
C	1.93541100	2.47245500	3.93932000
H	1.70029000	3.51037100	4.18363900
C	2.51606900	-0.21520700	3.33972100
C	4.10675900	-1.78963900	-2.35563400
C	1.58380500	1.45990900	4.82670900
H	1.08308600	1.71040300	5.76527100
C	3.93805600	-1.17819600	-4.69756300
H	3.86345200	-1.47940800	-5.74502300
C	4.00864800	-2.14794800	-3.70265100
H	3.98454800	-3.20485500	-3.97720100
C	4.03485100	2.05839900	-2.67978300
H	4.25469500	2.14788700	-1.60459600
C	2.76228200	-1.66938100	2.99330400
H	3.43074000	-1.69796400	2.11899400
C	3.45691800	-2.42862700	4.12121100
H	3.68634800	-3.45711100	3.80379400
H	2.82298000	-2.49888200	5.01865800
H	4.40030300	-1.94384500	4.41403900
C	5.10667300	2.84796600	-3.42846700
H	5.11077800	3.89756200	-3.09723700
H	4.92836800	2.84889100	-4.51488000
H	6.11005500	2.43108800	-3.25474400
C	1.44832500	-2.33724900	2.58233900
H	1.62275200	-3.38227500	2.28258100
H	0.72457400	-2.33586800	3.41242900
H	0.98364100	-1.80873700	1.73510500
C	2.63869800	2.64104700	-2.90556800
H	2.35735900	2.59596300	-3.96949500
H	1.88090900	2.08444000	-2.33166700
H	2.60321300	3.69592600	-2.59200600
C	2.92612500	3.27385500	1.74635900
H	3.68132900	2.87599600	1.05056800

C	1.68288700	3.61221400	0.91953100
H	1.29043500	2.71895400	0.40778400
H	0.88443000	4.01642700	1.56246700
H	1.91718400	4.36837900	0.15441000
C	3.52335200	4.51746700	2.39858100
H	4.40374800	4.27080700	3.01062300
H	3.83515100	5.23781900	1.62748800
H	2.79672500	5.03260600	3.04571900
C	4.13465600	-2.85128700	-1.27369900
H	4.36253100	-2.35220500	-0.31913000
C	5.22821100	-3.89035300	-1.51215300
H	5.27051600	-4.60132700	-0.67304400
H	5.04389900	-4.47488400	-2.42674500
H	6.21763600	-3.41915400	-1.61051600
C	2.75756000	-3.50081700	-1.12482400
H	1.98513800	-2.74411800	-0.91358200
H	2.46959600	-4.03180700	-2.04605500
H	2.76094300	-4.23083800	-0.30033300
C	-5.48425600	-6.69107700	-0.71654100
C	-6.51458400	-5.77699800	-0.49433600
C	-6.23121100	-4.41934300	-0.39764300
C	-4.91556700	-3.96364300	-0.53949600
C	-3.88227500	-4.88668800	-0.75089600
C	-4.16828100	-6.24608400	-0.83752500
H	-5.70677100	-7.75810400	-0.78851700
H	-7.54415700	-6.12672100	-0.39311400
H	-7.01960700	-3.68773400	-0.21217300
H	-2.83942900	-4.56390400	-0.81582500
H	-3.35884600	-6.96244300	-0.99238300
C	-4.68623000	-2.49853300	-0.41420200
O	-5.47717400	-1.76908200	0.17304700
N	-3.55092800	-2.03508600	-1.00275700
H	-2.93565000	-2.66377200	-1.50869100
N	-3.11760500	-0.71848400	-0.86955800
H	-3.15436400	-0.23743900	-1.77147500
H	-3.94104700	0.13883300	-0.05260200
H	-1.96248500	-0.52205900	5.09054500
C	-6.29781800	6.34598400	-1.63685700
C	-5.84254000	5.50181600	-2.65011200
C	-5.32217600	4.25232100	-2.33279000
C	-5.26695800	3.83394600	-0.99826200
C	-5.71236800	4.69029000	0.01756600
C	-6.22656700	5.94285000	-0.30358100

H	-6.70405700	7.32874900	-1.88665300
H	-5.89215300	5.82203000	-3.69293500
H	-4.95159400	3.57845000	-3.10745000
H	-5.62704200	4.40711100	1.06993700
H	-6.56427000	6.61204600	0.49044200
C	-4.70378700	2.48538100	-0.73629700
O	-3.99094700	1.88690300	-1.51680200
N	-5.04907500	1.92810800	0.47709600
H	-5.80986200	2.29746500	1.03365300
N	-4.58764600	0.66132300	0.78939400
H	-4.00614200	0.64978000	1.63638100
H	-5.31286400	-0.08078000	0.83327200

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Au	-0.11578600	-0.40042200	-0.40264500
C	0.69782600	1.25144800	-1.34825100
H	0.45359600	1.34828600	-2.41951400
C	1.86725600	1.87157600	-0.99900400
C	2.35716600	1.91930600	0.40492300
C	2.89243400	0.78488100	1.01957000
C	2.28732600	3.12462800	1.11697900
C	3.35400800	0.85847600	2.33273500
H	2.97364700	-0.13923900	0.44470700
C	2.72745600	3.18778000	2.43736400
H	1.89450800	4.02053000	0.62629800
C	3.26721000	2.05352100	3.04460200
H	3.78862400	-0.02592500	2.80291800
H	2.66090100	4.12765300	2.99036800
C	8.78870900	2.63006800	-0.26446100
C	8.53591200	1.58188600	-1.15064300
C	7.23483700	1.31964600	-1.56538800
C	6.17971600	2.11806500	-1.11132100
C	6.43466700	3.15924200	-0.21036300
C	7.73748500	3.41224900	0.21180000
H	9.81075200	2.83287400	0.06382900
H	9.35944500	0.96468200	-1.51647100
H	7.01101000	0.49570100	-2.24597200
H	5.61275400	3.75131200	0.20083700
H	7.93241100	4.21791300	0.92298600
C	4.80552900	1.78033600	-1.57388600
O	4.45365900	0.66026200	-1.88106200
N	3.92952900	2.84193500	-1.62529900

H	4.22905800	3.79026900	-1.43981500
N	2.60565500	2.62999300	-1.88339600
H	2.38967600	2.46636900	-2.86431000
H	3.62815100	2.10514400	4.07431000
C	-6.99841500	3.21600600	-2.02817200
C	-6.83330900	3.96513100	-0.86174700
C	-5.56959000	4.10517700	-0.29792300
C	-4.46807100	3.47646500	-0.88830400
C	-4.63120000	2.74788600	-2.07215500
C	-5.89594200	2.61890100	-2.63993000
H	-7.99079600	3.11085900	-2.47251100
H	-7.69487700	4.44695200	-0.39467100
H	-5.41379300	4.69579700	0.60734300
H	-3.76633000	2.30754300	-2.57344900
H	-6.02094800	2.05979200	-3.56976000
C	-3.15918700	3.60472000	-0.20637800
O	-2.85291200	4.51329800	0.54085700
N	-2.24663100	2.60500000	-0.46954600
H	-2.50865200	1.67761500	-0.79265300
N	-1.05457500	2.65545000	0.23802000
H	-0.21613800	2.06982100	-0.42160200
H	-0.85529800	3.64894400	0.41429300
H	-1.14009000	2.19647400	1.15753200
N	-0.65715400	-3.31381200	0.38301300
N	-2.16868000	-2.00282000	1.15155600
C	-1.56908000	-4.11132500	1.04703400
H	-1.45418500	-5.18991900	1.10689700
C	-4.03452700	-0.50942400	0.66387300
C	-1.01737000	-2.01361200	0.43910400
C	-2.52401100	-3.28071100	1.54188600
H	-3.41471800	-3.47964500	2.13111700
C	0.49801200	-3.90658700	-1.68197000
C	0.52162200	-3.78446000	-0.28434800
C	-2.90311600	-0.81074300	1.44694600
C	-4.72900400	0.66536200	0.96461200
H	-5.61190200	0.93684900	0.38384300
C	2.79875800	-4.50748000	-0.17581400
H	3.69975300	-4.74592200	0.39170300
C	1.67553400	-4.33184900	-2.30503300
H	1.69946000	-4.43648700	-3.39195400
C	1.65143600	-4.08381500	0.49741200
C	-2.45888400	0.00730400	2.49847400
C	2.81248700	-4.62554300	-1.56282700

H	3.72245400	-4.95399300	-2.06973900
C	-4.30331800	1.50463700	1.99128200
H	-4.85773600	2.42040200	2.20719700
C	-3.17955800	1.18321300	2.74448900
H	-2.87125700	1.84307600	3.55918500
C	-4.44755100	-1.39380100	-0.49830300
H	-4.11233700	-2.41791100	-0.27118600
C	1.64970200	-3.88824500	2.00204000
H	0.60920400	-3.97826900	2.35240500
C	2.46412800	-4.94056000	2.74773900
H	2.32845600	-4.82452600	3.83338700
H	3.54218800	-4.84473800	2.54705600
H	2.15869500	-5.96106200	2.47296000
C	-5.95735400	-1.44550800	-0.70798800
H	-6.20500200	-2.19277800	-1.47619200
H	-6.35542000	-0.48018300	-1.05751900
H	-6.48851300	-1.71850100	0.21585600
C	2.12148200	-2.47438500	2.34497300
H	2.07611200	-2.29720200	3.43106400
H	3.16335400	-2.32941900	2.01797400
H	1.50766600	-1.70997700	1.84563300
C	-3.73159000	-0.95849000	-1.77988100
H	-4.08160800	0.03761600	-2.09209300
H	-2.63888000	-0.91746000	-1.64646500
H	-3.94554200	-1.65728700	-2.60298400
C	-0.73814500	-3.61399900	-2.50869200
H	-1.52786100	-3.26623500	-1.82552500
C	-0.48524800	-2.49195900	-3.51464300
H	-0.12941800	-1.58033100	-3.00891600
H	0.27293000	-2.77912600	-4.25926900
H	-1.40998500	-2.24733700	-4.05970700
C	-1.25505100	-4.88081300	-3.19124700
H	-1.46647700	-5.67461600	-2.45913600
H	-2.18301600	-4.67016400	-3.74487900
H	-0.52224700	-5.27793400	-3.91057500
C	-1.27565400	-0.35607300	3.37369900
H	-0.85036100	-1.29675300	2.99414700
C	-1.72313000	-0.60407800	4.81482000
H	-0.87214800	-0.93592500	5.42868000
H	-2.12957900	0.30957500	5.27577300
H	-2.50286000	-1.37856600	4.86576800
C	-0.17038400	0.69492100	3.29861600
H	0.22448800	0.78863800	2.27379600

H	-0.51804100	1.68287200	3.64200400
H	0.67878700	0.41226000	3.93735900

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N	-3.16998200	1.20895800	-0.43461000
N	-3.39606800	-0.51718000	0.81759500
C	-4.50249200	1.15540300	-0.07306300
H	-5.22371600	1.89073400	-0.41869200
C	-2.52330700	-1.57685400	2.83073500
C	-2.48213100	0.17819400	0.10512800
C	-4.64424000	0.06624400	0.72782200
H	-5.51202000	-0.34516600	1.23555500
C	-2.32002300	3.47687700	-0.70310600
C	-2.58588900	2.21598400	-1.26998800
C	-3.08302200	-1.70797300	1.54990800
C	-2.17320000	-2.75501800	3.49809800
H	-1.73662600	-2.69762900	4.49787400
C	-1.72679100	2.89680900	-3.39510400
H	-1.50264600	2.69155900	-4.44425000
C	-1.74624600	4.43882400	-1.53637000
H	-1.53104700	5.43235900	-1.14101100
C	-2.31578600	1.89969800	-2.60989600
C	-3.31452800	-2.94880500	0.93157100
C	-1.44675600	4.15042000	-2.86590400
H	-1.00116700	4.92006800	-3.50077000
C	-2.37656600	-3.99838100	2.90931200
H	-2.09475800	-4.90658600	3.44669900
C	-2.94384700	-4.09357700	1.64188500
H	-3.10187800	-5.07786100	1.19723600
C	-2.28100400	-0.22754600	3.47965200
H	-2.70472400	0.54570400	2.82099800
C	-2.68174900	0.56236100	-3.22345600
H	-3.07120600	-0.08329600	-2.42227200
C	-3.79690600	0.72705000	-4.25696300
H	-4.09919800	-0.25234400	-4.65831100
H	-3.47066800	1.34900500	-5.10488600
H	-4.68509500	1.20421200	-3.81654400
C	-2.99276200	-0.11491100	4.82726900
H	-2.86720200	0.89574000	5.24442300
H	-2.58874900	-0.82740400	5.56273000
H	-4.07047000	-0.31207800	4.72880900
C	-1.46478300	-0.14487000	-3.81535800

H	-1.74394200	-1.14009100	-4.19369600
H	-1.03019200	0.41979000	-4.65439500
H	-0.67946500	-0.27298300	-3.05516300
C	-0.78495800	0.06365400	3.60966700
H	-0.28527500	-0.68433500	4.24592200
H	-0.29561100	0.06064900	2.62187800
H	-0.62009300	1.05318900	4.06219000
C	-2.61478800	3.76196400	0.75885000
H	-3.51897200	3.19298800	1.02862900
C	-1.47900400	3.25697400	1.65172500
H	-1.24161700	2.20153800	1.45568900
H	-0.56401500	3.84085300	1.47825700
H	-1.74919900	3.35776300	2.71419900
C	-2.91218700	5.23001500	1.04231600
H	-3.70014500	5.62450800	0.38370700
H	-3.24698500	5.35117400	2.08302800
H	-2.01685000	5.85899400	0.91933400
C	-3.89381300	-3.04999400	-0.46776300
H	-4.41051900	-2.10170100	-0.68416200
C	-4.92889100	-4.16416500	-0.59822200
H	-5.40651000	-4.12340800	-1.58843900
H	-4.47420400	-5.16180000	-0.50105900
H	-5.71665700	-4.07661300	0.16456700
C	-2.78034600	-3.20054500	-1.50692700
H	-2.07254700	-2.35884300	-1.45668600
H	-2.21294000	-4.13134600	-1.34675100
H	-3.20104300	-3.23378300	-2.52366400
Au	-0.52516200	-0.35294900	-0.15096400
C	7.91199200	1.50802900	-0.12935400
C	8.21596500	0.17635300	0.15523100
C	7.20848100	-0.69931100	0.54459400
C	5.88532700	-0.25424500	0.64082800
C	5.58755300	1.08751200	0.36712600
C	6.59888600	1.96353400	-0.01757300
H	8.70416400	2.19683100	-0.43180500
H	9.24573500	-0.17884500	0.07636200
H	7.42129700	-1.74292400	0.78462700
H	4.57320100	1.47808100	0.48038800
H	6.36138700	3.00991800	-0.22138800
C	4.86662700	-1.26041300	1.05899700
O	5.14405100	-2.30911600	1.59999500
N	3.56581500	-0.91862800	0.76303300
H	3.34629100	-0.10109800	0.20269600

N	2.51875300	-1.68852200	1.17346800
H	2.17459600	-1.49908400	2.11006700
C	1.64313500	-2.26550100	0.30008600
C	2.16553200	-2.79057300	-0.97696100
C	3.44992300	-3.35289300	-1.02909600
C	1.36184800	-2.81362700	-2.12800000
C	3.91908800	-3.90919600	-2.21572100
H	4.06402100	-3.38557500	-0.12562200
C	1.83786800	-3.36780900	-3.31144200
H	0.35634900	-2.38508700	-2.09378200
C	3.12168000	-3.91226300	-3.35937700
H	4.91714200	-4.35182300	-2.24288000
H	1.20469500	-3.37276300	-4.20147200
H	3.49818700	-4.34457400	-4.28911200
C	0.31175500	-2.41251000	0.65502700
H	-0.28673100	-3.15537500	0.12749000
H	0.01185800	-2.21762000	1.68976200
C	2.27001800	3.75153200	2.21691700
C	2.09306500	2.57605100	1.49821100
C	1.71714100	2.63084300	0.14265800
C	1.52063700	3.87730900	-0.47717000
C	1.70305900	5.04677900	0.25174000
C	2.07670300	4.98691800	1.59529400
H	2.56264900	3.70668000	3.26790500
H	2.24325400	1.60644900	1.97783000
H	1.22090700	3.91082400	-1.52528400
H	1.55381400	6.01473300	-0.23153100
H	2.21961500	5.90919400	2.16271700
C	1.56894500	1.43408900	-0.60968600
C	1.43871500	0.39194400	-1.25377200
H	1.69370200	-0.38034200	-1.97036800

IPr_TS5_2

1 1

N	3.14688500	-1.36710000	0.28950500
N	1.83212700	-3.06187700	0.26359800
C	3.92527000	-2.47690200	0.56354800
H	4.99452600	-2.40024800	0.73950500
C	0.32015300	-4.37644200	-1.12327900
C	1.85688300	-1.72003500	0.10022600
C	3.08969700	-3.54969700	0.55363300
H	3.27551500	-4.60634600	0.72376400
C	3.90844700	0.50512400	-1.07366100

C	3.64520700	-0.02782400	0.19911100
C	0.62678200	-3.82593300	0.13202900
C	-0.91186600	-5.02397500	-1.25121400
H	-1.19157600	-5.46226800	-2.21157400
C	4.38897500	1.97635900	1.27692400
H	4.57236600	2.56577000	2.17648200
C	4.42705700	1.80415500	-1.12914500
H	4.64974200	2.25387600	-2.09941400
C	3.86414800	0.68664700	1.39105500
C	-0.22493000	-3.91814600	1.24386000
C	4.67601300	2.52697600	0.03199400
H	5.08267800	3.53827700	-0.03338700
C	-1.78742700	-5.11722700	-0.17302000
H	-2.74595200	-5.62692100	-0.29621600
C	-1.44491000	-4.57573700	1.06130300
H	-2.13862200	-4.66093200	1.90056500
C	1.25242600	-4.24284700	-2.31219100
H	2.22614300	-3.89111300	-1.93670000
C	3.47936400	0.11539100	2.74210700
H	3.51870300	-0.98302100	2.66575800
C	4.42945200	0.52418700	3.86302300
H	4.17794200	-0.01824200	4.78630100
H	4.35631700	1.59811600	4.09302700
H	5.47688900	0.30104900	3.61131900
C	1.49502100	-5.58076200	-3.00754300
H	2.24627400	-5.46632400	-3.80334900
H	0.57923600	-5.96918400	-3.47888100
H	1.85805700	-6.34276200	-2.30192900
C	2.03320900	0.49538100	3.07365300
H	1.73241600	0.07041100	4.04344500
H	1.91876500	1.58999800	3.13158300
H	1.34016000	0.11678400	2.30759300
C	0.73854700	-3.18464700	-3.28999400
H	-0.24441000	-3.46700000	-3.69937300
H	0.63191000	-2.20857500	-2.79292400
H	1.43394800	-3.06808200	-4.13554500
C	3.64766700	-0.26442500	-2.35342600
H	3.29333100	-1.26960100	-2.07963900
C	2.53435000	0.39754900	-3.16585200
H	1.60333200	0.45819000	-2.57734800
H	2.81310700	1.41674000	-3.47733600
H	2.31874300	-0.18273000	-4.07576800
C	4.92274600	-0.43838900	-3.17733700

H	5.71379600	-0.93084200	-2.59258400
H	4.72339600	-1.05367500	-4.06773700
H	5.31748600	0.52850500	-3.52551700
C	0.13159800	-3.31950400	2.58964300
H	1.15057000	-2.90877800	2.51741400
C	0.14794900	-4.38137700	3.68868500
H	0.47059000	-3.94005900	4.64387600
H	-0.85135200	-4.81541500	3.84723300
H	0.83461400	-5.20529200	3.44355100
C	-0.80237800	-2.16231100	2.93694900
H	-0.78342700	-1.38894300	2.15324300
H	-1.84428200	-2.50102100	3.03591300
H	-0.50748700	-1.69468200	3.88866000
Au	0.23615300	-0.61441500	-0.38024900
C	4.31361800	6.44396400	-0.61840700
C	3.99720500	6.34032100	0.73768000
C	2.98017900	5.48579700	1.15114000
C	2.29123200	4.71239600	0.21169900
C	2.59725500	4.83179500	-1.14855300
C	3.60576300	5.69837000	-1.56164500
H	5.10734100	7.12084400	-0.94300700
H	4.54262500	6.93592000	1.47304900
H	2.70485300	5.39644200	2.20408300
H	2.03381200	4.25876800	-1.88836700
H	3.83674900	5.80012600	-2.62438300
C	1.23989700	3.78727300	0.70884900
O	0.63005100	3.95251600	1.74965000
N	0.97944800	2.69613400	-0.09049000
H	1.74335600	2.29684700	-0.63057500
N	0.03640900	1.78536800	0.36971100
H	0.03513200	1.82691600	1.39353000
H	-0.89148500	2.08443800	0.06047800
C	-8.57508200	3.46843400	-0.10582800
C	-8.57332500	2.13006700	-0.50049500
C	-7.38411900	1.51919900	-0.88208800
C	-6.18549300	2.24098000	-0.85843800
C	-6.19326100	3.58798600	-0.47377800
C	-7.38671200	4.19823900	-0.09855000
H	-9.51041600	3.94925500	0.18969500
H	-9.50625400	1.56245100	-0.51396700
H	-7.35699300	0.47654300	-1.20442100
H	-5.27730700	4.18395000	-0.49999900
H	-7.39185500	5.25132200	0.19048100

C	-4.95341000	1.51929100	-1.26992300
O	-4.94894800	0.50700000	-1.93699100
N	-3.76542800	2.06174400	-0.81299500
H	-3.75614700	2.75019300	-0.07176200
N	-2.58303200	1.43044900	-1.09946200
H	-2.22178900	1.67348300	-2.02087100
C	-2.45336000	0.08044400	-0.80822900
C	-3.13025100	-0.40600200	0.41169400
C	-3.79068300	-1.63983300	0.39288400
C	-3.13488600	0.35607200	1.58908500
C	-4.44880100	-2.09904100	1.52981100
H	-3.81674700	-2.22185300	-0.52970700
C	-3.78750900	-0.10819100	2.72566100
H	-2.60797300	1.31256400	1.62637200
C	-4.45176400	-1.33471400	2.69575500
H	-4.97514400	-3.05552900	1.50008300
H	-3.77796700	0.48946000	3.63948700
H	-4.97487200	-1.69370200	3.58492400
C	-1.67805700	-0.74102800	-1.60187100
H	-1.75907100	-1.82070500	-1.45256500
H	-1.42039000	-0.40820600	-2.61243200

N'-(1-phenylvinyl)benzohydrazide

01

C	4.39018800	-1.04554000	0.00323200
C	3.72973200	-0.84703700	1.21627300
C	2.56443500	-0.08907200	1.25860100
C	2.03984800	0.46422500	0.08638400
C	2.71289600	0.27355100	-1.12589400
C	3.88448500	-0.47913100	-1.16585500
H	5.30782500	-1.63778200	-0.02999900
H	4.12909700	-1.28405700	2.13446700
H	2.03376400	0.09394800	2.19511600
H	2.34538900	0.73949100	-2.04362400
H	4.41002400	-0.61671800	-2.11364300
C	0.77932600	1.26142800	0.21565200
O	0.42834700	1.76943300	1.25929700
N	0.03877800	1.36945000	-0.93513500
H	0.23736400	0.75494200	-1.71419900
N	-1.20246400	1.95993800	-0.93675300
H	-1.13982100	2.97221400	-0.87684400
C	-2.18877100	1.42096400	-0.09104700
C	-2.25157800	-0.05823400	-0.07262400

C	-2.37215600	-0.74413900	1.14073700
C	-2.18178600	-0.79384800	-1.26435600
C	-2.43914600	-2.13579700	1.16172300
H	-2.38881400	-0.17063200	2.06993000
C	-2.24749900	-2.18355600	-1.24227900
H	-2.09894900	-0.25980900	-2.21483100
C	-2.37640600	-2.85901500	-0.02799500
H	-2.52907200	-2.65971300	2.11638600
H	-2.20363800	-2.74513700	-2.17872300
H	-2.42352800	-3.95046900	-0.01027700
C	-3.05950200	2.19384100	0.57563400
H	-3.90306200	1.74842200	1.10232500
H	-2.96194200	3.28228600	0.58363500

Thiazol_Au_Cation

1 1

C	0.83792600	2.26100100	0.00010700
C	-0.20504200	3.14660100	0.00008800
C	-0.92911900	0.77484300	-0.00002400
N	0.39264600	0.93874100	0.00004000
S	-1.71028100	2.27749000	-0.00001200
C	1.30011600	-0.18562900	0.00005600
C	1.71342400	-0.70024200	-1.23943100
C	1.71323600	-0.70035000	1.23956200
C	2.57078200	-1.80352800	-1.20784200
C	2.57060200	-1.80363100	1.20800800
C	2.99206000	-2.34997100	0.00009100
H	2.91525700	-2.24214800	-2.14663600
H	2.91494400	-2.24232600	2.14681500
C	1.24486300	-0.12462200	-2.56160700
H	0.70245900	0.81235200	-2.35528500
C	1.24449900	-0.12482400	2.56171800
H	0.70208300	0.81214100	2.35538000
C	2.41505600	0.22491700	-3.48062600
H	3.12891600	0.90550600	-2.99255500
H	2.97112200	-0.67247900	-3.79089300
H	2.04907900	0.71523400	-4.39473600
C	0.26399600	-1.07634600	-3.24872000
H	0.74350600	-2.03793000	-3.48791100
H	-0.60670400	-1.28872000	-2.60650300
H	-0.10794700	-0.64130400	-4.18833000
C	0.26360200	-1.07661700	3.24869300
H	-0.60702600	-1.28901100	2.60638500

H	0.74312700	-2.03818800	3.48790500
H	-0.10845600	-0.64162100	4.18827800
C	2.41458600	0.22470800	3.48087700
H	2.97066400	-0.67268600	3.79112600
H	3.12846100	0.90537000	2.99292900
H	2.04849600	0.71493600	4.39499000
C	-0.18664200	4.63466000	0.00015400
H	-0.69141600	5.04177600	-0.88900100
H	-0.69132000	5.04169300	0.88940300
H	0.84589600	5.00577400	0.00011600
C	2.29632900	2.54296600	0.00019000
H	2.78114700	2.10727900	-0.88579900
H	2.48019300	3.62318100	0.00026800
H	2.78106400	2.10716900	0.88617000
H	3.66227700	-3.21233100	0.00010400
Au	-1.83875300	-0.97478900	-0.00012700

Thiazol_INT1

1 1

Au	0.33319100	1.62877500	-0.13295100
C	4.83325600	-1.63396100	0.57712800
C	3.88623300	-1.70869500	-0.44556500
C	3.14036100	-0.58873000	-0.78918000
C	3.35062500	0.61975300	-0.10210600
C	4.29849800	0.69234900	0.93387000
C	5.03756300	-0.43650200	1.26515300
H	5.41960100	-2.51716300	0.84056800
H	3.72720200	-2.64679500	-0.97980300
H	2.38886500	-0.64195400	-1.57954800
H	4.44777800	1.63342300	1.46611600
H	5.77915000	-0.38291000	2.06465500
C	2.59526200	1.78434700	-0.44054600
C	2.03097400	2.85291600	-0.72480700
H	1.88380500	3.85962500	-1.09304300
C	-3.09770400	-0.81775700	0.50979400
C	-3.82698500	0.27831700	0.87190500
C	-1.45644900	0.81416100	0.28767500
N	-1.78083200	-0.47747200	0.18989200
S	-2.81746700	1.68990600	0.79996600
C	-0.83402100	-1.48811100	-0.21665900
C	-0.09424300	-2.15205500	0.78395600
C	-0.74754200	-1.81550500	-1.58517200
C	0.72116800	-3.21073700	0.36795500

C	0.09205300	-2.88351000	-1.92685700
C	0.80560800	-3.58618200	-0.96587700
H	1.30023400	-3.75052900	1.12128700
H	0.17090500	-3.17037800	-2.97863900
C	0.00374400	-1.78393000	2.26292100
H	0.28628600	-2.73056200	2.75207500
C	-1.38604600	-1.07820800	-2.76080900
H	-1.49011500	-1.85493600	-3.53624600
C	1.17520400	-0.82056500	2.47932500
H	2.10060400	-1.19602700	2.01971600
H	0.96074100	0.16789000	2.04092100
H	1.35750900	-0.67529200	3.55479700
C	-1.23897900	-1.29190500	3.00003300
H	-1.52823200	-0.26776100	2.72517100
H	-2.10420800	-1.95353700	2.85862000
H	-1.02193100	-1.27621700	4.07820000
C	-2.77388400	-0.46314000	-2.60207800
H	-3.50762700	-1.17434900	-2.19977200
H	-2.77838000	0.44083000	-1.97680600
H	-3.13610600	-0.15888800	-3.59500700
C	-0.40130600	-0.04337500	-3.31529100
H	-0.24235300	0.77649700	-2.59565200
H	0.57789300	-0.49351000	-3.53604300
H	-0.78926000	0.39779200	-4.24570700
C	-5.25475700	0.37672400	1.28002100
H	-5.35459300	0.80784900	2.28760100
H	-5.82637500	1.01161300	0.58602900
H	-5.72362400	-0.61524600	1.29111200
C	-3.54580100	-2.23252100	0.42920200
H	-2.94088000	-2.88054000	1.07945700
H	-4.59533800	-2.31994100	0.73265200
H	-3.44671500	-2.62519400	-0.59321300
H	1.43140400	-4.43225700	-1.25898700

Thaizol_INT1_2

1 1

Au	0.04207400	-1.40699000	-0.83754200
C	4.74969900	2.26500700	-1.03001300
C	5.69237100	1.33430400	-0.59086700
C	5.27896200	0.16362800	0.03728500
C	3.91380900	-0.09193600	0.20979100
C	2.96821600	0.85298200	-0.21351400
C	3.39087300	2.02904600	-0.83134200

H	5.07853100	3.18466400	-1.51900600
H	6.75805600	1.52655500	-0.73227600
H	6.01045100	-0.55965100	0.40422000
H	1.89977400	0.70026200	-0.02446300
H	2.65089400	2.76756200	-1.14528900
C	3.51015500	-1.33962200	0.93292200
O	3.88009300	-1.62273400	2.04512600
N	2.69255500	-2.21660500	0.24212300
H	2.24703400	-2.94653600	0.78985300
N	2.09088800	-1.93332700	-1.00142400
H	2.59183900	-1.11738900	-1.38137100
H	2.29319000	-2.70405500	-1.64563000
C	-3.56007000	0.45442600	0.34489400
C	-4.29981900	-0.54102100	-0.22864800
C	-1.83708400	-0.84750900	-0.51717700
N	-2.19164300	0.24930000	0.16040300
S	-3.23488600	-1.69574100	-0.97343700
C	-1.20393700	1.17684000	0.65862200
C	-0.86080000	2.27161600	-0.15322300
C	-0.64236700	0.94603000	1.92506900
C	0.09381200	3.16007500	0.34880600
C	0.31901400	1.85953600	2.36962900
C	0.68034800	2.95525200	1.59402700
H	0.38304500	4.02858000	-0.24669100
H	0.78969100	1.71065600	3.34365500
C	-1.45267300	2.47125900	-1.53501000
H	-2.32222700	1.80209500	-1.63336200
C	-1.02704900	-0.23774800	2.79041700
H	-1.85692400	-0.76697900	2.29564800
C	-1.95235000	3.89718800	-1.75758200
H	-2.66587300	4.20626100	-0.97889700
H	-1.12702700	4.62519600	-1.76063800
H	-2.45758000	3.97552400	-2.73149300
C	-0.44304500	2.05953800	-2.60873800
H	0.45236800	2.69992300	-2.57509200
H	-0.11686400	1.01601300	-2.47196200
H	-0.88292700	2.14983600	-3.61327000
C	0.13580200	-1.22375100	2.90953600
H	0.44395200	-1.58517000	1.91550500
H	1.01685000	-0.76342600	3.38222100
H	-0.15397800	-2.09620200	3.51400700
C	-1.52527300	0.20521100	4.16602600
H	-0.72930900	0.69331600	4.74843400

H	-2.36276800	0.91470700	4.08733200
H	-1.87049400	-0.66390500	4.74536900
C	-5.77702300	-0.71739100	-0.27579600
H	-6.14721900	-0.71921100	-1.31233500
H	-6.08263300	-1.66644000	0.19009300
H	-6.28101100	0.09733000	0.25930400
C	-4.03180200	1.64853900	1.09322200
H	-3.72389000	2.57816700	0.59188400
H	-5.12467600	1.64600300	1.17426100
H	-3.60824200	1.67002500	2.10817800
H	1.43034800	3.65764400	1.96389800

Thiazol_INT3

1 1

C	-1.23019200	0.31967700	-1.39833200
H	-1.36834400	-0.55190100	-2.05708500
C	-2.33104300	1.06301000	-1.21078300
C	-2.55019400	2.24460800	-0.35359000
C	-3.40485100	3.29018200	-0.74287200
C	-1.90864100	2.33651100	0.89132400
C	-3.59438600	4.40087100	0.07621400
H	-3.91656900	3.27199800	-1.71065700
C	-2.09421500	3.44909800	1.70469000
H	-1.26319500	1.51712000	1.21434600
C	-2.93619000	4.48550800	1.30125100
H	-4.25179900	5.20892100	-0.25170600
H	-1.58515400	3.50204500	2.66961900
C	-7.81632900	-2.42280900	1.71511800
C	-6.99934300	-3.30947900	1.01232500
C	-6.07661800	-2.82364000	0.09405300
C	-5.96387000	-1.44300700	-0.11634800
C	-6.79314000	-0.55462500	0.58360300
C	-7.71653800	-1.04774000	1.49828700
H	-8.54367600	-2.80660800	2.43414600
H	-7.08592700	-4.38478400	1.18059700
H	-5.42934100	-3.49662300	-0.47139800
H	-6.75075400	0.52138800	0.39763800
H	-8.36915000	-0.35876500	2.03801400
C	-4.96281900	-0.98850100	-1.09232800
O	-4.37331800	-1.70390000	-1.88307700
N	-4.68780300	0.38112800	-1.12681000
H	-4.71989500	0.94867400	-0.28194700
N	-3.57113800	0.65921800	-1.93593400

H	-3.41946500	-0.27505800	-2.40100000
H	-3.83474500	1.34357000	-2.65608100
H	-3.08403700	5.35630100	1.94348600
Au	0.63297300	0.64045700	-0.66046700
C	4.64650800	0.42809500	0.85684900
C	4.73852300	1.78943400	0.85424500
C	2.51864300	0.93810800	0.03883900
N	3.39947900	-0.00379700	0.39693700
S	3.24255200	2.46131900	0.27173900
C	3.06384000	-1.40276000	0.31324300
C	3.36724200	-2.09007000	-0.87241900
C	2.44828700	-2.00729500	1.42033700
C	3.01563500	-3.44121400	-0.93318100
C	2.11866700	-3.36056700	1.30621400
C	2.39757900	-4.06974900	0.14276300
H	3.22864400	-4.01076500	-1.84024100
H	1.63431800	-3.86753400	2.14364200
C	4.00844200	-1.40457800	-2.06278100
H	4.35647800	-0.41200400	-1.73566900
C	2.11404500	-1.23780200	2.68312900
H	2.57514900	-0.24073300	2.60508900
C	5.22793100	-2.16447600	-2.58145000
H	5.97063200	-2.33605800	-1.78741000
H	4.95201200	-3.14604300	-2.99605900
H	5.71713000	-1.59648700	-3.38682900
C	2.97571500	-1.17980500	-3.16887400
H	2.59066400	-2.13920700	-3.54877500
H	2.11901900	-0.59511100	-2.79813000
H	3.42418200	-0.63600400	-4.01422200
C	0.60306800	-1.02979600	2.80019600
H	0.20611900	-0.52452500	1.90520000
H	0.07747500	-1.99219800	2.90239500
H	0.36210700	-0.41761500	3.68296400
C	2.68585900	-1.90616600	3.93241200
H	2.22944900	-2.89142800	4.11277100
H	3.77356500	-2.05397200	3.85334800
H	2.49169800	-1.28718800	4.82127300
C	5.87570200	2.66259000	1.25503000
H	6.22826000	3.27419800	0.41038000
H	5.58825800	3.34927400	2.06579200
H	6.72219100	2.06043800	1.60942500
C	5.66630000	-0.57183000	1.26903000
H	5.92803200	-1.23795300	0.43341500

H	6.57980700	-0.07285100	1.61249500
H	5.29000700	-1.20792400	2.08396900
H	2.13226900	-5.12716500	0.07434400

Thiazol_INT4

1 1

Au	0.70997200	-1.20203200	0.14141300
C	-1.06812200	-0.64012500	-0.65035300
H	-1.14515300	-0.64975100	-1.74971800
C	-2.15637800	-0.16324800	-0.02920300
C	-2.35230700	0.10727600	1.41283500
C	-1.36765500	0.82124400	2.11119900
C	-3.51837000	-0.26898800	2.09769000
C	-1.53959000	1.14677900	3.45371100
H	-0.46761700	1.13236900	1.57865500
C	-3.69330700	0.06501000	3.43963500
H	-4.29143100	-0.84956900	1.59116000
C	-2.70575400	0.77452600	4.12236600
H	-0.75856300	1.70146400	3.97949500
H	-4.60354100	-0.24444300	3.95822900
C	-8.68343700	-3.18066900	-0.89517200
C	-8.99186800	-1.82453100	-1.00687900
C	-7.97852000	-0.87446100	-0.95330200
C	-6.64656300	-1.27719600	-0.80152300
C	-6.34214300	-2.63963900	-0.67891000
C	-7.36022300	-3.58715000	-0.72491700
H	-9.48045500	-3.92664800	-0.93406500
H	-10.02911100	-1.50763300	-1.13398200
H	-8.19591200	0.19257100	-1.02886700
H	-5.31641000	-2.97941600	-0.51128900
H	-7.12106600	-4.64729900	-0.61958600
C	-5.62132800	-0.20523500	-0.74620900
O	-5.86736800	0.95676200	-0.48631700
N	-4.33320700	-0.60126300	-1.01832600
H	-4.06198800	-1.54469900	-1.26539000
N	-3.28783400	0.30936800	-0.86536100
H	-2.89938100	0.62084300	-1.76635300
H	-3.65348200	1.24891800	-0.43935500
H	-2.84350000	1.03129000	5.17510200
C	1.84831000	5.67998200	-0.45360900
C	1.49473700	5.00871600	-1.62500600
C	0.33418400	4.24296500	-1.66624200
C	-0.48872300	4.15098900	-0.53850600

C	-0.11985700	4.81162400	0.64073700
C	1.04327600	5.57571100	0.68048300
H	2.75801400	6.28419800	-0.42189000
H	2.12566100	5.08781300	-2.51321400
H	0.04122100	3.70196500	-2.56772600
H	-0.71390200	4.70648700	1.55206700
H	1.32870800	6.08370100	1.60400500
C	-1.71039800	3.30311700	-0.65439700
O	-1.84351400	2.47078700	-1.53681000
N	-2.67078000	3.51970500	0.29224300
H	-2.62351600	4.34121600	0.88366800
N	-3.78962700	2.71398200	0.33716100
H	-3.98184200	2.40835500	1.29220400
H	-4.62524500	3.15729400	-0.04788800
C	4.89119500	-1.71542500	0.96148400
C	4.61498700	-2.52896100	2.02095800
C	2.55605700	-1.69089900	0.84462600
N	3.72262400	-1.27061600	0.33692500
S	2.88881100	-2.69508800	2.17837500
C	3.75454600	-0.39972200	-0.81119800
C	3.76925100	0.98743600	-0.59475700
C	3.75482500	-0.97963800	-2.08906100
C	3.75515800	1.81056700	-1.72336000
C	3.74532800	-0.11051200	-3.18395300
C	3.74036900	1.26823200	-3.00423100
H	3.74943100	2.89451300	-1.59481200
H	3.73905700	-0.52289300	-4.19529600
C	3.74607700	1.58556400	0.79772000
H	4.00186800	0.78792000	1.51339800
C	3.73643700	-2.48052900	-2.30032500
H	3.85844800	-2.96292800	-1.31794300
C	4.77323200	2.70168800	0.97322900
H	5.78729000	2.37145600	0.70111400
H	4.52903000	3.57941300	0.35527300
H	4.79443700	3.03793000	2.02076600
C	2.33586600	2.06949700	1.13530700
H	2.02342400	2.87226400	0.45151800
H	1.61061500	1.24727000	1.03844300
H	2.29040700	2.45875400	2.16439500
C	2.38667200	-2.93093700	-2.86074300
H	1.56240300	-2.62166200	-2.19897300
H	2.20493300	-2.49438200	-3.85548100
H	2.35564800	-4.02648200	-2.96217500

C	4.89385900	-2.94606100	-3.18293600
H	4.81217200	-2.54671900	-4.20551100
H	5.86778800	-2.62896800	-2.77988500
H	4.89959400	-4.04378500	-3.25898500
C	5.54805800	-3.21806300	2.95416800
H	5.37801000	-2.90502300	3.99569200
H	5.42336900	-4.31094600	2.91125400
H	6.59135200	-2.98926200	2.70102000
C	6.21447500	-1.28377900	0.43922500
H	6.31551000	-0.18847400	0.47118000
H	7.02567500	-1.72332100	1.03112200
H	6.34452300	-1.58994200	-0.60949500
H	3.72943500	1.92861400	-3.87445300

Thiazol_INT5

1 1

C	-0.24701100	0.84109600	-1.87984300
H	-0.39053600	1.54423500	-2.71771100
C	1.00118200	0.84806200	-1.37170900
C	1.44906500	-0.04663400	-0.26689200
C	1.20147500	-1.42758400	-0.35876500
C	2.12042800	0.42470500	0.87351800
C	1.59263100	-2.30152400	0.65313700
H	0.67872300	-1.80787900	-1.23950500
C	2.51953300	-0.45032000	1.88543100
H	2.29508300	1.49285000	1.00413400
C	2.25109700	-1.81626000	1.78314200
H	1.37945800	-3.36873700	0.55798200
H	3.01772600	-0.05451800	2.77379400
C	4.82848100	6.24712500	1.52194700
C	5.55221100	5.05849500	1.62050400
C	5.18903800	3.95785000	0.85275000
C	4.08836200	4.03541800	-0.00933800
C	3.37254300	5.23599800	-0.11530500
C	3.74362100	6.33709800	0.64983000
H	5.11777400	7.11347100	2.12111700
H	6.40758400	4.99281100	2.29615900
H	5.74886000	3.02244800	0.90434500
H	2.54548100	5.33636000	-0.82271500
H	3.19159300	7.27450200	0.55617600
C	3.74489800	2.82233200	-0.78965200
O	4.58568200	1.93701600	-0.98687300
N	2.47452000	2.72556100	-1.23200800

H	1.77693200	3.39145500	-0.90530800
N	2.05089300	1.63762400	-1.97757100
H	1.73172500	1.97001200	-2.88701100
H	2.54047500	-2.49558000	2.58856500
C	7.52866900	-4.49200000	1.80066400
C	8.19417000	-4.20907100	0.60747400
C	7.58835900	-3.40662900	-0.35248000
C	6.31415700	-2.87661400	-0.11677200
C	5.64433800	-3.16906000	1.07808200
C	6.25363400	-3.97544600	2.03352600
H	8.00474500	-5.12454700	2.55341700
H	9.18984600	-4.61856400	0.42512700
H	8.08536600	-3.17441900	-1.29622600
H	4.63539100	-2.79353900	1.26101400
H	5.72965200	-4.20945900	2.96265000
C	5.73197400	-2.02773300	-1.17522300
O	6.18561300	-1.92203300	-2.30257900
N	4.59309100	-1.31204800	-0.86277400
H	4.26711300	-1.09621300	0.07590300
N	4.18534300	-0.44067200	-1.86707700
H	3.21434400	-0.61250500	-2.15185200
H	4.27437800	0.61560000	-1.56611800
Au	-1.84331900	-0.24175800	-1.24524000
H	4.84569000	-0.65923800	-2.64697200
C	-5.37266500	-1.75960200	0.68434300
C	-5.27269200	-2.93152600	-0.00568500
C	-3.45729000	-1.28156600	-0.57016400
N	-4.34771700	-0.87184300	0.34219800
S	-3.88575900	-2.85716100	-1.05618900
C	-4.24817600	0.43574000	0.93890200
C	-4.94384900	1.49517600	0.33496200
C	-3.46204800	0.58786600	2.09137400
C	-4.82644000	2.75556600	0.92645200
C	-3.37961600	1.86967100	2.64260100
C	-4.05384800	2.94155200	2.06814900
H	-5.34811600	3.60661700	0.48368600
H	-2.77530500	2.02976200	3.53835100
C	-5.75065000	1.30977000	-0.93489400
H	-5.86776400	0.22817900	-1.10708600
C	-2.69874200	-0.56373700	2.71483500
H	-2.97369400	-1.48413300	2.17666300
C	-7.15269000	1.90594500	-0.82737200
H	-7.70091100	1.50778500	0.04017100

H	-7.12504700	3.00194300	-0.72899800
H	-7.73508800	1.67546900	-1.73197200
C	-4.98868400	1.87828800	-2.13377400
H	-4.84712100	2.96556300	-2.02882600
H	-3.99325200	1.41593800	-2.22590300
H	-5.54237500	1.69663800	-3.06759800
C	-1.19253800	-0.36955600	2.53713500
H	-0.92997600	-0.25732500	1.47394000
H	-0.84236500	0.52967500	3.06810200
H	-0.63900200	-1.23294300	2.93641300
C	-3.06984700	-0.76551700	4.18343500
H	-2.77971800	0.10031100	4.79839500
H	-4.15213600	-0.91675400	4.31430400
H	-2.55317400	-1.64721600	4.59198900
C	-6.14539500	-4.13668300	0.04271600
H	-6.60646600	-4.33710900	-0.93666600
H	-5.57629300	-5.03350400	0.33161200
H	-6.95415100	-4.00277500	0.77273200
C	-6.39122000	-1.35699800	1.68962400
H	-6.94727900	-0.46791100	1.35646600
H	-7.10792900	-2.16880700	1.85967300
H	-5.91991500	-1.10169400	2.65029900
H	-3.97801800	3.93486200	2.51649700

Thiazol_INT6

1 1

Au	-0.49744800	0.46932400	-0.12415100
C	1.06534500	-0.36804500	0.87313200
H	0.88245600	-0.59829900	1.93505300
C	2.35724200	-0.51698900	0.48428400
C	2.79437700	-0.28292400	-0.91359200
C	2.45061100	0.90088200	-1.57881300
C	3.46233400	-1.29236100	-1.62432400
C	2.70487100	1.04614600	-2.94257900
H	1.98667900	1.70718200	-1.00779400
C	3.70654300	-1.15271700	-2.99089600
H	3.74512300	-2.21254800	-1.10788900
C	3.31612200	0.01437900	-3.65707800
H	2.43330300	1.97541600	-3.44868100
H	4.20780900	-1.95418900	-3.53906500
C	8.90746400	2.03455100	0.50445100
C	8.07445000	2.77526200	1.34391700
C	6.77410000	2.34727500	1.58817600

C	6.30187900	1.16537300	1.00750700
C	7.13638700	0.43298700	0.15418200
C	8.43548500	0.86794200	-0.09568100
H	9.92791000	2.37279500	0.31017400
H	8.44200200	3.69347300	1.80736700
H	6.09866800	2.91628900	2.23014800
H	6.76695400	-0.46218200	-0.35275300
H	9.08010000	0.29883600	-0.76912100
C	4.89632200	0.76844600	1.30724300
O	4.03616700	1.55535600	1.64611000
N	4.62002300	-0.57129100	1.16799100
H	5.35213300	-1.24851100	1.00207500
N	3.34471900	-1.05193400	1.32764700
H	3.04732500	-1.04725700	2.30222400
H	3.51339400	0.12652000	-4.72567100
C	-0.65612500	-6.07705000	2.14551900
C	-1.51138400	-6.24493400	1.05551200
C	-1.37825300	-5.42910300	-0.06157100
C	-0.38915300	-4.43837300	-0.08906800
C	0.47623000	-4.27748200	1.00284400
C	0.33717700	-5.09725300	2.11749800
H	-0.76000100	-6.71954100	3.02296200
H	-2.28257400	-7.01762800	1.07805000
H	-2.03310500	-5.53964000	-0.92790100
H	1.26998800	-3.52639200	0.99012500
H	1.01099600	-4.97655900	2.96810300
C	-0.31790500	-3.58331900	-1.28575000
O	-1.00125500	-3.71780800	-2.28957100
N	0.61044600	-2.55351900	-1.25037500
H	0.81561400	-2.03434200	-0.37033900
N	0.44090600	-1.67087100	-2.31735600
H	1.33396800	-1.50379600	-2.81283300
H	-0.27155200	-2.15036600	-2.92172500
C	-4.29947700	2.15704700	-1.14662100
C	-3.87872800	2.45591600	-2.40964000
C	-2.11772900	1.33248200	-1.00558200
N	-3.29476900	1.53377500	-0.40211200
S	-2.22448900	1.94136700	-2.59361500
C	-3.49208300	1.13135400	0.96852300
C	-3.16449500	2.04564800	1.98246600
C	-3.98486900	-0.15908600	1.22029600
C	-3.34492300	1.62236300	3.30234900
C	-4.14759300	-0.52904600	2.55762600

C	-3.83184600	0.35134000	3.58738200
H	-3.09659700	2.30075900	4.12129000
H	-4.52363900	-1.52608600	2.79686900
C	-2.60153200	3.42182900	1.68673400
H	-2.66687000	3.59045900	0.60018800
C	-4.27957800	-1.14485300	0.10726400
H	-4.21226300	-0.60538700	-0.85079400
C	-3.40737000	4.52839400	2.36599300
H	-4.47296600	4.48387800	2.09388600
H	-3.34162200	4.46518200	3.46282800
H	-3.02274100	5.51636200	2.07190700
C	-1.12188100	3.49193300	2.06943700
H	-0.98404700	3.34522100	3.15193200
H	-0.53290600	2.71722500	1.55251100
H	-0.69871700	4.47302000	1.80598700
C	-3.21801800	-2.24573900	0.08261800
H	-2.20760200	-1.80964000	0.02821400
H	-3.26047700	-2.86273500	0.99369800
H	-3.35787800	-2.90880700	-0.78444600
C	-5.68814900	-1.72763800	0.20264500
H	-5.81834300	-2.33005500	1.11452200
H	-6.45608600	-0.93939800	0.21322400
H	-5.88897200	-2.38561500	-0.65615600
C	-4.61292500	3.11708300	-3.52287800
H	-4.11623600	4.04896500	-3.83364900
H	-4.67835400	2.46319400	-4.40594600
H	-5.63618500	3.36904900	-3.21616300
C	-5.62396200	2.41318600	-0.52298000
H	-5.52310000	3.05446900	0.36529700
H	-6.29752900	2.90723500	-1.23256400
H	-6.09348900	1.47462700	-0.19296300
H	-3.96592200	0.04209900	4.62637500
H	0.07324800	-0.75469200	-1.93896600

Thiazol_INT7

1 1

C	2.14634800	-4.00150200	0.42966200
C	2.81998700	-3.40457800	1.49571000
C	3.68219100	-2.33873800	1.26305000
C	3.86111000	-1.84385800	-0.03480400
C	3.19025400	-2.45445100	-1.10099000
C	2.33747200	-3.53075200	-0.86841000
H	1.48255000	-4.85052900	0.60771600

H	2.68688700	-3.78418700	2.51108700
H	4.24885400	-1.88285900	2.07794300
H	3.36662000	-2.13694400	-2.12988200
H	1.83529400	-4.01616200	-1.70795200
C	4.85140000	-0.73625800	-0.19064800
O	5.81399800	-0.61463600	0.52576000
N	4.64706800	0.19316100	-1.20697900
H	5.33063900	0.94679000	-1.23301600
N	3.46273900	0.40976500	-1.84141300
H	3.32309200	-0.06884000	-2.72715000
C	2.47415400	1.20453400	-1.40831200
C	2.69229600	2.03343000	-0.19750900
C	2.62784500	3.42636100	-0.32430200
C	2.92338900	1.45837800	1.05844400
C	2.81632600	4.23554400	0.79357200
H	2.44442500	3.87821500	-1.30189200
C	3.09950900	2.27273300	2.17175600
H	2.92365900	0.37349700	1.17300300
C	3.05339900	3.66055700	2.04063900
H	2.77810800	5.32164600	0.68732300
H	3.27303800	1.81862900	3.14942600
H	3.19989700	4.29697600	2.91606300
C	1.26092700	1.27404700	-2.12603500
Au	0.13306900	-0.00031400	-0.80946400
H	0.70270600	2.21032900	-2.01175600
H	1.25637600	0.86286600	-3.14348100
C	-3.14799800	-1.41942500	1.49297500
C	-2.44274600	-2.50600700	1.92324300
C	-1.13984500	-1.03009900	0.37195300
N	-2.38793000	-0.62457700	0.63311700
S	-0.85107800	-2.47465200	1.22079400
C	-2.91011300	0.58289600	0.04164900
C	-3.58491100	0.48005200	-1.18564800
C	-2.70406100	1.79872500	0.71272700
C	-4.05512600	1.66661100	-1.75434500
C	-3.19621200	2.95395600	0.09847400
C	-3.86228900	2.89007400	-1.12070000
H	-4.58103000	1.63215000	-2.71071200
H	-3.05508900	3.92134100	0.58555500
C	-3.76648100	-0.84433200	-1.90115400
H	-3.49118400	-1.64950000	-1.20142200
C	-1.96507100	1.88992700	2.03334000
H	-1.72820900	0.86603700	2.36297600

C	-5.21641000	-1.08357800	-2.31854200
H	-5.90531100	-1.00634300	-1.46373000
H	-5.54770500	-0.35999800	-3.07871300
H	-5.32727800	-2.08759500	-2.75445300
C	-2.81736100	-0.94005300	-3.09736800
H	-3.04224800	-0.16121300	-3.84272400
H	-1.76870700	-0.81243000	-2.78394200
H	-2.91154600	-1.91893300	-3.59159400
C	-0.63775300	2.63031400	1.86568600
H	0.00172100	2.14356500	1.11307700
H	-0.79791000	3.67218100	1.54760800
H	-0.08267100	2.65222600	2.81536800
C	-2.82698400	2.53168600	3.12056600
H	-3.06440000	3.57991900	2.88311100
H	-3.78045200	1.99885100	3.25468700
H	-2.29652700	2.52436400	4.08456100
C	-2.85992900	-3.60360000	2.83843600
H	-2.82725700	-4.58141700	2.33390800
H	-2.20513900	-3.66103800	3.72126800
H	-3.88632800	-3.44413200	3.19280600
C	-4.54346800	-1.02594200	1.81943300
H	-5.16507400	-0.98511200	0.91257600
H	-4.99447900	-1.74246400	2.51545000
H	-4.57498300	-0.02733400	2.27944900
H	-4.23973800	3.80543600	-1.58198900

Thiazol_TS1

1 1

Au	0.29249700	0.21153500	-1.62962400
C	-6.34974400	1.72319700	1.89216400
C	-6.07665700	0.35600100	1.94983600
C	-5.24893800	-0.22815900	0.99754800
C	-4.68064000	0.55508500	-0.01316100
C	-4.97158700	1.92382700	-0.07892400
C	-5.80245800	2.50488400	0.87445100
H	-7.00345000	2.18118100	2.63798800
H	-6.51672100	-0.25676900	2.73947200
H	-5.02554600	-1.29646000	1.01621800
H	-4.58284200	2.53821800	-0.89490300
H	-6.03657600	3.56989200	0.81567800
C	-3.78141300	-0.12354500	-0.97690400
O	-3.72381800	-1.33720900	-1.11276500
N	-2.96845200	0.68514000	-1.73157400

H	-2.68424800	1.58056500	-1.35147900
N	-1.99004300	0.03118700	-2.48510300
H	-2.23326700	-0.96649600	-2.40010000
H	-2.10765700	0.27752000	-3.47051500
C	-0.31824600	-4.90232000	1.46679300
C	-1.37168500	-4.10672500	1.01325000
C	-1.20735500	-3.29273200	-0.10075900
C	0.03825200	-3.26185200	-0.75668700
C	1.10289900	-4.05355800	-0.28773000
C	0.91478400	-4.87780000	0.81374100
H	-0.46180000	-5.55333400	2.33239600
H	-2.33810000	-4.13459100	1.52107000
H	-2.04016400	-2.68940800	-0.47041300
H	2.06401500	-4.02047900	-0.80352700
H	1.73523300	-5.50584900	1.16734100
C	0.22332300	-2.46247400	-1.91719800
C	0.40448000	-1.75062400	-2.90719400
H	0.55522600	-1.49668200	-3.94712500
C	2.51878000	2.59538600	1.11028500
C	2.39437800	3.67822700	0.29009600
C	1.28400500	1.61187900	-0.60721800
N	1.89360500	1.46379600	0.57554000
S	1.47761000	3.22545900	-1.11888700
C	1.92616300	0.19391900	1.25646800
C	3.03731500	-0.64038200	1.04808200
C	0.86192500	-0.13858500	2.10837600
C	3.06154800	-1.85220700	1.74172800
C	0.93272000	-1.36864500	2.76880600
C	2.02315000	-2.21158300	2.59447200
H	3.90833000	-2.52882900	1.60870900
H	0.12051900	-1.66820000	3.43442000
C	4.15092100	-0.28376900	0.08308100
H	4.02577200	0.77116100	-0.20789900
C	-0.33620700	0.76701300	2.30869900
H	-0.14867200	1.70550300	1.76370200
C	5.53580100	-0.42083700	0.71282800
H	5.62626000	0.16887700	1.63763000
H	5.76946900	-1.46703800	0.96234200
H	6.30936900	-0.07307800	0.01215300
C	4.03274600	-1.12054900	-1.19255400
H	4.16859800	-2.19146800	-0.97303000
H	3.04548200	-0.99363800	-1.66158000
H	4.80293600	-0.82797500	-1.92228400

C	-1.59111200	0.13592300	1.70795500
H	-1.43652000	-0.10665200	0.64486100
H	-1.85536300	-0.80206300	2.22035400
H	-2.45202600	0.81598300	1.79142300
C	-0.54292100	1.12771500	3.77910900
H	-0.77930700	0.23975000	4.38495200
H	0.35273100	1.59687800	4.21332800
H	-1.38102500	1.83260500	3.88681700
C	2.91432800	5.06260400	0.45969400
H	3.63188100	5.32042200	-0.33440900
H	2.10192900	5.80439900	0.42837200
H	3.42883100	5.16842300	1.42332100
C	3.20645600	2.50436400	2.42488100
H	4.03947600	1.78687400	2.38879600
H	3.60514800	3.48175600	2.71983800
H	2.51546900	2.15906500	3.20798300
H	2.06232500	-3.16392200	3.12659500

Thaizol_TS2

1 1

Au	-0.39042900	0.84507200	-1.32361600
C	1.64330100	1.09019000	-1.69525200
H	2.04021400	2.07676000	-1.93671700
C	2.18209800	-0.03984100	-1.49054500
C	2.33739100	-1.41133100	-1.14305700
C	2.51814700	-2.39047700	-2.13828400
C	2.29887100	-1.78267800	0.21233500
C	2.67272500	-3.72155300	-1.77567700
H	2.52805000	-2.09575700	-3.18987800
C	2.45039400	-3.11896700	0.56195100
H	2.14283100	-1.01770800	0.97411100
C	2.64287700	-4.08503700	-0.42613300
H	2.81216700	-4.48368600	-2.54502500
H	2.42222300	-3.40708800	1.61474800
C	3.66763300	-0.20239400	3.14973400
C	2.79406900	0.85107100	2.87203400
C	2.97701000	1.62885200	1.73334200
C	4.02183600	1.34180400	0.84843100
C	4.89697900	0.28832500	1.13209100
C	4.72359600	-0.47846800	2.28245800
H	3.53386500	-0.79995700	4.05461000
H	1.97645800	1.07728700	3.55885100
H	2.32344000	2.47656400	1.51897200

H	5.75179900	0.09210600	0.48041100
H	5.42360400	-1.28553700	2.50890800
C	4.24075900	2.26807700	-0.30168800
O	4.06363000	3.46295400	-0.22023500
N	4.73949500	1.71839100	-1.47086100
H	4.97175000	2.40690200	-2.18133200
N	4.44593900	0.42780500	-1.88689600
H	4.32430500	0.41456600	-2.89752500
H	5.18537100	-0.23649000	-1.64872200
H	2.76764800	-5.13357300	-0.14555700
C	-4.28352600	0.08092800	0.24877600
C	-4.86451500	0.74557100	-0.79276400
C	-2.36215900	0.69443700	-0.92074800
N	-2.89099600	0.07615700	0.14137200
S	-3.62448900	1.33245900	-1.86247900
C	-2.04637300	-0.55296500	1.12571600
C	-1.60603800	0.21891200	2.21270700
C	-1.70053300	-1.90111700	0.94243100
C	-0.76447300	-0.40692400	3.13645900
C	-0.85253600	-2.47460800	1.89388200
C	-0.38749200	-1.73622700	2.97706400
H	-0.40512800	0.15651300	4.00014300
H	-0.55518800	-3.51934500	1.78383700
C	-1.99270000	1.67491000	2.38392000
H	-2.75817000	1.91347800	1.62908000
C	-2.19121300	-2.71000400	-0.24217700
H	-2.97260300	-2.12440200	-0.75180100
C	-2.60743100	1.94748100	3.75601200
H	-3.47041400	1.29407100	3.95462900
H	-1.87959200	1.79182700	4.56702100
H	-2.94995900	2.99092700	3.82050600
C	-0.79661400	2.58971800	2.11699300
H	-0.00359900	2.43139900	2.86441100
H	-0.36561900	2.40284000	1.12086900
H	-1.09706500	3.64694600	2.16819400
C	-1.06231100	-2.93312200	-1.24915600
H	-0.64532600	-1.97579100	-1.59845200
H	-0.23904900	-3.51057200	-0.80127800
H	-1.42903400	-3.48750300	-2.12629000
C	-2.82419100	-4.03230700	0.18807900
H	-2.08490700	-4.71026000	0.64138500
H	-3.62994200	-3.88028200	0.92217100
H	-3.25164000	-4.55133400	-0.68269700

C	-6.30541300	0.99200100	-1.07369900
H	-6.52725000	2.06938500	-1.11230500
H	-6.60639000	0.55493700	-2.03796800
H	-6.93472800	0.54738900	-0.29219200
C	-4.93537600	-0.59200200	1.40265300
H	-4.60469100	-0.15295200	2.35558900
H	-6.02547800	-0.49800800	1.33890300
H	-4.68089200	-1.66198900	1.43184400
H	0.26978400	-2.20536600	3.71311700

Thiazol_TS3

1 1

Au	1.32903300	-0.83475700	-0.04951500
C	-0.55567900	-0.58749500	-0.75746000
H	-0.69610500	-0.34099000	-1.82250000
C	-1.69800600	-0.68088700	-0.05656200
C	-1.81101900	-0.90163600	1.40929800
C	-1.12574700	-0.04371300	2.28550900
C	-2.64083100	-1.89044300	1.96108600
C	-1.26832100	-0.16774100	3.66610900
H	-0.48201600	0.73119000	1.86362700
C	-2.78454300	-2.01239100	3.34287100
H	-3.16200400	-2.59371500	1.30973700
C	-2.10274500	-1.15024800	4.20040200
H	-0.72451600	0.50954300	4.32916200
H	-3.42705600	-2.79601600	3.75097800
C	-6.76590400	-5.53807600	-1.51036600
C	-7.55188600	-4.42403300	-1.21430900
C	-6.94933200	-3.20896800	-0.90873300
C	-5.55439100	-3.09501600	-0.91358300
C	-4.76870400	-4.21978000	-1.20004200
C	-5.37519500	-5.43703400	-1.49599700
H	-7.23966100	-6.49362500	-1.74640700
H	-8.64087200	-4.50558500	-1.21914300
H	-7.54416200	-2.32764200	-0.66244000
H	-3.67684600	-4.17237700	-1.16189800
H	-4.75900100	-6.31309100	-1.70842800
C	-4.97966500	-1.76663800	-0.56856200
O	-5.61218800	-0.93552300	0.07322200
N	-3.71711000	-1.54295800	-1.02321700
H	-3.23666200	-2.23879500	-1.58429300
N	-2.98774200	-0.40440500	-0.68999000
H	-2.84197100	0.18096500	-1.51614100

H	-3.63366600	0.51834200	0.20748200
H	-2.21569100	-1.24844600	5.28241800
C	-4.19861000	7.28336000	-0.52258200
C	-3.89548000	6.49324300	-1.63187100
C	-3.73717300	5.11987800	-1.48505000
C	-3.89544900	4.52626100	-0.22743300
C	-4.18602200	5.32498300	0.88664300
C	-4.33704200	6.70022800	0.73677700
H	-4.32058600	8.36272100	-0.63821100
H	-3.78061200	6.95240800	-2.61598400
H	-3.49150100	4.48260100	-2.33657300
H	-4.25868400	4.89012300	1.88692300
H	-4.55435700	7.32161400	1.60798400
C	-3.71817000	3.05418600	-0.14829300
O	-3.11840000	2.39971000	-0.97741800
N	-4.29466400	2.45011000	0.94916000
H	-4.98120800	2.92899100	1.51875800
N	-4.19948500	1.07634300	1.08633600
H	-3.71855600	0.79803300	1.95029500
H	-5.09007800	0.55267700	0.97984800
C	5.52392900	-0.71319900	0.89027100
C	5.35825900	-1.68383700	1.83384600
C	3.22514400	-1.06915500	0.64841100
N	4.31767800	-0.40151000	0.25569700
S	3.68318600	-2.15728100	1.87682700
C	4.24156800	0.60104100	-0.77594300
C	3.94732300	1.92163400	-0.40298300
C	4.46314500	0.20681600	-2.10470700
C	3.86868600	2.87132900	-1.42519300
C	4.37196200	1.19593300	-3.08752900
C	4.07813900	2.51355100	-2.75258300
H	3.63657700	3.90927800	-1.17656800
H	4.53111800	0.92846800	-4.13425600
C	3.68553300	2.31923300	1.03631800
H	3.90876400	1.44991500	1.67423900
C	4.74083300	-1.23469400	-2.48248400
H	4.95623300	-1.79193900	-1.55711000
C	4.59201600	3.46232200	1.49021900
H	5.65620700	3.21656800	1.35447000
H	4.39136700	4.38816200	0.92952100
H	4.42853300	3.68173000	2.55620200
C	2.20774800	2.65980000	1.23705700
H	1.91939800	3.54110200	0.64278500

H	1.56766800	1.81950700	0.92430500
H	2.00180300	2.88278100	2.29558200
C	3.49784100	-1.86706500	-3.11178400
H	2.63190100	-1.79689200	-2.43468200
H	3.23254400	-1.35939000	-4.05257400
H	3.67520200	-2.92969600	-3.33783700
C	5.96147700	-1.37346900	-3.39006500
H	5.79737400	-0.90231900	-4.37126100
H	6.85621500	-0.91180900	-2.94507400
H	6.18250900	-2.43586700	-3.57215500
C	6.36534000	-2.31271400	2.73203300
H	6.10233500	-2.17114200	3.79148900
H	6.44298300	-3.39583600	2.55103300
H	7.35859800	-1.87391700	2.57125000
C	6.76913800	-0.00401000	0.49446200
H	6.66555500	1.08267600	0.63212100
H	7.61858200	-0.35090100	1.09424400
H	7.00169600	-0.17430000	-0.56741900
H	4.01204600	3.27132200	-3.53658700

Thiazol_TS4

1 1

Au	-1.13761700	-1.14246800	-0.74520600
C	0.57213500	-0.53122600	-1.75310400
H	0.56364100	-0.65603000	-2.84913200
C	1.83297700	-0.50016900	-1.21259800
C	2.09021100	-0.38985400	0.24508900
C	1.60380300	-1.36183800	1.12538800
C	2.83858100	0.68060100	0.75473000
C	1.84161000	-1.25011400	2.49402000
H	1.07162300	-2.22474700	0.72058600
C	3.05561000	0.80248900	2.12354900
H	3.25100500	1.43142600	0.07610100
C	2.55675500	-0.16507500	2.99673700
H	1.46935900	-2.02206000	3.17109800
H	3.62130800	1.65457100	2.50747200
C	7.81067900	-3.45830300	0.90124900
C	7.05634200	-4.37893400	0.17254600
C	5.89304200	-3.97138400	-0.47101500
C	5.48662600	-2.63439700	-0.40543100
C	6.23751200	-1.71662400	0.33942400
C	7.39649000	-2.13006900	0.99134600
H	8.72211600	-3.78039500	1.41016500

H	7.37667700	-5.42124900	0.11049100
H	5.27809800	-4.67660900	-1.03372700
H	5.89935800	-0.68321900	0.45317200
H	7.97406200	-1.41500800	1.58124500
C	4.22468600	-2.26206000	-1.10160100
O	3.31569300	-3.03666900	-1.31275900
N	4.14180700	-0.94606200	-1.50288700
H	4.90970000	-0.30021100	-1.37891500
N	2.96969700	-0.45345200	-2.00711700
H	2.79685000	-0.72794000	-2.97270200
H	2.73705800	-0.07755100	4.07052400
C	5.11590500	5.15247100	0.09070300
C	4.31614000	5.03744000	1.22874900
C	3.03227200	4.51373600	1.12576300
C	2.54686800	4.09164700	-0.11755300
C	3.34622200	4.22180600	-1.26111900
C	4.62896000	4.75113700	-1.15361100
H	6.12273300	5.56849000	0.17172600
H	4.69588400	5.36327100	2.19946200
H	2.38445000	4.41642600	1.99910300
H	2.96087800	3.94601700	-2.24586100
H	5.24755400	4.86441500	-2.04635800
C	1.18842400	3.50437600	-0.15044000
O	0.36443300	3.62682800	0.73429000
N	0.87924900	2.75390700	-1.27625500
H	1.63125800	2.25473300	-1.74645300
N	-0.28535600	2.00095000	-1.18062600
H	-0.00608400	0.80637500	-1.38532200
H	-0.65527900	2.12116400	-0.22018900
H	-1.01492000	2.33436600	-1.81966700
C	-4.96376200	-1.19453700	1.14462700
C	-4.89912000	-2.54385300	1.33629300
C	-2.87181800	-1.60764200	0.18474800
N	-3.81876900	-0.71305900	0.50324500
S	-3.39491000	-3.14283800	0.69564800
C	-3.65040200	0.68197100	0.18431200
C	-4.07096600	1.13431900	-1.07700800
C	-3.06515100	1.52287700	1.14723800
C	-3.87563800	2.48955200	-1.36923700
C	-2.89221800	2.86825900	0.80471200
C	-3.29407000	3.34728700	-0.43986900
H	-4.19766400	2.87949900	-2.33776500
H	-2.42299400	3.54931000	1.51667400

C	-4.69108300	0.21258900	-2.10788000
H	-4.83272500	-0.77308500	-1.63884000
C	-2.58979100	1.00907400	2.49146700
H	-2.96881000	-0.01757800	2.61422900
C	-6.06521300	0.70674400	-2.55894000
H	-6.74926700	0.84454700	-1.70797700
H	-5.99892300	1.66810100	-3.09118200
H	-6.52370600	-0.01833800	-3.24766700
C	-3.74714000	0.01641700	-3.29525200
H	-3.57583400	0.96515300	-3.82880200
H	-2.77213800	-0.37597900	-2.96469300
H	-4.17424200	-0.69751500	-4.01533300
C	-1.06210100	0.93858000	2.52522800
H	-0.67273400	0.28501000	1.72875200
H	-0.61144800	1.93560200	2.40165000
H	-0.71440600	0.52767900	3.48473600
C	-3.13657100	1.84144600	3.64992500
H	-2.73774200	2.86713900	3.63772000
H	-4.23483000	1.90964800	3.62418200
H	-2.84724000	1.39030700	4.61064600
C	-5.88714000	-3.45831500	1.97165800
H	-6.22423000	-4.23483500	1.26816000
H	-5.45643700	-3.96741700	2.84739400
H	-6.77195800	-2.90268000	2.30788800
C	-6.05020700	-0.25220600	1.52114300
H	-6.44332500	0.27327400	0.63810200
H	-6.87779800	-0.78885200	1.99911600
H	-5.68632200	0.51480600	2.22113100
H	-3.15645300	4.40379800	-0.68268900

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Au	1.26373300	0.08023200	-1.33462200
C	-3.85631800	4.91556600	1.87474900
C	-4.64809000	3.85252500	1.43914600
C	-4.19924200	3.02492500	0.41533600
C	-2.94592500	3.24637400	-0.16747200
C	-2.15970200	4.32278200	0.26379100
C	-2.61635200	5.15439800	1.28196100
H	-4.21218300	5.56926900	2.67428700
H	-5.62321400	3.67222200	1.89661300
H	-4.80854100	2.19144700	0.06027500
H	-1.20342600	4.54169500	-0.21813600

H	-2.00799600	6.00100800	1.60697900
C	-2.50272300	2.30093100	-1.22306600
O	-3.27404900	1.58921900	-1.85683200
N	-1.15523100	2.20800900	-1.41334600
H	-0.52474200	2.53851500	-0.69251400
N	-0.64785500	1.21205300	-2.23983300
H	-1.38031500	0.49451700	-2.35038200
H	-0.45331700	1.59650200	-3.16583800
C	-8.11697900	-1.47265000	0.14364300
C	-7.52197700	-2.70903700	0.39397700
C	-6.20662600	-2.93852200	0.00515800
C	-5.47383100	-1.93452400	-0.63654300
C	-6.07593900	-0.69311700	-0.88668500
C	-7.39336300	-0.46700700	-0.49721700
H	-9.15123500	-1.29194500	0.44565700
H	-8.08810700	-3.49824900	0.89348200
H	-5.71430000	-3.89550200	0.18845300
H	-5.53885400	0.11406800	-1.39143600
H	-7.86057200	0.49907800	-0.70110000
C	-4.06524800	-2.26419700	-0.99742600
O	-3.54325200	-3.33458600	-0.76575800
N	-3.35575100	-1.25057000	-1.60052500
H	-3.70695600	-0.30453700	-1.73051400
N	-2.01867600	-1.39416200	-1.83129800
H	-1.79546100	-1.89622000	-2.68937800
C	-1.11579700	-1.61887000	-0.81063500
C	-1.52421600	-1.36229200	0.58838700
C	-1.09666700	-2.24486000	1.58896400
C	-2.33478000	-0.27738800	0.95054700
C	-1.46951800	-2.04456600	2.91421700
H	-0.49601600	-3.11474200	1.31991800
C	-2.69688500	-0.07084300	2.27682000
H	-2.69761800	0.40950700	0.19207600
C	-2.26741100	-0.95658300	3.26433300
H	-1.14532100	-2.75460100	3.67824200
H	-3.32261900	0.78659100	2.53439900
H	-2.56521400	-0.80582100	4.30445900
C	0.16558300	-2.02368000	-1.12397600
H	0.81793000	-2.35386100	-0.31411100
H	0.36499400	-2.44538000	-2.11548600
C	5.14152700	0.80937700	0.28327600
C	5.46444200	1.60801600	-0.77477100
C	3.15537700	0.62532500	-0.93311900

N	3.85629400	0.27368100	0.15347100
S	4.11829200	1.66437200	-1.87828600
C	3.31066800	-0.64478600	1.11947300
C	3.64862000	-2.00312100	0.99782000
C	2.46423900	-0.14596300	2.12142900
C	3.08433400	-2.88398100	1.92478200
C	1.93149900	-1.07012000	3.02429100
C	2.23624900	-2.42275100	2.92687800
H	3.31707400	-3.94885400	1.86436000
H	1.25997200	-0.72388800	3.81240200
C	4.55186400	-2.51356000	-0.10946500
H	5.10778900	-1.65346900	-0.51563800
C	2.11074000	1.32377400	2.23523600
H	2.67834400	1.86981000	1.46568700
C	5.58391500	-3.51991200	0.39437100
H	6.16048000	-3.12450400	1.24452000
H	5.11549700	-4.46179800	0.71793600
H	6.29153600	-3.77165600	-0.40933100
C	3.72471200	-3.09195200	-1.25948200
H	3.11781900	-3.94522700	-0.91736000
H	3.04469900	-2.33578000	-1.67882000
H	4.38190600	-3.44756500	-2.06740500
C	0.62482800	1.54452800	1.95310100
H	0.34778800	1.12999200	0.96969300
H	-0.01038200	1.03948000	2.69610300
H	0.37448400	2.61726200	1.97247700
C	2.51248100	1.89851800	3.59320700
H	1.95365600	1.42440800	4.41444700
H	3.58465600	1.75363200	3.79389400
H	2.30369900	2.97834800	3.63149300
C	6.72275900	2.35408400	-1.05018800
H	7.21184100	1.98799900	-1.96607500
H	6.53244500	3.42999700	-1.18195200
H	7.43324100	2.23722100	-0.22179300
C	5.96007000	0.47763200	1.47920400
H	6.18292000	-0.59882400	1.52598700
H	6.90962600	1.02481200	1.46045900
H	5.42615100	0.73865700	2.40500800
H	1.80927700	-3.12888500	3.64277000

Thiazol_TS5_2

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Au	-0.70759100	-1.20690000	-0.13887200
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C	7.12851100	2.73057400	-0.77150000
C	7.70106700	1.70601400	-0.01693600
C	6.88871500	0.79914400	0.65468000
C	5.49585300	0.90091700	0.56655500
C	4.92557900	1.94006400	-0.18101000
C	5.74138300	2.85011600	-0.84772200
H	7.76704600	3.44496700	-1.29624500
H	8.78753000	1.61739600	0.05027800
H	7.31157600	-0.00376000	1.26179900
H	3.84233500	2.07686900	-0.22642700
H	5.29097100	3.66284600	-1.42173100
C	4.69846000	-0.11420000	1.31257300
O	5.14514600	-0.78826100	2.21534200
N	3.39586100	-0.25106200	0.88432700
H	3.05644600	0.22606500	0.05539800
N	2.51488600	-1.05409900	1.54191600
H	2.07025500	-0.65071600	2.36095700
C	1.90991100	-2.12842200	0.96393100
C	2.66213400	-2.90229000	-0.04167500
C	4.04452000	-3.08933900	0.11485000
C	2.00358000	-3.52954400	-1.11124100
C	4.74824100	-3.87416100	-0.79320400
H	4.55662200	-2.64960500	0.97427600
C	2.71422200	-4.30916400	-2.01827300
H	0.92404100	-3.40036200	-1.23379000
C	4.09022800	-4.47803500	-1.86418700
H	5.82160400	-4.02196900	-0.65619600
H	2.19168000	-4.78722500	-2.84964200
H	4.64916400	-5.08820200	-2.57715900
C	0.63288200	-2.49569900	1.36087600
H	0.30470100	-3.51671500	1.15858800
H	0.20807800	-2.02640000	2.25462200
C	1.22332400	4.04799400	0.80081900
C	1.19120800	2.68758100	0.52534200
C	0.87856800	2.23880200	-0.77266800
C	0.58394600	3.17663200	-1.78014800
C	0.62512200	4.53543300	-1.49405800
C	0.94671100	4.97244100	-0.20814100
H	1.47479100	4.39240900	1.80610500
H	1.41820700	1.95973600	1.30590300
H	0.34430300	2.82400700	-2.78461000
H	0.41019200	5.26151700	-2.28095500
H	0.98495500	6.04229000	0.00953600

C	0.94492400	0.85744600	-1.08994900
C	1.03259900	-0.34791200	-1.35208000
H	1.51965900	-1.19619800	-1.82520500
C	-4.93266900	-0.58476900	0.35117200
C	-5.14688100	-1.92995900	0.27281700
C	-2.73274400	-1.28716800	0.00743700
N	-3.57878200	-0.26638600	0.19258600
S	-3.62568600	-2.73605700	0.01897900
C	-3.12877600	1.10189300	0.19648000
C	-3.22382900	1.82827800	-1.00286600
C	-2.65109800	1.65435400	1.39453100
C	-2.83347700	3.16861700	-0.96909100
C	-2.27451300	3.00068700	1.37106800
C	-2.37368000	3.75207500	0.20689800
H	-2.89178600	3.76765200	-1.87988900
H	-1.90117500	3.46924700	2.28433900
C	-3.67600100	1.18472100	-2.29922500
H	-4.17130500	0.23252100	-2.05183800
C	-2.52074000	0.85024500	2.67256900
H	-2.88336700	-0.16961800	2.47291200
C	-4.68746300	2.03647300	-3.06235400
H	-5.55302200	2.30361100	-2.43726900
H	-4.24097500	2.97272200	-3.43056600
H	-5.05960600	1.48866900	-3.94071300
C	-2.46189500	0.84720400	-3.16782000
H	-1.93165500	1.76487300	-3.46783900
H	-1.74975300	0.20534200	-2.62737100
H	-2.77260500	0.32360300	-4.08462500
C	-1.05243800	0.73437600	3.08473000
H	-0.45204200	0.31692000	2.26041500
H	-0.63017600	1.71719900	3.34656900
H	-0.94468400	0.07879300	3.96259800
C	-3.37332300	1.42909800	3.80100100
H	-3.04609400	2.44343100	4.07632500
H	-4.43445700	1.48863200	3.51655300
H	-3.30029500	0.80084700	4.70144900
C	-6.41988200	-2.69514000	0.37172200
H	-6.64159400	-3.22526200	-0.56733000
H	-6.37588100	-3.44577600	1.17528500
H	-7.26174500	-2.02385600	0.58434900
C	-5.92662900	0.49882800	0.57025900
H	-5.98042000	1.17278400	-0.29771000
H	-6.92392900	0.07724700	0.74080100

H	-5.65508300	1.11360500	1.44095200
H	-2.08065700	4.80357400	0.21277700