# *Supporting Information*

# Rh-Catalyzed Regio- and Stereoselective Route to Enamides: Benzamides as an Assembling Reagent

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(**Acknowledgment**. We acknowledge the Korea Basic Science Institute (KBSI) for the mass analysis.)

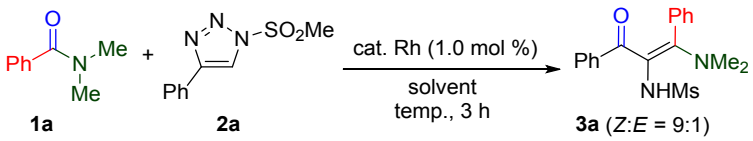
# I. General Methods.

Unless otherwise stated, all commercial reagents and solvents were used without additional purification. Analytical thin layer chromatography (TLC) was performed on Merck precoated silica gel 60 $F_{254}$ plates. Visualization on TLC was achieved by use of UV light (254 nm). Flash column chromatography was undertaken on silica gel (Merck Kiesel gel 60 $F_{254}$ 400-630 mesh). $^{1}H$ NMR was recorded on Brucker DPX FT (300 and 400 MHz). Chemical shifts were quoted in parts per million (ppm) referenced to the appropriate solvent peak or 0.0 ppm for tetramethylsilane. The following abbreviations were used to describe peak splitting patterns when appropriate: br = broad, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet. Coupling constants, ***J***, were reported in hertz unit (Hz). $^{13}C$ NMR was recorded on Brucker FT AM 400 (100 MHz) and was fully decoupled by broad band proton decoupling. Chemical shifts were reported in ppm referenced to the center line of a triplet at 77.0 ppm of chloroform-*d*. Infrared spectra were recorded on a JASCO FT/IR-460 plus FT-IR spectrometer. Frequencies are given in reciprocal centimeters ($cm^{-1}$) and only selected absorbance is reported. High resolution mass spectra were recorded on a Jeol JMS-HX110/110A by using EI method.

# II. Experimental Procedure

**1. Experimental Procedure for the Optimization Studies (Table S1).** To a test tube with a triangular-shaped stir bar were added *N*,*N*-dimethylbenzamide (**1a**, 0.6 mmol, 89.4 mg), 1-methanesulfonyl-4-phenyl-1,2,3-triazole (**2a**, 0.2 mmol, 44.6 mg), and rhodium catalyst (1.0 mol %) and solvent (2.0 mL) under atmospheric conditions. After 4h at indicated temperature, the reaction mixture filtered through a pad of celite and concentrated in *vacuo*. The NMR yield of desired product **3a**, (Z)-*N*-(1-(dimethylamino)-3-oxo-1,3-diphenylprop-1-en-2-yl)methanesulfonamide, was determined by integration using an internal standard ($CH_2Br_2$).

***Table S1.*** Optimization of the reaction conditions.[a]




**1a** **2a** **3a** (*Z*:*E* = 9:1)

| entry | cat. [Rh] | solvent | temp [°C] | yield [%][b] |
|---|---|---|---|---|
| 1 | $Rh_2(esp)_2$ | 1,2-DCE | 25 | n.d. |
| 2 | $Rh_2(esp)_2$ | 1,2-DCE | 40 | 50 |
| 3 | $Rh_2(esp)_2$ | 1,2-DCE | 60 | 48 |
| 4 | $Rh_2(esp)_2$ | 1,2-DCE | 80 | 63 |
| 5 | $Rh_2(esp)_2$ | 1,2-DCE | 100 | 67 |
| 6 | $Rh_2(OAc)_4$ | 1,2-DCE | 80 | n.d. |
| 7 | $Rh_2(Oct)_4$ | 1,2-DCE | 80 | n.d. |
| 8 | $Rh_2(esp)_2$ | chloroform | 80 | n.d. |
| 9 | $Rh_2(esp)_2$ | toluene | 80 | 83[c] |
| 10 | $Rh_2(esp)_2$ | 1,2-DCE | 80 | n.d.[d] |

[a] Reaction conditions: **1a** (3.0 equiv), **2a** (0.2 mmol), [Rh] catalyst (1.0 mol %) and solvent (2.0 mL). [b] $^{1}H$ NMR yields using $CH_2Br_2$ as an internal standard. [c] 5.0 equiv of **1a** was used. [d] When N,N-dimethylacetamide was used instead of **1a**, corresponding product was not determined.

**2. General Procedure for $Rh_2(esp)_2$ catalyzed reaction of 4-phenyl-1-toluenesulfonyl-1,2,3-triazole (2b) with *N*,*N*-disubstituted benzamides (Table 1).** To a test tube with a triangular-shaped stir bar were added 4-phenyl-1-toluenesulfonyl-1,2,3-triazole (**2b**, 0.5 mmol, 149.5 mg), *N*,*N*-disubstituted benzamide (**1**, 1.5 mmol) and $Rh_2(esp)_2$ (1.0 mol%, 3.8 mg) and toluene (5.0 mL). The reaction mixture was stirred at 80 °C for 4 h, filtered through a pad of celite and then washed with $CH_2Cl_2$ (10 mL x 3). Organic solvents were removed under reduced pressure and the residue was purified by chromatography on silica gel to give the desired product **3**.

**3. General Procedure for $Rh_2(esp)_2$ catalyzed reaction of 1-sulfonyl-1,2,3-triazoles with *N*,*N*-dimethylbenzamide (1a) (Table 2).** To a test tube with a triangular-shaped stir bar were added *N*,*N*-dimethylbenzamide (**1a**, 1.0 mmol, 149.1 mg), 1-sulfonyl-1,2,3-triazole (**1**, 0.2 mmol), and $Rh_2(esp)_2$ (1.0 mol%, 1.5 mg) and toluene (2.0 mL). The reaction mixture was stirred at 80 °C for 4 h, filtered through a pad of celite and then washed with $CH_2Cl_2$ (10 mL x 3). Organic solvents were removed under reduced pressure and the residue was purified by chromatography on silica gel to give the desired product **3**.

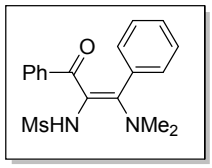
**4. Representative Experimental Procedure of the Scale-up Reactions**. To a round bottom flask with a octagon-shaped stir bar were added *N*,*N*-dimethylbenzamide (**1a**, 9.0 mmol, 1.3427 g), 4-phenyl-1-toluenesulfonyl-1,2,3-triazole (**2b**, 3.0 mmol, 898.0 mg), and $Rh_2(esp)_2$ (0.5 mol%, 11.8 mg) and toluene (30 mL). The reaction mixture was stirred at 80 °C for 4 h, filtered through a pad of celite and then washed with $CH_2Cl_2$ (10 mL x 3). Organic solvents were removed under reduced pressure and the residue was purified by chromatography on silica gel to give the desired product **3b** in 83% (1.04 g).

**5. General procedure for the reaction of endiamines with $NaBH_4$ (Scheme 3).** To 10 mL round bottom flask with a stir bar were added endiamines **3** (0.3 mmol), $NaBH_4$ (1.2 mmol) and acetic acid (2.0 mL) under $N_2$ atmosphere. The reaction mixture was stirred at room temperature for 4 h, and then neutralized with an aqueous solution of 10% NaOH. The reaction mixture was extracted with $CH_2Cl_2$, the organic phases were combined, dried over $MgSO_4$, and concentrated. The residue was purified by chromatography on silica gel to give the corresponding product **4**.

**6. Representative Experimental Procedure of the One-pot Reactions**. To a test tube with a triangular-shaped stir bar were added *N*,*N*-dimethylbenzamide (**1a**, 1.5 mmol, 223.8 mg), 4-phenyl-1-toluenesulfonyl-1,2,3-triazole (**2b**, 0.5 mmol), and $Rh_2(esp)_2$ (1.0 mol%, 1.5 mg) and toluene (2.0 mL). The reaction mixture was stirred at 80 °C for 4 h, and then toluene was removed under reduced pressure. To the above mixture, $NaBH_4$ (2.0 mmol, 75.7 mg) and acetic acid (2.0 mL) under $N_2$ atmosphere were added. The reaction mixture was stirred at room temperature for 4 h, and then neutralized with an aqueous solution of 10% NaOH. The reaction mixture was extracted with $CH_2Cl_2$, the organic phases were combined, dried over $MgSO_4$, and concentrated. The residue was purified by chromatography on silica gel to give the corresponding product **4a** in 82%.

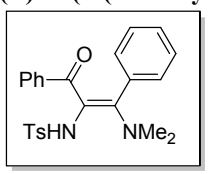
**7. Spectroscopic Data of Products 3 and 4 Obtained in this Study**

**(Z)-N-(1-(dimethylamino)-3-oxo-1,3-diphenylprop-1-en-2-yl)methanesulfonamide (3a):**



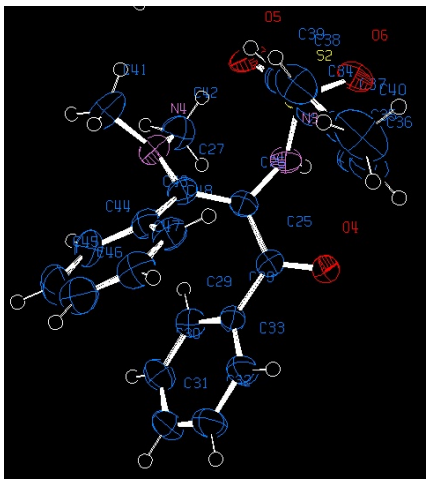

yellow solid (83%); $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.10-7.08 (m, 3H), 7.03-7.00 (m, 5H), 6.94-6.91 (m, 2H), 6.30 (s, 1H), 3.23 (s, 3H), 3.03 (s, 6H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 193.4, 166.7, 141.9, 136.6, 131.8, 130.7, 129.1, 128.1, 128.0, 127.2, 108.9, 44.0, 40.2, 29.6; IR (solid) ν 2927, 1444, 1512 1390, 1301, 1143 cm$^{-1}$; HRMS (EI) m/z calcd. for $C_{18}H_{20}N_2O_3S$ [*M*]: 344.1195, found: 344.1198.

**(Z)-N-(1-(dimethylamino)-3-oxo-1,3-diphenylprop-1-en-2-yl)-4-methylbenzenesulfonamide (3b):**

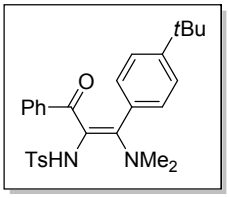



yellow solid (87%); $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 8.2 Hz 2H), 7.35 (d, *J* = 8.0 Hz 2H), 7.05-7.01 (m, 1H), 6.93-6.87 (m, 3H), 6.85-6.75 (m, 7H), 3.10 (s, 6H), 2.48 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 191.3, 164.7, 143.5, 141.5, 136.8, 136.2, 132.2, 130.7, 129.1, 128.6, 128.4, 127.8, 126.9, 109.2, 44.0, 29.7, 21.7; IR (solid) ν 3155, 1584, 1566, 1504, 1391, 1155 cm$^{-1}$; HRMS (EI) m/z calcd. for $C_{24}H_{24}N_2O_3S$ [*M*]: 420.1508, found: 420.1510.

***Figure S1.*** ORTEP plot of **3b**

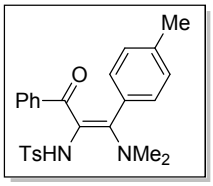



**(Z)-N-(1-(4-(tert-butyl)phenyl)-1-(dimethylamino)-3-oxo-3-phenylprop-1-en-2-yl)-4-methylbenzenesulfonamide (3c):**



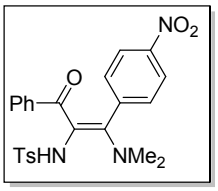

yellow solid (90%); $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 8.2 Hz 2H), 7.35 (d, *J* = 8.0 Hz 2H), 6.88-6.86 (m, 3H), 6.84-6.80 (m, 1H), 6.77-6.74 (m, 4H), 6.71-6.68 (m, 2H), 3.11 (s, 6H), 2.49 (s, 3H), 1.11 (s, 9H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 191.2, 164.7, 154.0, 143.4, 141.6, 136.7, 133.1, 132.2, 129.0, 128.5, 128.2, 127.6, 126.8, 124.7, 109.1, 44.0, 34.6, 30.7, 21.7; IR (solid) ν 2960, 2922, 2854, 1595, 1529, 1392 cm$^{-1}$; HRMS (EI) m/z calcd. for $C_{28}H_{32}N_2O_3S$ [*M*]: 476.2134, found: 476.2133.

**(Z)-N-(1-(dimethylamino)-3-oxo-3-phenyl-1-(p-tolyl)prop-1-en-2-yl)-4-methylbenzenesulfonamide (3d):**



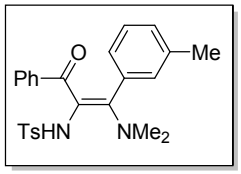

yellow solid (73%); $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.93 (d, *J* = 8.2 Hz 2H), 7.33 (d, *J* = 8.0 Hz 2H), 6.91-6.87 (m, 2H), 6.81-6.77 (m, 2H), 6.75-6.72 (m, 2H), 6.69 (m, 4H), 3.10 (s, 6H), 2.47 (s, 3H), 2.10 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 191.2, 164.7, 143.5, 141.6, 141.2, 136.7, 133.3, 132.3, 129.0, 128.5, 128.4, 128.2, 127.7, 126.8, 108.9, 43.9, 21.7, 21.1; IR (solid) ν 1509, 1472, 1390, 1300, 1152, 1088 cm$^{-1}$; HRMS (EI) m/z calcd. for $C_{25}H_{26}N_2O_3S$ [*M*]: 434.1664, found: 434.1667.

**(Z)-N-(1-(dimethylamino)-1-(4-nitrophenyl)-3-oxo-3-phenylprop-1-en-2-yl)-4-methylbenzenesulfonamide ( 3e):**



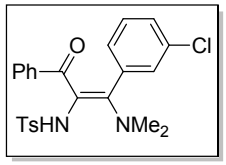

yellow solid (86%); $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, J = 8.2 Hz 2H), 7.76 (d, J = 8.7 Hz 2H), 7.37 (d, J = 7.9 Hz 2H), 7.04 (d, J = 8.6 Hz 2H), 6.96-6.92 (m, 1H), 6.89 (s, 1H), 6.83 (t, J = 7.6 Hz 2H), 6.77-6.75 (m, 2H), 3.07 (s, 6H), 2.50 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 191.4, 161.3, 148.4, 144.0, 142.8, 141.1, 136.6, 132.8, 129.4, 129.2, 128.3, 127.9, 127.4, 127.3, 122.8, 110.8, 43.9, 21.7; IR (solid) ν 1596, 1518, 1391, 1345, 1300, 1152 cm$^{-1}$; HRMS (EI) m/z calcd. for $C_{24}H_{23}N_3O_5S$ [*M*]: 465.1358, found: 465.1360.

**(Z)-N-(1-(dimethylamino)-3-oxo-3-phenyl-1-(m-tolyl)prop-1-en-2-yl)-4-methylbenzenesulfonamide (3f):**



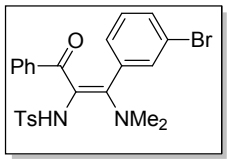

yellow solid (73%); $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, *J* = 82. Hz 2H), 7.34 (d, *J* = 8.0 Hz 2H), 6.94 (s, 1H), 6.89-6.85 (m, 1H), 6.81-6.78 (m, 4H), 6.75-6.71 (m, 3H), 6.37 (s, 1H), 3.11 (s, 6H), 2.48 (s, 3H), 1.98 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 191.1, 164.6, 143.5, 141.5, 137.2, 136.6, 135.9, 133.6, 131.3, 129.0, 128.9, 128.7, 128.3, 127.7, 127.6, 127.4, 126.7, 109.2, 43.9, 21.7, 20.6; IR (solid) ν 2922, 1596, 1520, 1388, 1298, 1287, 1154 cm$^{-1}$; HRMS (EI) m/z calcd. for $C_{25}H_{26}N_2O_3S$ [*M*]: 434.1664, found: 434.1662.

**(Z)-N-(1-(3-chlorophenyl)-1-(dimethylamino)-3-oxo-3-phenylprop-1-en-2-yl)-4-methylbenzenesulfonamide (3g):**



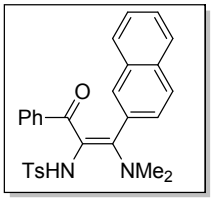

yellow solid (84%); $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 8.2 Hz 2H), 7.36 (d, *J* = 8.0 Hz 2H), 6.97-6.90 (m, 3H), 6.87-6.81 (m, 4H), 6.75-6.73 (m, 2H), 6.50 (s, 1H), 3.08 (s, 6H), 2.48 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 191.2, 162.4, 144.0, 141.2, 137.9, 136.3, 133.7, 132.5, 130.4, 129.8, 129.2, 129.0, 128.8, 128.5, 127.5, 127.1, 110.0, 43.9, 21.7; IR (solid) ν 1596, 1524, 1413, 1388, 1286, 1167, 1155 cm$^{-1}$; HRMS (EI) m/z calcd. for $C_{24}H_{23}ClN_2O_3S$ [*M*]: 454.1118, found: 454.1117.

**(Z)-N-(1-(3-bromophenyl)-1-(dimethylamino)-3-oxo-3-phenylprop-1-en-2-yl)-4-methylbenzenesulfonamide (3h):**



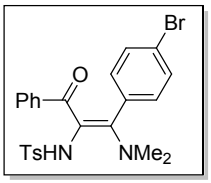

yellow solid (54%); $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.84 (d, *J* = 8.2 Hz 2H), 7.29 (d, *J* = 8.0 Hz 2H), 7.03 (d, *J* = 8.6 Hz 1H), 6.87-6.77 (m, 5H), 6.74-6.70 (m, 1H), 6.67-6.65 (m, 2H), 6.57 (s, 1H), 3.01 (s, 6H), 2.41 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 191.2, 162.2, 144.0, 141.2, 138.1, 136.2, 135.4, 133.4, 130.1, 129.2, 129.2, 128.8, 128.5, 127.4, 127.1, 121.9, 110.0, 43.9, 21.8; IR (solid) ν 1595, 1522, 1409, 1388, 1316, 1287, 1154 cm$^{-1}$; HRMS (EI) m/z calcd. for $C_{24}H_{23}BrN_2O_3S$ [*M*]: 498.0613, found: 498.0611.

**(Z)-N-(1-(dimethylamino)-1-(naphthalen-2-yl)-3-oxo-3-phenylprop-1-en-2-yl)-4-methylbenzenesulfonamide (3i):**



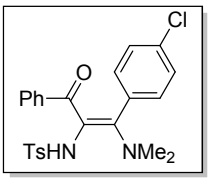

yellow solid (81%); $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, J = 8.1 Hz 2H), 7.56 (d, J = 7.6 Hz 1H), 7.43-7.40 (m, 3H), 7.37-7.35 (m, 2H), 7.31-7.29 (m, 1H), 7.09-7.06 (m, 2H), 6.89 (s, 1H), 6.66-6.64 (m, 2H), 6.59-6.53 (m,3H), 3.15 (s, 6H), 2.56 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 191.3, 164.0, 143.7, 141.5, 136.9, 134.4, 133.9, 133.7, 132.0, 129.2, 128.9, 128.0, 128.0, 127.6, 127.5, 127.4, 127.2, 127.1, 126.7, 126.3, 110.1, 43.9, 21.8; IR (solid) ν 1515, 1435, 1394, 1300, 1152, 1001 cm$^{-1}$; HRMS (EI) m/z calcd. for $C_{28}H_{26}N_2O_3S$ [*M*]: 470.1664, found: 470.1662.

**(Z)-N-(1-(4-bromophenyl)-1-(dimethylamino)-3-oxo-3-phenylprop-1-en-2-yl)-4-methylbenzenesulfonamide (3j):**



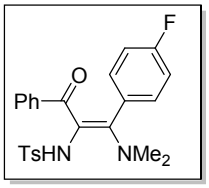

yellow solid (82%); $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.91 (d, *J* = 8.2 Hz 2H), 7.33 (d, *J* = 7.9 Hz 2H), 7.02 (d, *J* = 8.5 Hz 2H),6.99-6.96 (m, 1H), 6.88 (s, 1H), 6.85 (t, *J* = 7.6 Hz 2H), 6.74-6.72 (m, 2H), 6.67 (d, *J* = 8.3 Hz 2H), 3.06 (s, 6H), 2.47 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 191.3, 163.2, 143.7, 141.4, 136.7, 135.2, 133.4, 131.0, 129.1, 128.7, 128.4, 127.7, 127.1, 125.3, 109.6, 43.9, 21.7; IR (solid) ν 1586, 1516, 1443, 1391, 1300, 1152, 1089 cm$^{-1}$; HRMS (EI) m/z calcd. for $C_{24}H_{23}BrN_2O_3S$ [*M*]: 498.0613, found: 498.0609.

**(Z)-N-(1-(4-chlorophenyl)-1-(dimethylamino)-3-oxo-3-phenylprop-1-en-2-yl)-4-methylbenzenesulfonamide (3k):**



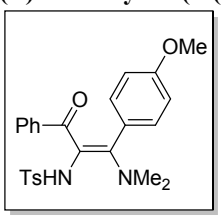

yellow solid (78%); $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.91 (d, *J* = 8.2 Hz 2H), 7.33 (d, *J* = 8.0 Hz 2H), 6.98-6.95 (m, 1H), 6.88-6.83 (m, 5H), 6.75-6.73 (m, 4H), 3.06 (s, 6H), 2.47 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 191.3, 163.1, 143.7, 141.4, 136.8, 136.7, 134.8, 133.3, 129.1, 128.8, 128.4, 128.0, 127.7, 127.1, 109.6, 43.9, 21.7; IR (solid) ν 1591, 1517, 1472, 1392, 1301, 1152, 1014 cm$^{-1}$; HRMS (EI) m/z calcd. for $C_{24}H_{23}ClN_2O_3S$ [*M*]: 454.1118, found: 454.1119.

**(Z)-N-(1-(dimethylamino)-1-(4-fluorophenyl)-3-oxo-3-phenylprop-1-en-2-yl)-4-methylbenzenesulfonamide (3l):**



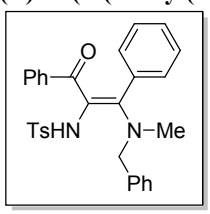

yellow solid (73%); $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 8.1 Hz 2H), 7.34 (d, *J* = 8.0 Hz 2H), 6.97-69.3 (m, 1H), 6.86-6.80 (m, 5H), 6.77-6.75 (m, 2H), 6.59 (t, *J* = 8.5 Hz 2H), 3.08 (s, 6H), 2.48 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 191.3, 165.1, 163.2, 162.6, 143.6, 141.4, 136.7, 134.2, 134.1, 132.4, 132.4, 129.1, 128.8, 128.4, 127.7, 127.1, 115.1, 114.8, 109.4, 43.9, 21.7; IR (solid) ν 2922, 2853, 1589, 1512, 1389, 1290, 1150 cm$^{-1}$; HRMS (EI) m/z calcd. for $C_{24}H_{23}FN_2O_3S$ [*M*]: 438.1413, found: 438.1415.

**(Z)-4-methyl-N-(1-(methyl(phenyl)amino)-3-oxo-1,3-diphenylprop-1-en-2-yl)benzenesulfonamide (3m):**



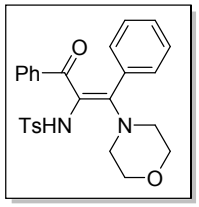

yellow solid (66%); $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.92 (d , J = 8.2 Hz 2H), 7.33 (d, J = 8.0 Hz 2H), 6.91-6.87 (m, 2H), 6.82 (t, J = 7.4 Hz 2H), 6.77-6.73 (m, 4H), 6.41 (s, 1H), 6.38 (s, 1H), 3.63 (s, 3H), 3.09 (s, 6H), 2.47 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 191.0, 164.4, 161.6, 143.5, 141.6, 136.8, 133.9, 129.0, 128.5, 128.4, 128.4, 127.7, 126.9, 113.3, 108.6, 55.2, 43.9, 21.7; IR (solid) ν 2923, 1602, 1509, 1390, 1300, 1248, 1151 cm$^{-1}$; HRMS (EI) m/z calcd. for $C_{25}H_{26}N_2O_4S$ [*M*]: 450.1613 , found: 450.1615.

**(Z)-N-(1-(benzyl(methyl)amino)-3-oxo-1,3-diphenylprop-1-en-2-yl)-4-methylbenzenesulfonamide (3n):**



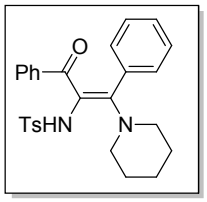

yellow solid (88%); $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, J = 8.2 Hz 2H), 7.37-7.21 (m, 7H), 6.93-6.89 (m, 1H), 6.87 (s, 1H), 6.81-6.74 (m, 5H), 6.67 (t, J = 7.5 Hz 2H), 6.50 (d, J = 7.2 Hz 2H), 4.60 (s, 2H), 2.77 (s, 3H), 2.38 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 191.0, 162.3, 142.6, 140.3, 136.0, 135.7, 135.6, 131.0, 129.7, 128.1, 127.7, 127.6, 127.4, 126.8, 126.6, 125.9, 109.7, 57.7, 40.8, 20.6; IR (solid) ν 1595, 1507, 1443, 1390, 1314, 1287, 1150 cm$^{-1}$; HRMS (EI) m/z calcd. for $C_{30}H_{28}N_2O_3S$ [*M*]: 496.1821, found: 496.1819.

**(Z)-4-methyl-N-(1-morpholino-3-oxo-1,3-diphenylprop-1-en-2-yl)benzenesulfonamide (3o):**



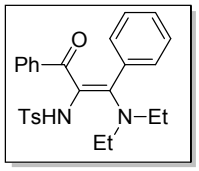
yellow solid (85%); $^1$H NMR (400 MHz, $CDCl_3$) δ 7.93 (d, *J* = 8.2 Hz 2H), 7.35 (d, *J* = 8.1 Hz 2H), 7.07-7.02 (m, 1H), 6.94-6.93 (m, 4H), 6.91-6.89 (m, 1H), 6.87 (s, 1H), 6.84-6.76 (m, 4H), 3.82 (t, *J* = 9.3 Hz 4H), 3.40 (t, *J* = 8.5 Hz 4H), 2.47 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 192.3, 163.8, 143.6, 141.2, 136.8, 135.9, 132.1, 131.0, 129.1, 128.9, 128.4, 128.1, 127.9, 127.0, 110.0, 67.1, 51.7, 21.7; IR (solid) ν 1594, 1508, 1487, 1315, 1285, 1270, 1251 cm$^{-1}$; HRMS (EI) m/z calcd. for $C_{26}H_{26}N_2O_4S$ [*M*]: 462.1613, found: 462.1617.

**(Z)-4-methyl-N-(3-oxo-1,3-diphenyl-1-(piperidin-1-yl)prop-1-en-2-yl)benzenesulfonamide (3p):**



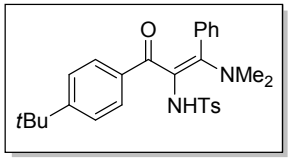
yellow solid (91%); $^1$H NMR (400 MHz, $CDCl_3$) δ 7.94(d, *J* = 8.2 Hz 2H), 7.34 (d, *J* = 8.1 Hz 2H), 7.04-7.00 (m, 1H), 6.92-6.87 (m, 6H), 6.82-6.75(m, 4H), 3.37 (s, 4H), 2.46 (s, 3H), 1.72 (s, 6H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 191.6, 164.9, 143.4, 141.5, 136.8, 131.9, 130.8, 129.0, 128.6, 128.4, 127.8, 127.8, 126.9, 109.5, 52.8, 26.7, 23.7, 21.7; IR (solid) ν 1595, 1500, 1442, 1299, 1269, 1251, 1149 cm$^{-1}$; HRMS (EI) m/z calcd. for $C_{27}H_{28}N_2O_3S$ [*M*]: 460.1821, found: 460.1821.

**(Z)-N-(1-(diethylamino)-3-oxo-1,3-diphenylprop-1-en-2-yl)-4-methylbenzenesulfonamide (3q):**



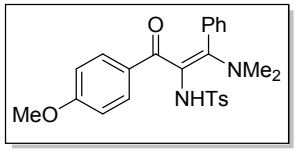
yellow solid (88%); $^1$H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, *J* = 8.1 Hz 2H), 7.35 (d, *J* = 8.1 Hz 2H), 7.02-6.99 (m, 1H), 6.94 (s, 1H), 6.90-6.86 (m, 3H), 6.81-6.77 (m, 4H), 6.67-6.65 (m, 2H), 3.49 (q, *J* = 6.8 Hz 4H), 2.47 (s, 3H), 1.23 (t, *J* = 7.1 Hz 6H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 191.3, 162.2, 143.6, 142.0, 137.3, 136.7, 132.0, 130.3, 129.0, 128.5, 128.1, 127.6, 127.3, 126.9, 109.8, 47.0, 21.7, 13.4; IR (solid) ν 2924, 1505, 1458, 1443, 1313, 1278, 1150 cm$^{-1}$; HRMS (EI) m/z calcd. for $C_{26}H_{28}N_2O_3S$ [*M*]: 448.1821, found: 448.1823.

**(Z)-N-(3-(4-(tert-butyl)phenyl)-1-(dimethylamino)-3-oxo-1-phenylprop-1-en-2-yl)-4-methylbenzenesulfonamide (3r):**



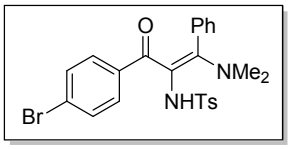

yellow solid (86%); $^1$H NMR (400 MHz, $CDCl_3$) δ 7.93 (d, *J* = 8.2 Hz 2H), 7.34 ( d, *J* = 8.0 Hz 2H), 6.99-6.95 (m, 1H), 6.89-6.85 (m, 3H), 6.81-6.78 (m, 4H), 6.69-6.67 (m, 2H), 3.08 (s, 6H), 2.47 (s, 3H), 1.09 (s, 9H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 191.3, 164.4, 151.2, 143.5, 138.5, 136.7, 136.3, 132.2, 130.4, 129.0, 128.5, 127.7, 127.6, 123.8, 109.5, 43.9, 34.3, 30.8, 21.7; IR (solid) ν 2954, 1589, 1519, 1471, 1390, 1301, 1246 cm$^{-1}$; HRMS (EI) m/z calcd. for $C_{28}H_{32}N_2O_3S$ [*M*]: 476.2134, found: 476.2132.

**(Z)-N-(1-(dimethylamino)-3-(4-methoxyphenyl)-3-oxo-1-phenylprop-1-en-2-yl)-4-methylbenzenesulfonamide (3s):**



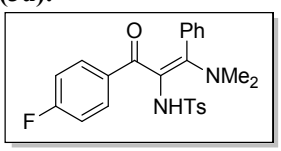

yellow solid (88%); $^1$H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 8.2 Hz 2H), 7.33 (d, *J* = 8.0 Hz 2H), 7.07-7.03 (m, 1H), 6.95-6.92 (m, 2H), 6.88-6.86 (m, 2H), 6.82-6.80 (m, 3H), 6.33 (d, *J* = 8.7 Hz 2H), 3.60 (s, 3H), 3.08 (s, 6H), 2.47 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 190.7, 164.1, 160.0, 143.5, 136.9, 136.4, 134.1, 132.1, 130.6, 129.9, 129.0, 128.4, 127.7, 112.3, 109.2, 55.1, 43.8, 21.6; IR (solid) ν 2923, 1603, 1504, 1394, 1297, 1243, 1149 cm$^{-1}$; HRMS (EI) m/z calcd. for $C_{25}H_{26}N_2O_4S$ [*M*]: 450.1613, found: 450.1609.

**(Z)-N-(3-(4-bromophenyl)-1-(dimethylamino)-3-oxo-1-phenylprop-1-en-2-yl)-4-methylbenzenesulfonamide (3t):**




yellow solid (81%); $^1$H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 8.1 Hz 2H), 7.34 (d, *J* = 7.9 Hz 2H), 7.11 (t, *J* = 7.3 Hz 1H), 6.97-6.91 (m, 4H), 6.85-6.82 (m, 3H), 6.61 (d, *J* = 8.3 Hz 2H), 3.09 (s, 6H), 2.47 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 190.0, 164.9, 143.6, 140.4, 136.8, 136.1, 132.2, 130.9, 130.0, 129.3, 129.1, 128.4, 127.9, 122.8, 109.1, 44.0, 21.7; IR (solid) ν 2925, 1586, 1512, 1395, 1329, 1310, 1152 cm$^{-1}$; HRMS (EI) m/z calcd. for $C_{24}H_{23}BrN_2O_3S$ [*M*]: 498.0613, found: 498.0610.

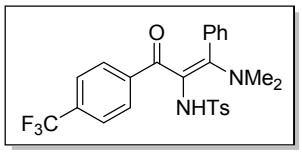
**(Z)-N-(1-(dimethylamino)-3-(4-fluorophenyl)-3-oxo-1-phenylprop-1-en-2-yl)-4-methylbenzenesulfonamide (3u):**




yellow solid (82%); $^1$H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 8.2 Hz 2H), 7.34 (d, *J* = 8.0 Hz 2H), 7.09-

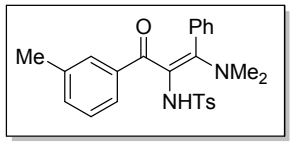
7.06 (m, 1H), 6.94 (t, $J$ = 7.7 Hz 2H), 6.86-6.84 (m, 3H), 6.80-6.76 (m, 2H), 6.48 (t, $J$ = 8.7 Hz 2H), 3.08 (s, 6H), 2.46 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 190.0, 164.7, 163.7, 161.2, 143.6, 137.7, 137.7, 136.8, 136.2, 132.1, 130.9, 130.0, 129.9, 129.1, 128.4, 127.9, 114.0, 113.8, 109.1, 44.0, 21.7; IR (solid) ν 2919, 1597, 1575, 1512, 1386, 1327, 1312 cm$^{-1}$; HRMS (EI) m/z calcd. for $C_{24}H_{23}FN_2O_3S$ [$M$]: 438.1413, found: 438.1413.

**(Z)-N-(1-(dimethylamino)-3-oxo-1-phenyl-3-(4-(trifluoromethyl)phenyl)prop-1-en-2-yl)-4-methylbenzenesulfonamide (3v):**



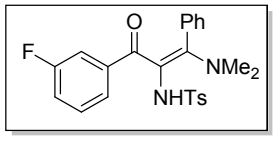

yellow solid (79%); $^1$H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, $J$ = 8.2 Hz 2H), 7.36 (d, $J$ = 8.0 Hz 2H), 7.07-7.03 (m, 3H), 6.91 (t, $J$ = 7.7 Hz 2H), 6.87 (s, 1H), 6.84-6.82 (m, 2H), 6.79 (d, $J$ = 7.9 Hz 2H), 3.11 (s, 6H), 2.48 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 189.7, 165.4, 145.0, 143.7, 136.7, 136.0, 132.1, 131.1, 129.1, 128.3, 128.0, 127.8, 123.9, 123.8, 109.3, 44.1, 21.7; IR (solid) ν 1591, 1523, 1394, 1315, 1151, 1106, 1059 cm$^{-1}$; HRMS (EI) m/z calcd. for $C_{25}H_{23}F_3N_2O_3S$ [$M$]: 488.1381, found: 488.1379.

**(Z)-N-(1-(dimethylamino)-3-oxo-1-phenyl-3-(m-tolyl)prop-1-en-2-yl)-4-methylbenzenesulfonamide (3w):**




yellow solid (81%); $^1$H NMR (400 MHz, $CDCl_3$) δ 7.93 (d, $J$ = 8.0 Hz 2H), 7.34 (d, $J$ = 7.9 Hz 2H), 7.04-7.00 (m, 1H), 6.93-6.83 (m, 5H), 6.72-6.66 (m, 2H), 6.59-6.58 (m, 1H), 6.49 (s, 1H), 3.09 (s, 6H), 2.47 (s, 3H), 2.01 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 191.4, 164.5, 143.5, 141.3, 136.8, 136.3, 136.1, 132.1, 130.5, 129.2, 129.0, 128.5, 128.4, 127.6, 127.0, 124.8, 109.3, 44.0, 21.7, 20.8; IR (solid) ν 2920, 1516, 1392, 1308, 1281, 1214, 1151 cm$^{-1}$; HRMS (EI) m/z calcd. for $C_{25}H_{26}N_2O_3S$ [$M$]: 434.1664, found: 434.1661.

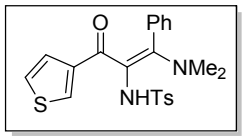
**(Z)-N-(1-(dimethylamino)-3-(3-fluorophenyl)-3-oxo-1-phenylprop-1-en-2-yl)-4-methylbenzenesulfonamide (3x):**




yellow solid (86%); $^1$H NMR (400 MHz, $CDCl_3$) δ 7.93 (d, $J$ = 8.2 Hz 2H), 7.35 (d, $J$ = 8.0 Hz 2H), 7.10-7.06 (m, 1H), 6.96 (t, $J$ = 7.6 Hz 2H), 6.88-6.86 (m, 2H), 6.81-6.75 (m, 2H), 6.60-6.54 (m, 2H), 6.41 (d, $J$ = 9.3 Hz 1H), 3.11 (s, 6H), 2.48 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 189.6, 189.6, 165.0, 162.4, 159.9, 143.7, 143.6, 136.7, 136.1, 132.2, 131.0, 129.1, 128.7, 128.6, 128.4, 127.9, 123.4, 123.4, 115.4, 115.2, 114.8, 114.6, 109.0, 44.1, 21.7; IR (solid) ν 2924, 1569, 1506, 1430, 1393, 1319, 1219 cm$^{-1}$; HRMS (EI)

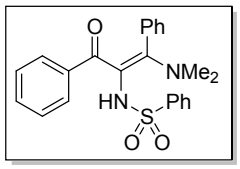
m/z calcd. for $C_{24}H_{23}FN_2O_3S$ [*M*]: 438.1413, found: 438.1412.

**(Z)-N-(1-(dimethylamino)-3-oxo-1-phenyl-3-(thiophen-3-yl)prop-1-en-2-yl)-4-methylbenzenesulfonamide ( 3y):**



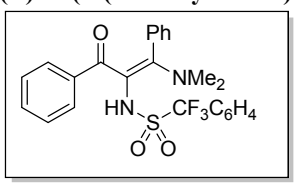

yellow solid (79%); $^1$H NMR (400 MHz, $CDCl_3$) δ 7.91 (d, *J* = 8.1 Hz 2H), 7.33 (d, *J* = 8.0 Hz 2H), 7.14-7.11 (m, 1H), 7.01 (t, *J* = 7.6 Hz 2H), 6.95-6.93 (m, 2H), 6.86-6.85 (m, 1H), 6.81 (s, 1H), 6.70-6.68 (m, 1H), 6.54 (d, *J* = 5.0 Hz 1H), 3.09 (s, 6H), 2.46 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 185.5, 164.4, 143.5, 143.0, 136.9, 136.3, 132.0, 130.8, 129.1, 128.4, 127.9, 127.3, 124.2, 110.2, 43.9, 21.7; IR (solid) ν 2922, 1508, 1385, 1286, 1206, 1147, 1088 cm$^{-1}$; HRMS (EI) m/z calcd. for $C_{22}H_{22}N_2O_3S_2$ [*M*]: 426.1072, found: 426.1072.

**(Z)-N-(1-(dimethylamino)-3-oxo-1,3-diphenylprop-1-en-2-yl)benzenesulfonamide (3z):**



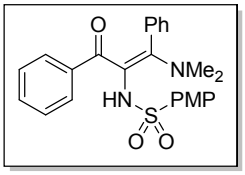

yellow solid (80%); $^1$H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, *J* = 7.3 Hz 2H), 7.66-7.63 (m, 1H), 7.58-7.54 (m, 2H), 7.04-7.00 (m, 1H), 6.93-6.86 (m, 4H), 6.82-6.73 (m, 6H), 3.10 (s, 6H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 191.2, 164.7, 141.4, 139.6, 136.1, 132.9, 132.2, 130.8, 128.6, 128.5, 128.4, 127.8, 127.7, 127.0, 109.0, 44.0; IR (solid) ν 2924, 1507, 1394, 1321, 1153, 1115, 1088 cm$^{-1}$; HRMS (EI) m/z calcd. for $C_{23}H_{22}N_2O_3S$ [*M*]: 406.1351, found: 406.1355.

**(Z)-N-(1-(dimethylamino)-3-oxo-1,3-diphenylprop-1-en-2-yl)-4-(trifluoromethyl)benzenesulfonamide (3aa):**



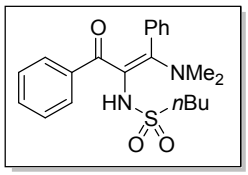

yellow solid (64%); $^1$H NMR (400 MHz, $CDCl_3$) δ 8.21 (d, *J* = 8.2 Hz 2H), 7.82 (d, *J* = 8.2 Hz 2H), 7.07-7.03 (s, 1H), 6.96-6.89 (m, 4H), 6.83-6.79 (m, 4H), 6.76-6.73 (m, 2H), 3.10 (s, 6H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 191.5, 165.3, 143.6, 141.2, 136.0, 132.0, 131.0, 129.0, 128.8, 127.9, 127.7, 127.1, 125.5, 125.4, 108.2, 44.0; IR (solid) ν 2923, 1516, 1395, 1319, 1156, 1125, 1105 cm$^{-1}$; HRMS (EI) m/z calcd. for $C_{24}H_{21}F_3N_2O_3S$ [*M*]: 474.1225, found: 474.1226.

**(Z)-N-(1-(dimethylamino)-3-oxo-1,3-diphenylprop-1-en-2-yl)-4-methoxybenzenesulfonamide (3ab):**



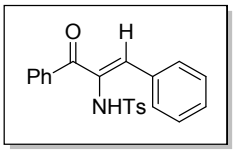

yellow solid (92%); $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, *J* = 8.7 Hz 2H), 7.03-7.01 (m, 3H), 6.93-6.77 (m, 10H), 3.90 (s, 3H), 3.10 (s, 6H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 191.4, 164.7, 163.1, 141.5, 136.2, 132.2, 131.4, 130.7, 130.6, 128.6, 127.8, 127.0, 113.6, 109.3, 55.6, 44.0; IR (solid) ν 2925, 1593, 1512, 1389, 1316, 1290, 1255 cm$^{-1}$; HRMS (EI) m/z calcd. for $C_{24}H_{24}N_2O_4S$ [*M*]: 436.1457, found: 436.1458.

**(Z)-N-(1-(dimethylamino)-3-oxo-1,3-diphenylprop-1-en-2-yl)butane-1-sulfonamide (3ac):**



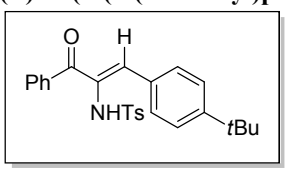

yellow solid (84%); $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.11-7.07 (m, 3H), 7.03-6.98 (m, 5H), 6.94-6.90 (m, 2H), 6.19 (s, 1H), 3.36-3.32 (m, 2H), 3.01 (s, 6H), 2.06-1.98 (m, 2H), 1.59-1.53 (m, 2H), 1.01 (t, J = 7.3 Hz 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 193.4, 166.7, 142.1, 136.8, 131.8, 130.6, 129.0, 128.0, 127.9, 127.2, 109.0, 52.6, 44.0, 25.6, 21.8, 13.7; IR (solid) ν 2921, 2854, 1588, 1567, 1505, 1386, 1318 cm$^{-1}$; HRMS (EI) m/z calcd. for $C_{21}H_{26}N_2O_3S$ [*M*]: 386.1664, found: 386.1662.

**(Z)-4-methyl-N-(3-oxo-1,3-diphenylprop-1-en-2-yl)benzenesulfonamide (4a):**




yellow solid (88%); $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.80-7.78 (m, 2H), 7.71 (d, *J* = 8.2 Hz 2H), 7.57-7.52 (m, 3H), 7.44-7.40 (m, 2H), 7.37-7.35 (m, 3H), 7.18 (d, *J* = 8.0 Hz 2H), 7.03 (s, 1H), 6.91 (s, 1H), 2.30 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 193.6, 144.1, 139.2, 136.3, 136.2, 132.7, 132.3, 131.3, 130.9, 130.6, 129.5, 129.1, 128.6, 128.3, 127.5, 21.5; IR (solid) ν 3233, 1644, 1623, 1595, 1404, 1263, 1171 cm$^{-1}$; HRMS (EI) m/z calcd. for $C_{22}H_{19}NO_3S$ [*M*]: 377.1072, found: 377.1088.

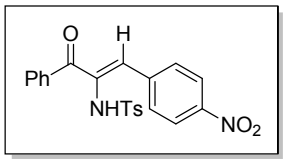
**(Z)-N-(1-(4-(tert-butyl)phenyl)-3-oxo-3-phenylprop-1-en-2-yl)-4-methylbenzenesulfonamide (4b):**




yellow solid (74%); $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, *J* = 8.4 Hz 2H), 7.73 (d, *J* = 8.2 Hz 2H), 7.55-7.51 (m, 3H), 7.43-7.39 (m, 4H), 7.19 (d, *J* = 8.0 Hz 2H), 7.04 (s, 1H), 6.88 (s, 1H), 2.31 (s, 3H), 1.32 (s, 9H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 193.7, 154.4, 144.0, 140.0, 136.5, 136.2, 132.2, 131.0, 130.5, 129.8,

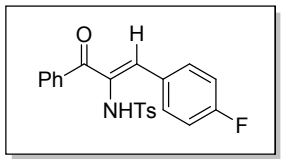
129.5, 129.1, 128.3, 127.6, 125.6, 34.9, 31.1, 21.5; IR (solid) ν 2916, 1598, 1398, 1317, 1262, 1163, 1090 $cm^{-1}$; HRMS (EI) m/z calcd. for $C_{26}H_{27}NO_3S$ [*M*]: 433.1712, found: 433.1714.

**(Z)-4-methyl-N-(1-(4-nitrophenyl)-3-oxo-3-phenylprop-1-en-2-yl)benzenesulfonamide (4c):**



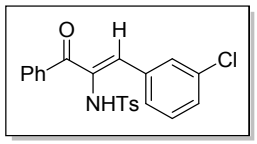

yellow solid (85%); $^1$H NMR (400 MHz, DMSO-$d_6$) δ 10.25 (s, 1H), 8.10 (d, *J* = 8.8 Hz 2H), 7.80 (d, *J* = 7.3 Hz 2H), 7.68-7.64 (m, 3H) 7.58-7.52 (m, 4H), 7.29 (d, *J* = 8.0 Hz 2H), 6.93 (s, 1H) 2.33 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 193.2, 147.9, 144.6, 139.4, 135.9, 135.6, 135.5, 133.7, 132.8, 131.3, 129.7, 129.1, 128.5, 127.4, 123.5, 21.5; IR (solid) ν 1650, 1595, 1515, 1404, 1342, 1302, 1167 $cm^{-1}$; HRMS (EI) m/z calcd. for $C_{22}H_{18}N_2O_5S$ [*M*]: 422.0936, found: 422.0938.

**(Z)-N-(1-(4-fluorophenyl)-3-oxo-3-phenylprop-1-en-2-yl)-4-methylbenzenesulfonamide (4d):**




yellow solid (86%); $^1$H NMR (400 MHz, $CDCl_3$) δ 7.90-7.87 (m, 2H), 7.70 (d, *J* = 8.2 Hz 2H), 7.56-7.52 (m, 1H), 7.51-7.48 (m, 2H), 7.44-7.40 (m, 2H), 7.81 (d, *J* = 8.0 Hz 2H), 7.07-7.03 (m, 3H), 6.97 (s, 1H), 2.30 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 193.7, 165.1, 162.6, 144.2, 139.4, 136.2, 135.9, 133.4, 133.3, 132.3, 130.7, 130.7, 129.5, 129.0, 128.4, 127.5, 115.8, 115.6, 21.5; IR (solid) ν 1623, 1597, 1445, 1337, 1305, 1263, 1230 $cm^{-1}$; HRMS (EI) m/z calcd. for $C_{22}H_{18}FNO_3S$ [*M*]: 395.0991, found: 395.0994.

**(Z)-N-(1-(3-chlorophenyl)-3-oxo-3-phenylprop-1-en-2-yl)-4-methylbenzenesulfonamide (4e):**

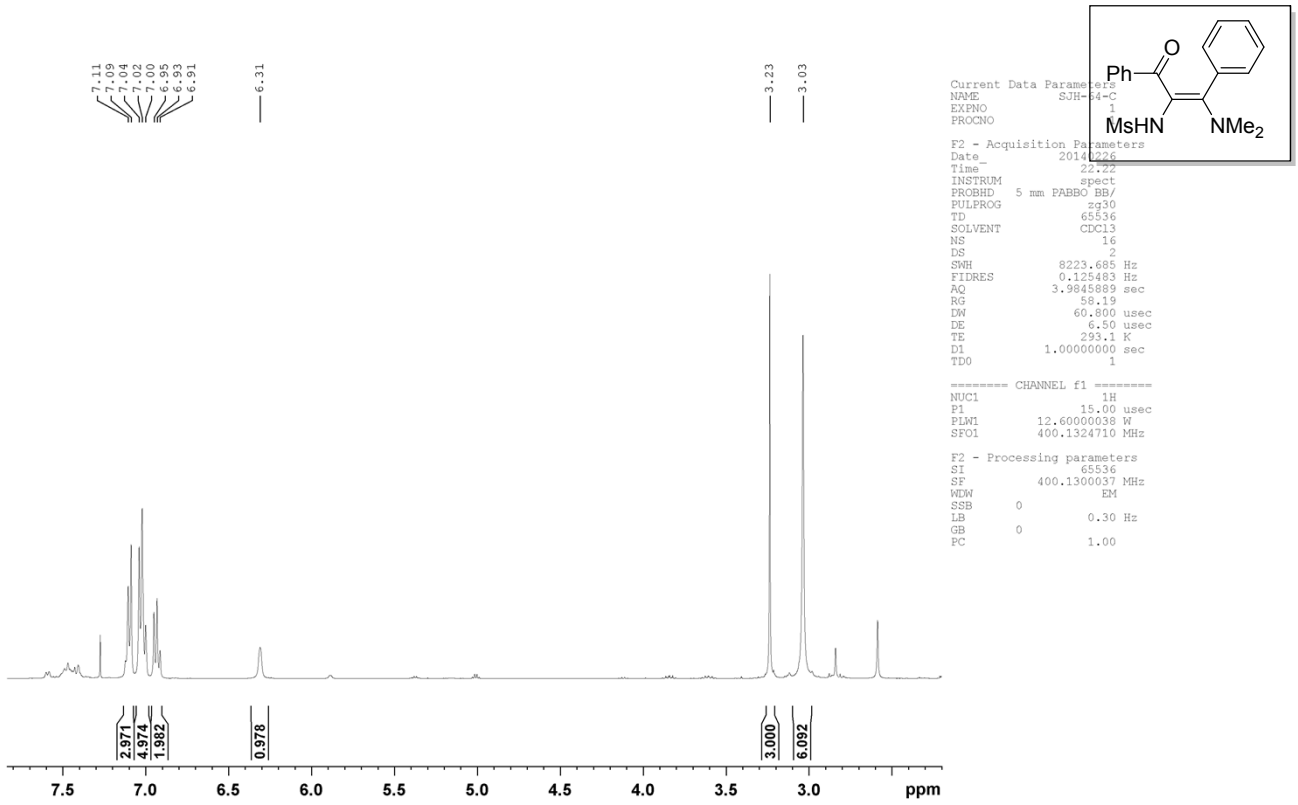


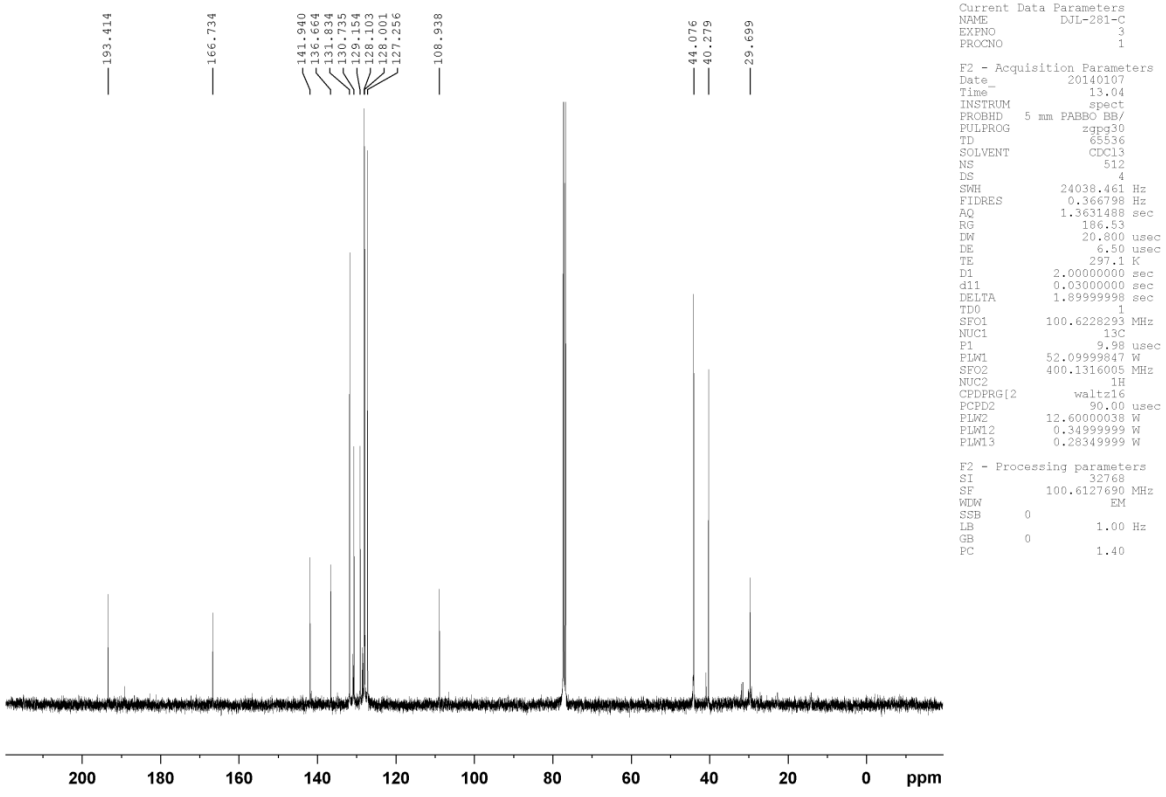

yellow solid (81%); $^1$H NMR (400 MHz, $CDCl_3$) δ 7.76-7.73 (m, 1H), 7.69 (d, *J* = 8.3 Hz 2H), 7.59 (s, 1H), 7.57-7.54 (m, 3H), 7.45-7.42 (m, 2H), 7.31-7.30 (m, 2H), 7.20 (d, *J* = 8.0 Hz 2H), 6.94 (s, 1H), 6.92 (s, 1H), 2.33 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 193.5, 144.3, 137.1, 136.0, 136.0, 134.5, 134.4, 132.5, 132.3, 130.5, 130.2, 129.8, 129.6, 129.1, 128.6, 128.4, 127.5, 21.5; IR (solid) ν 2924, 1667, 1613, 1594, 1427, 1340, 1204 $cm^{-1}$; HRMS (EI) m/z calcd. for $C_{22}H_{18}ClNO_3S$ [*M*]: 411.0696, found: 411.0698.

# Appendix

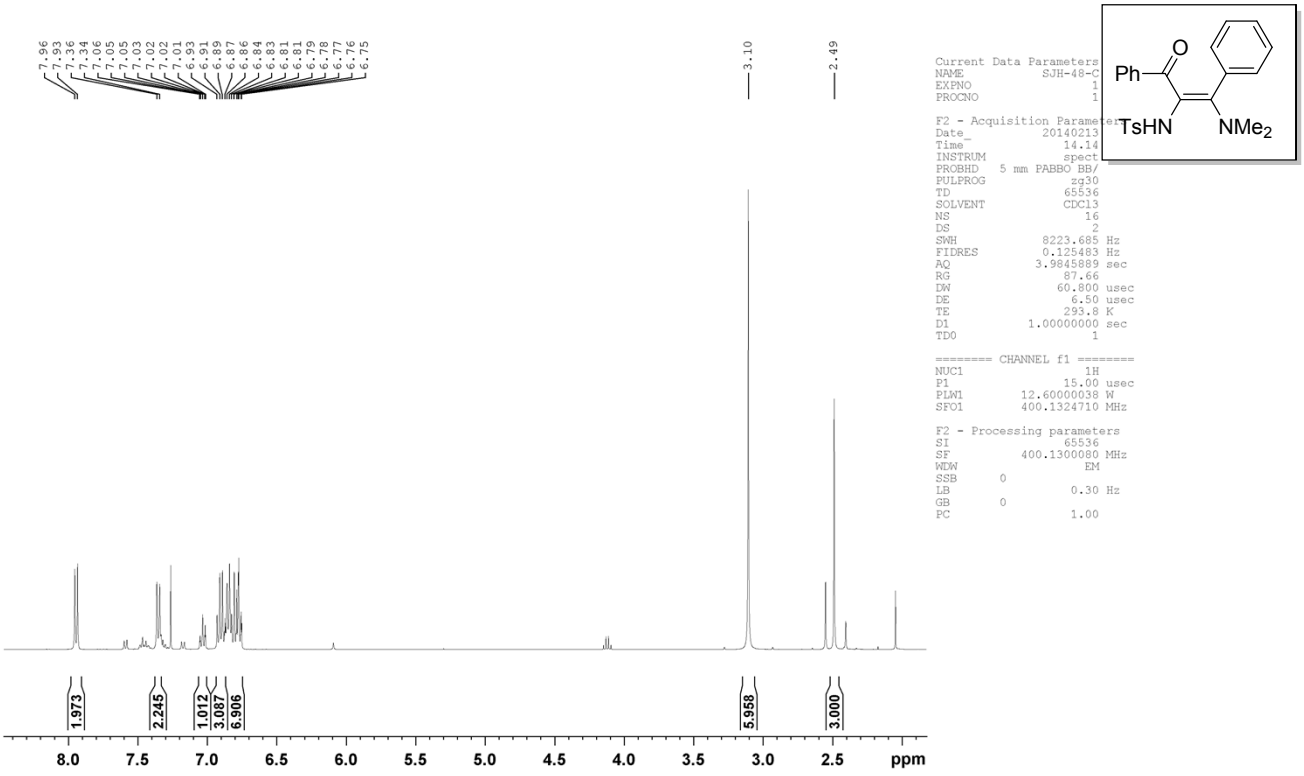
## Copies of $^{1}H$ and $^{13}C$ NMR Spectra of Compounds Obtained in this Study

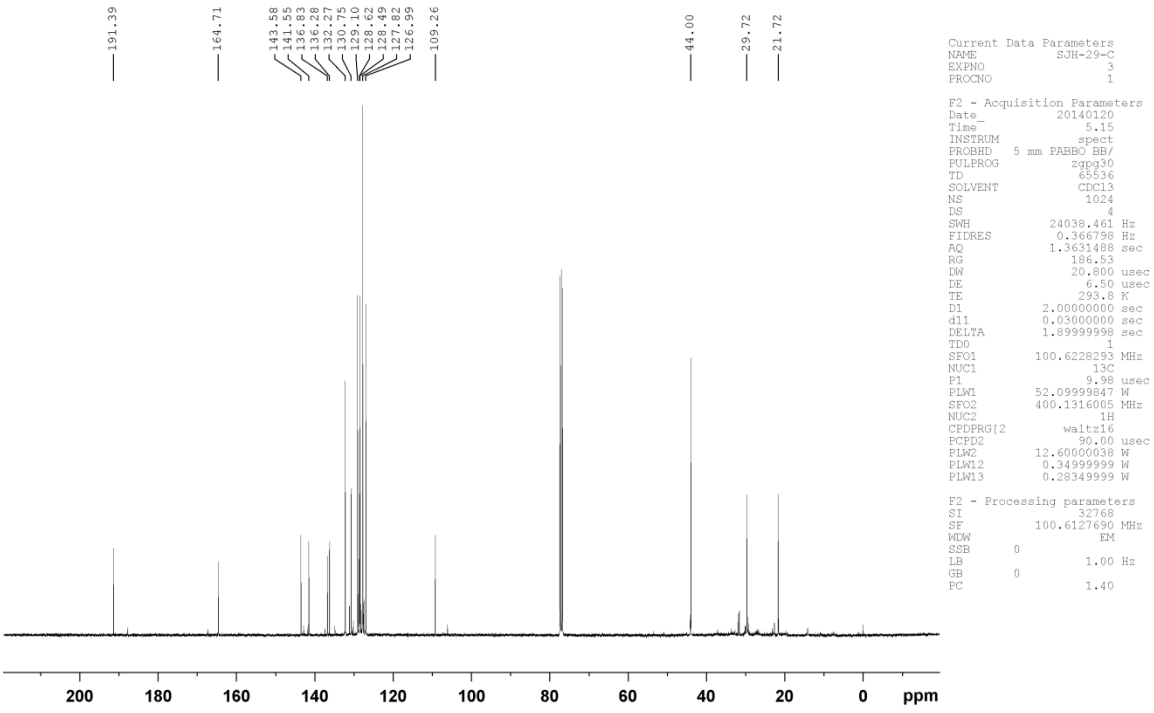
**(Z)-N-(1-(dimethylamino)-3-oxo-1,3-diphenylprop-1-en-2-yl)methanesulfonamide (3a):**



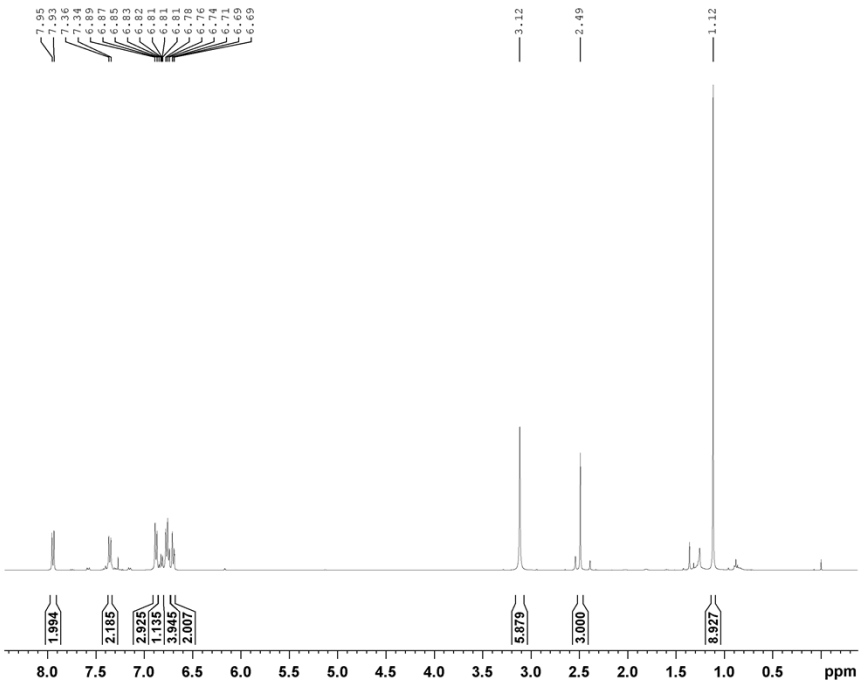



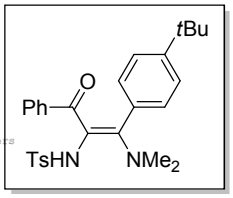
**(Z)-N-(1-(dimethylamino)-3-oxo-1,3-diphenylprop-1-en-2-yl)-4-methylbenzenesulfonamide (3b):**



**(Z)-N-(1-(4-(tert-butyl)phenyl)-1-(dimethylamino)-3-oxo-3-phenylprop-1-en-2-yl)-4-methylbenzenesulfonamide (3c):**

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Current Data Parameters
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EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_               20140226
Time_                  22.26
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         2
SWH                 8223.685 Hz
FIDRES              0.125483 Hz
AQ                  3.9845889 sec
RG                      32.47
DW                     60.800 usec
DE                      6.50 usec
TE                     293.1 K
D1                  1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     15.00 usec
PLW1               12.60000038 W
SFO1               400.1324710 MHz

F2 - Processing parameters
SI                     65536
SF                 400.1300055 MHz
WDW                       EM
SSB          0
LB                      0.30 Hz
GB           0
PC                      1.00
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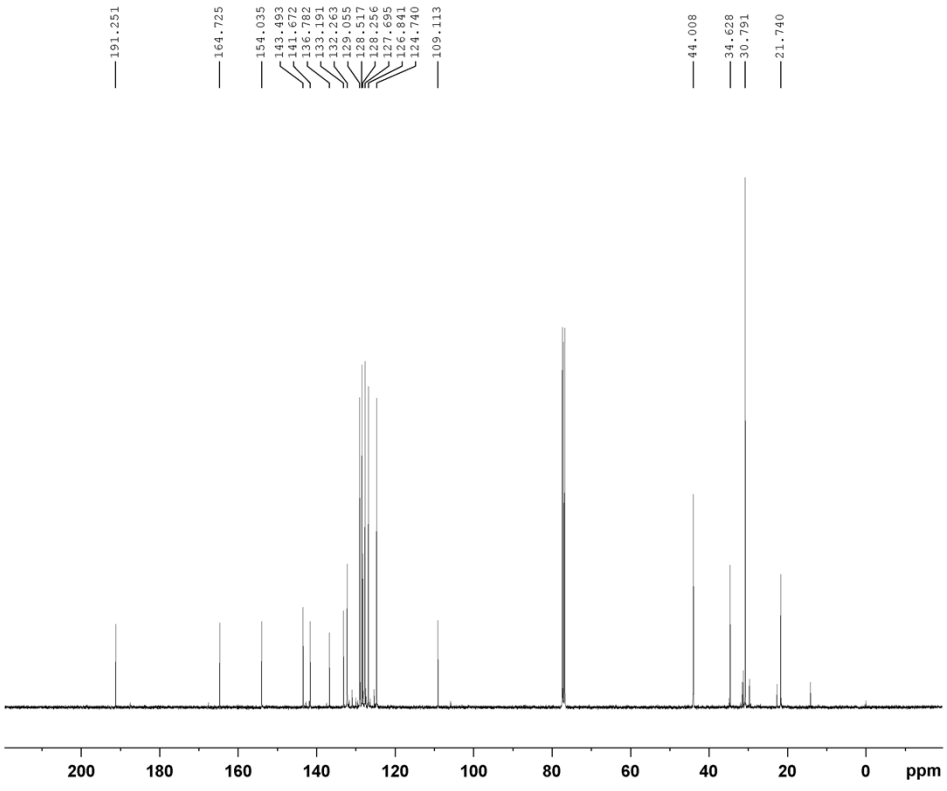


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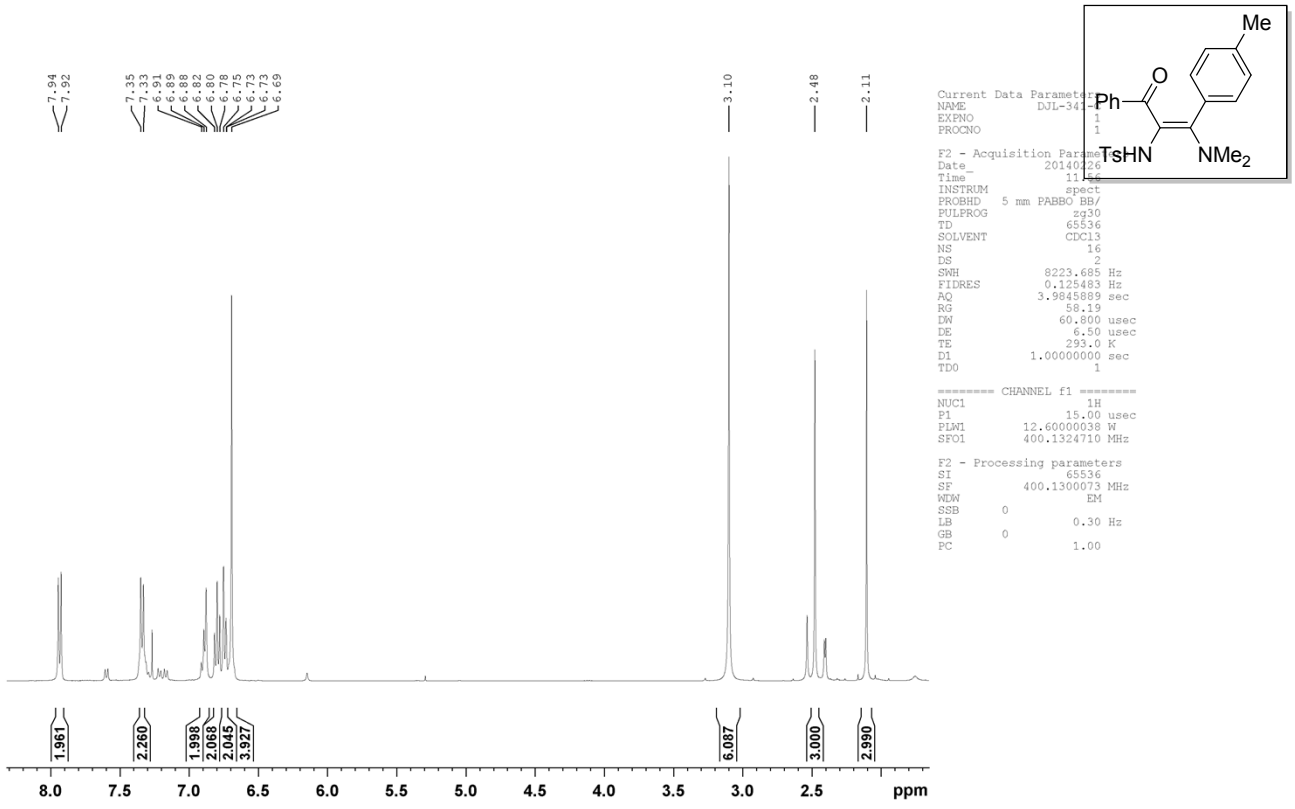
Current Data Parameters
NAME                  SJH-66-C
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_               20140227
Time_                   7.11
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                     65536
SOLVENT                CDCl3
NS                      1024
DS                         4
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                  1.3631488 sec
RG                     186.53
DW                     20.800 usec
DE                      6.50 usec
TE                     294.4 K
D1                  2.00000000 sec
d11                 0.03000000 sec
DELTA               1.89999998 sec
TD0                        1
SFO1               100.6228293 MHz
NUC1                      13C
P1                      9.98 usec
PLW1               52.09999847 W
SFO2               400.1316005 MHz
NUC2                      1H
CPDPRG[2             waltz16
PCPD2                  90.00 usec
PLW2               12.60000038 W
PLW12               0.34999999 W
PLW13               0.28349999 W

F2 - Processing parameters
SI                     32768
SF                 100.6127690 MHz
WDW                       EM
SSB          0
LB                      1.00 Hz
GB           0
PC                      1.40
```

**(Z)-N-(1-(dimethylamino)-3-oxo-3-phenyl-1-(p-tolyl)prop-1-en-2-yl)-4-methylbenzenesulfonamide (3d):**

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Current Data Parameters
NAME            DJL-341-H
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20140226
Time                11.56
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ              3.9845889 sec
RG                 58.19
DW                60.800 usec
DE                 6.50 usec
TE                293.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 15.00 usec
PLW1          12.60000038 W
SFO1          400.1324710 MHz

F2 - Processing parameters
SI                 65536
SF            400.1300073 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
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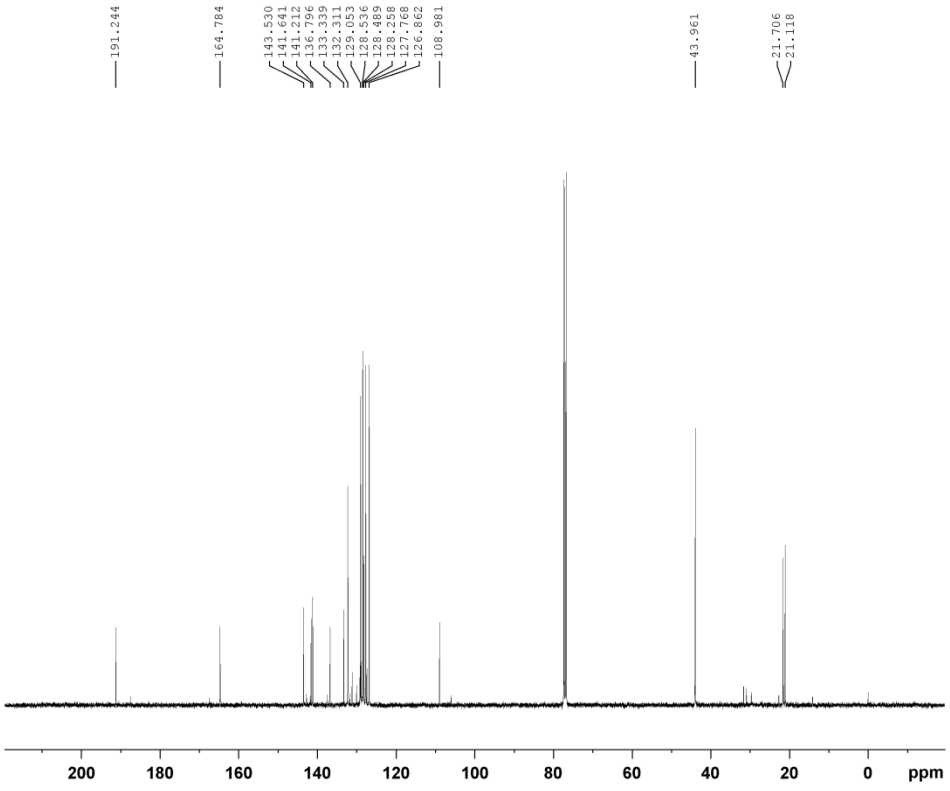


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Current Data Parameters
NAME            DJL-341-C
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
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Time                3.03
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ              1.3631488 sec
RG                186.53
DW                20.800 usec
DE                 6.50 usec
TE                294.5 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                    1
SFO1          100.6228293 MHz
NUC1                  13C
P1                 9.98 usec
PLW1          52.09999847 W
SFO2          400.1316005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2             90.00 usec
PLW2          12.60000038 W
PLW12          0.34999999 W
PLW13          0.28349999 W

F2 - Processing parameters
SI                 32768
SF            100.6127690 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
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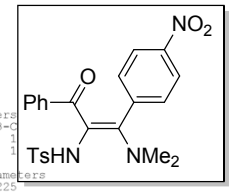
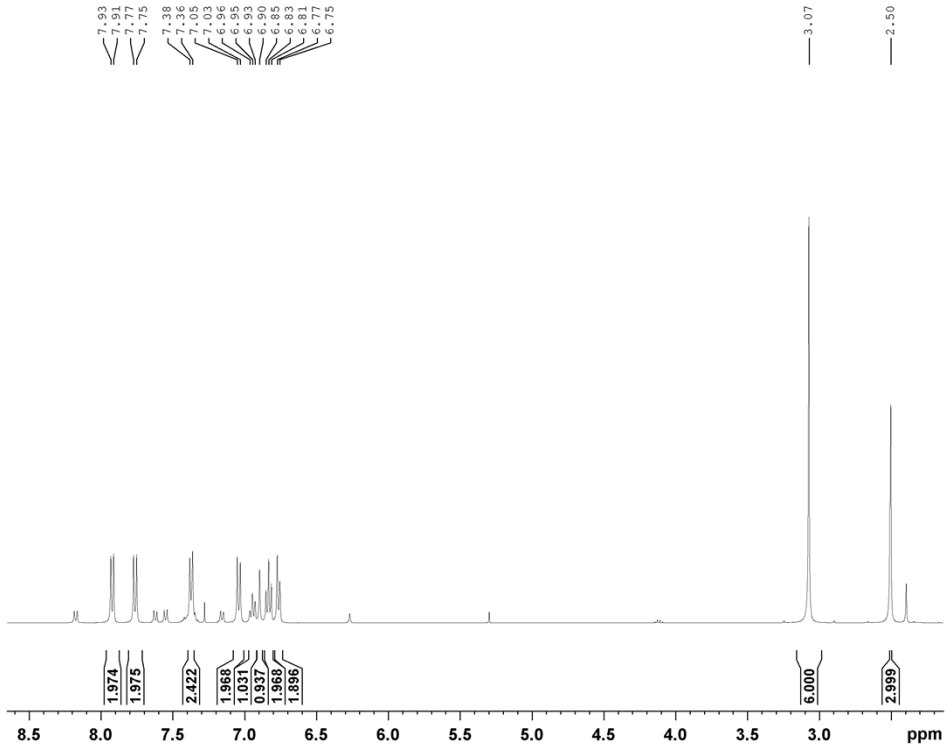
**(Z)-N-(1-(dimethylamino)-1-(4-nitrophenyl)-3-oxo-3-phenylprop-1-en-2-yl)-4-methylbenzenesulfonamide ( 3e):**

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Current Data Parameters
NAME                 DJL-333-C
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_               20140225
Time                   14.16
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8223.685 Hz
FIDRES             0.125483 Hz
AQ                 3.9845889 sec
RG                     32.47
DW                    60.800 usec
DE                     6.50 usec
TE                    293.1 K
D1                 1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                      1H
P1                     15.00 usec
PLW1              12.60000038 W
SFO1              400.1324710 MHz

F2 - Processing parameters
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SF                400.1300025 MHz
WDW                         EM
SSB          0
LB                      0.30 Hz
GB           0
PC                      1.00
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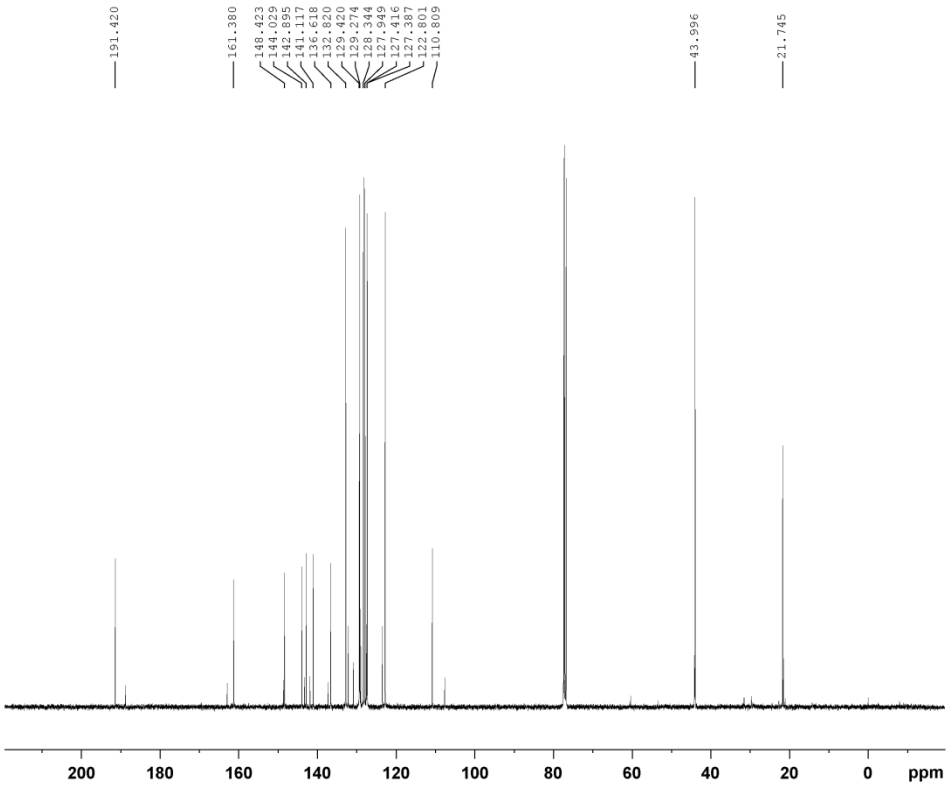


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Current Data Parameters
NAME                 DJL-333-C
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
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Time                    3.01
INSTRUM                spect
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PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     1024
DS                        4
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631488 sec
RG                    186.53
DW                    20.800 usec
DE                     6.50 usec
TE                    294.3 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
TD0                          1
SFO1              100.6228293 MHz
NUC1                      13C
P1                     9.98 usec
PLW1              52.09999847 W
SFO2              400.1316005 MHz
NUC2                      1H
CPDPRG[2             waltz16
PCPD2                 90.00 usec
PLW2              12.60000038 W
PLW12              0.34999999 W
PLW13              0.28349999 W

F2 - Processing parameters
SI                        32768
SF                100.6127690 MHz
WDW                         EM
SSB          0
LB                      1.00 Hz
GB           0
PC                      1.40
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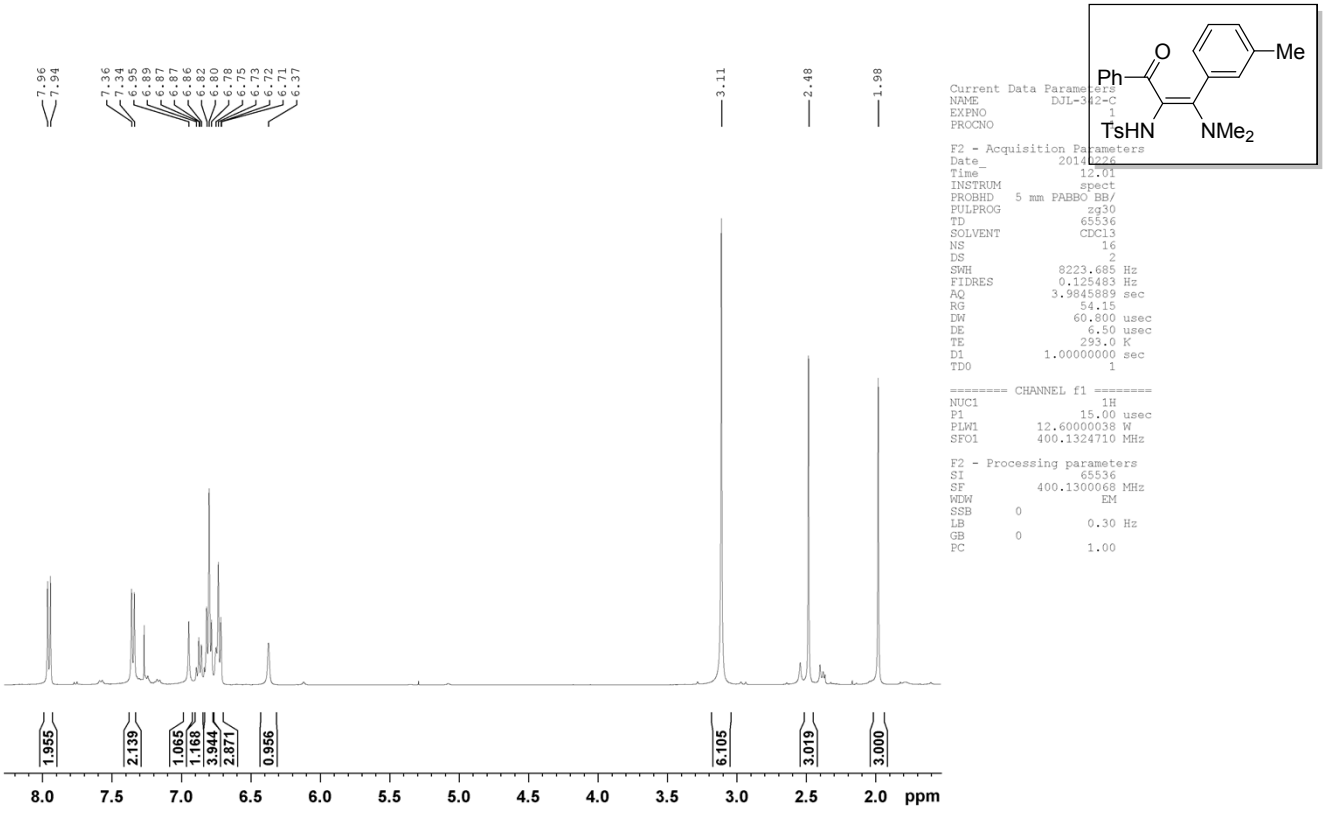
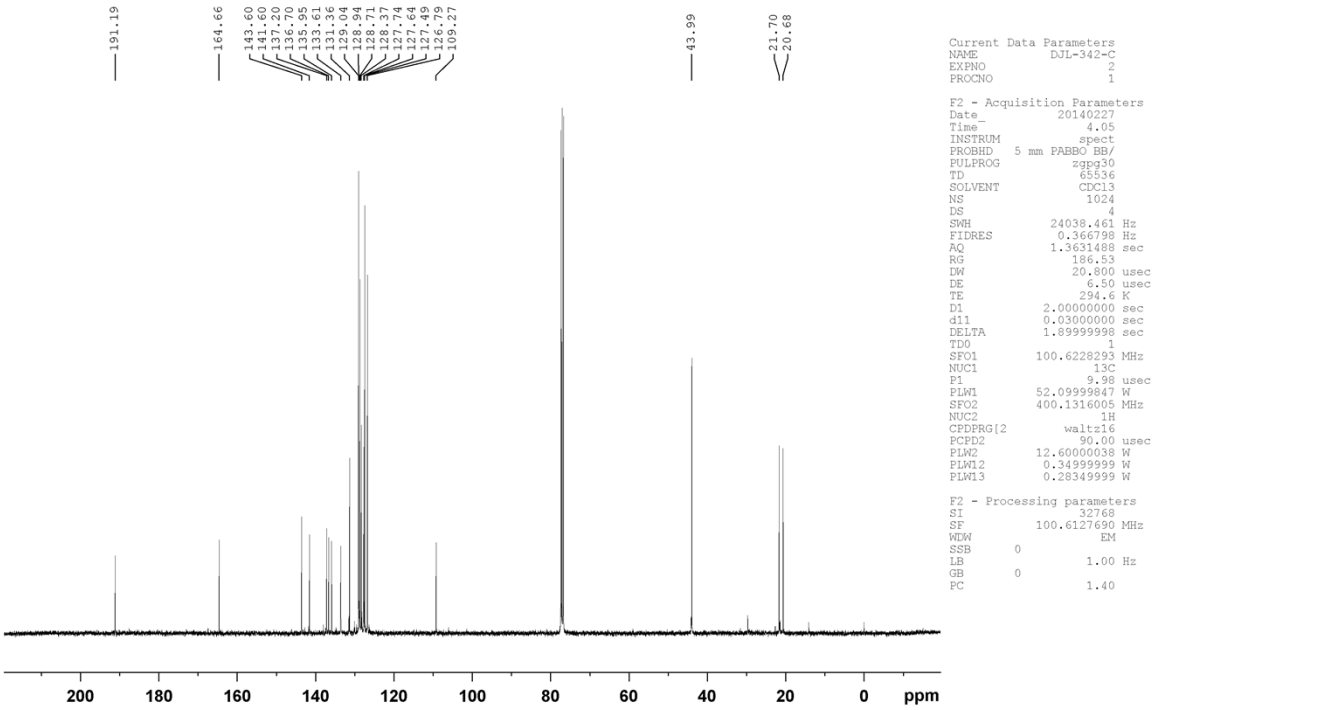
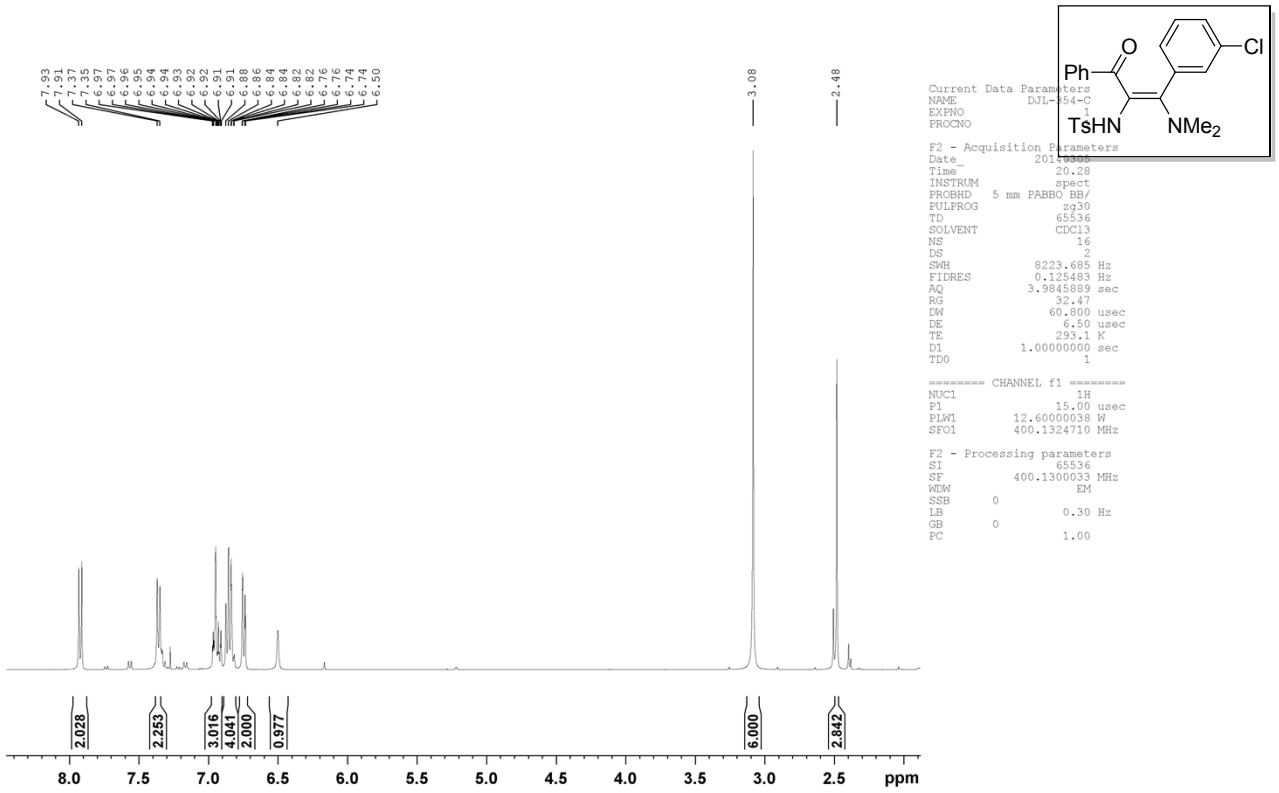
**(Z)-N-(1-(dimethylamino)-3-oxo-3-phenyl-1-(m-tolyl)prop-1-en-2-yl)-4-methylbenzenesulfonamide (3f):**



**(Z)-N-(1-(3-chlorophenyl)-1-(dimethylamino)-3-oxo-3-phenylprop-1-en-2-yl)-4-methylbenzenesulfonamide (3g):**

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PROCNO                        1

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Time                      20.28
INSTRUM                   spect
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PULPROG                   zg30
TD                       65536
SOLVENT                  CDCl3
NS                          16
DS                           2
SWH                   8223.685 Hz
FIDRES                0.125483 Hz
AQ                    3.9845889 sec
RG                        32.47
DW                       60.800 usec
DE                        6.50 usec
TE                       293.1 K
D1                    1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                         1H
P1                       15.00 usec
PLW1                 12.60000038 W
SFO1                 400.1324710 MHz

F2 - Processing parameters
SI                       65536
SF                   400.1300033 MHz
WDW                         EM
SSB                  0
LB                        0.30 Hz
GB                   0
PC                        1.00
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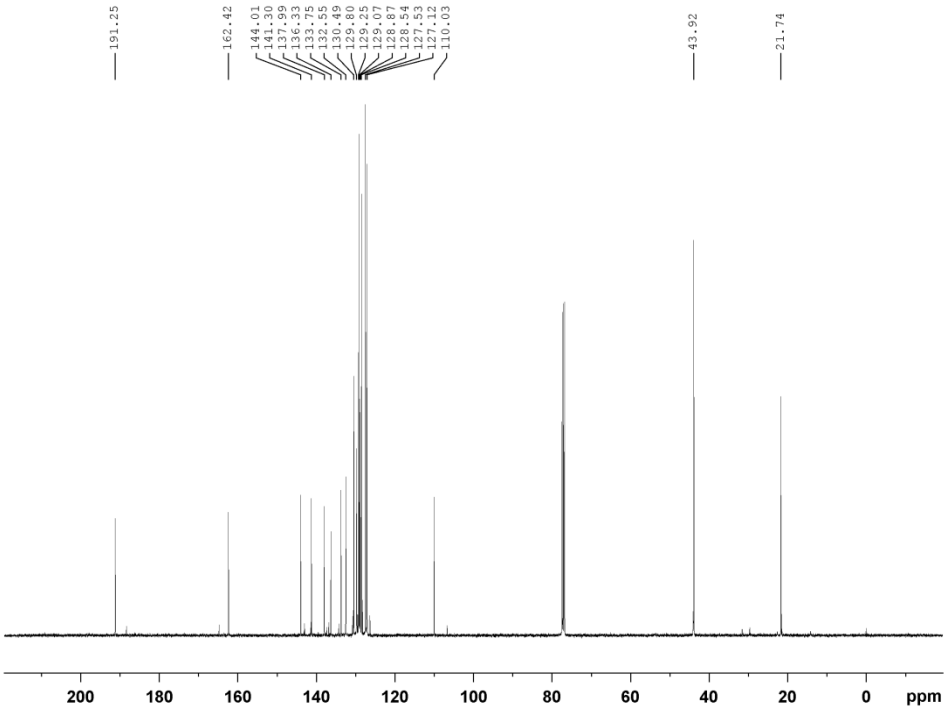


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Current Data Parameters
NAME                  DJL-354-C
EXPNO                         2
PROCNO                        1

F2 - Acquisition Parameters
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Time                       4.03
INSTRUM                   spect
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PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                        1024
DS                           4
SWH                  24038.461 Hz
FIDRES                0.366798 Hz
AQ                    1.3631488 sec
RG                       186.53
DW                       20.800 usec
DE                        6.50 usec
TE                       294.8 K
D1                    2.00000000 sec
d11                   0.03000000 sec
DELTA                 1.89999998 sec
TD0                          1
SFO1                100.6228293 MHz
NUC1                        13C
P1                        9.98 usec
PLW1                52.09999847 W
SFO2                400.1316005 MHz
NUC2                         1H
CPDPRG[2                waltz16
PCPD2                    90.00 usec
PLW2                 12.60000038 W
PLW12                 0.34999999 W
PLW13                 0.28349999 W

F2 - Processing parameters
SI                       32768
SF                   100.6127690 MHz
WDW                         EM
SSB                  0
LB                        1.00 Hz
GB                   0
PC                        1.40
```
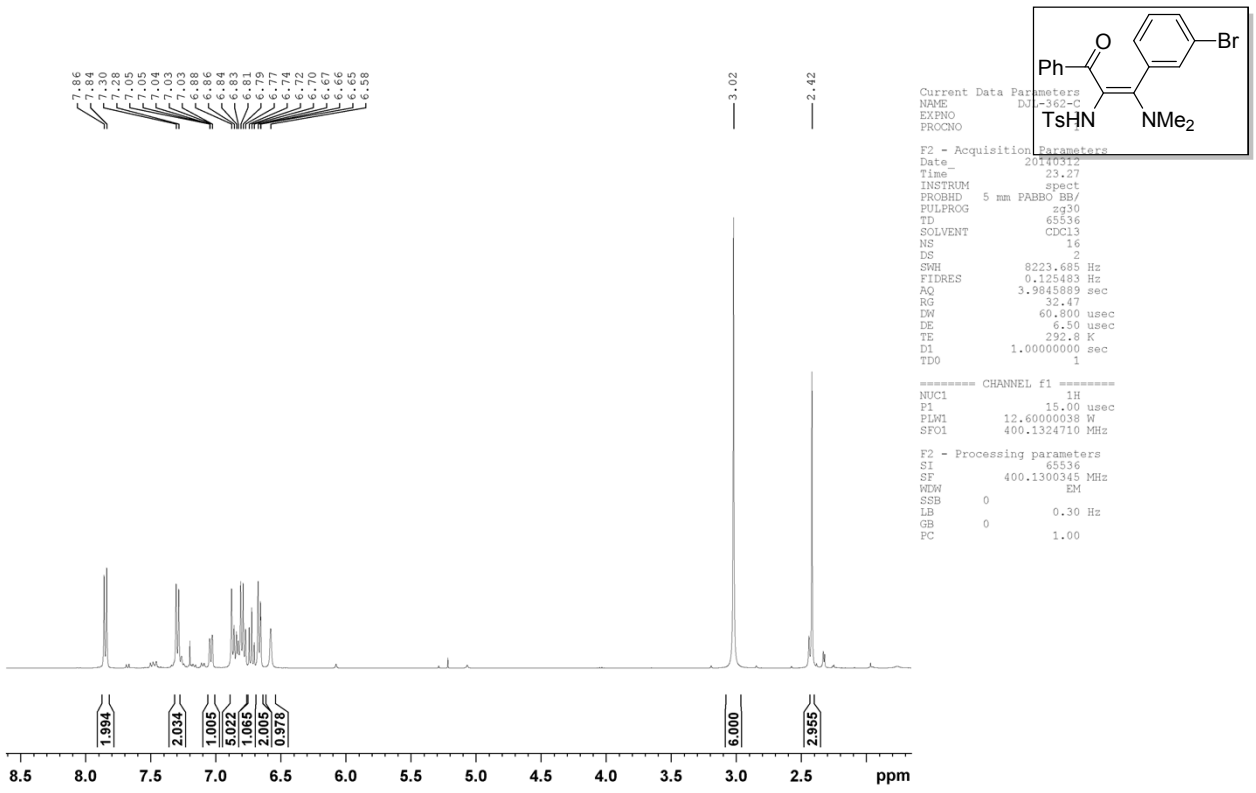
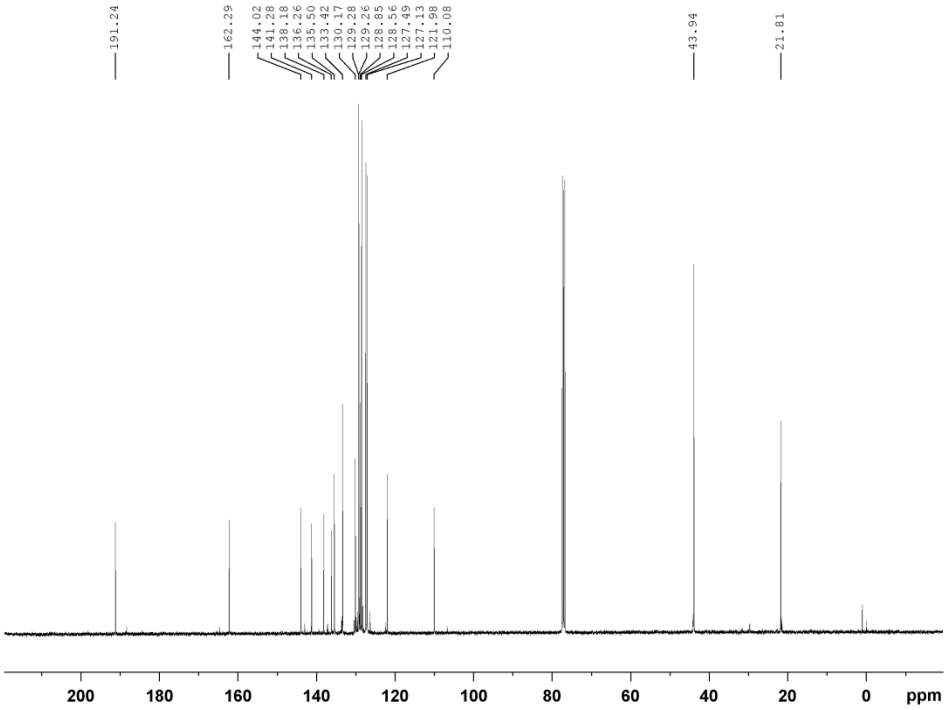

**(Z)-N-(1-(3-bromophenyl)-1-(dimethylamino)-3-oxo-3-phenylprop-1-en-2-yl)-4-methylbenzenesulfonamide (3h):**

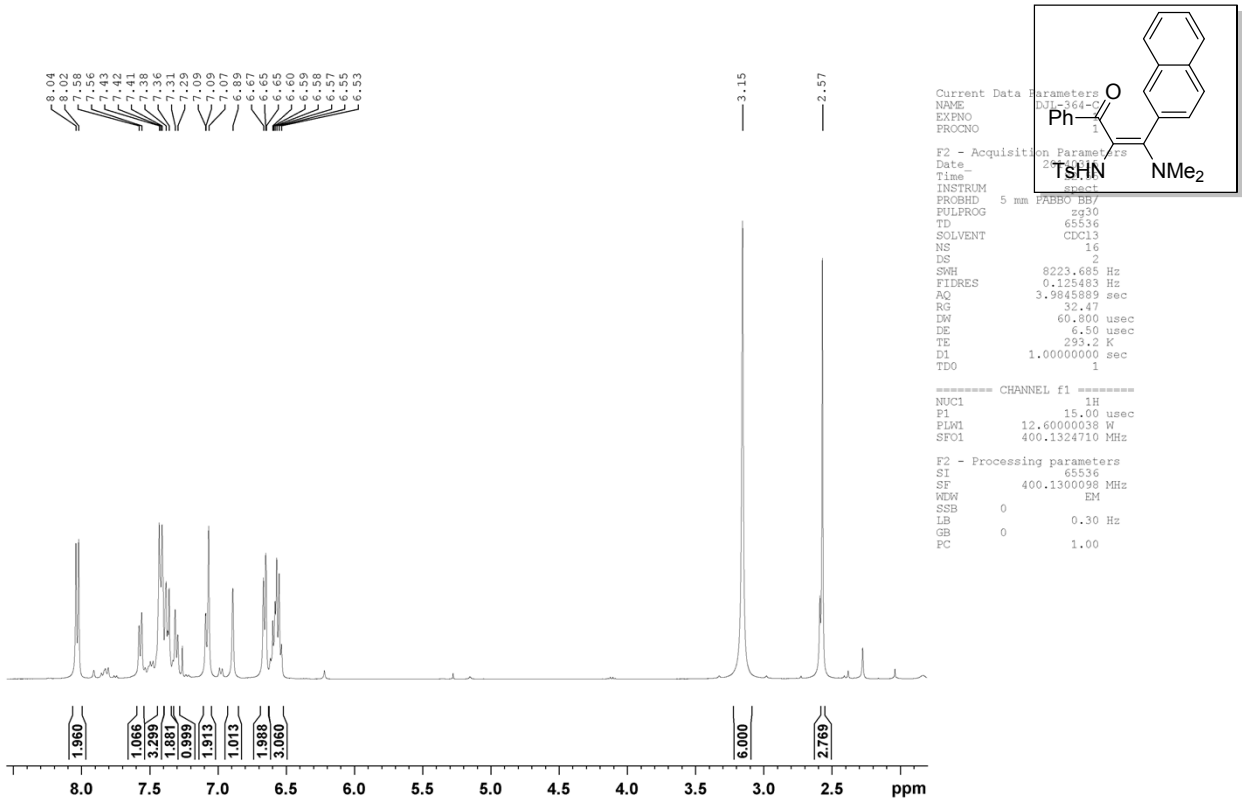


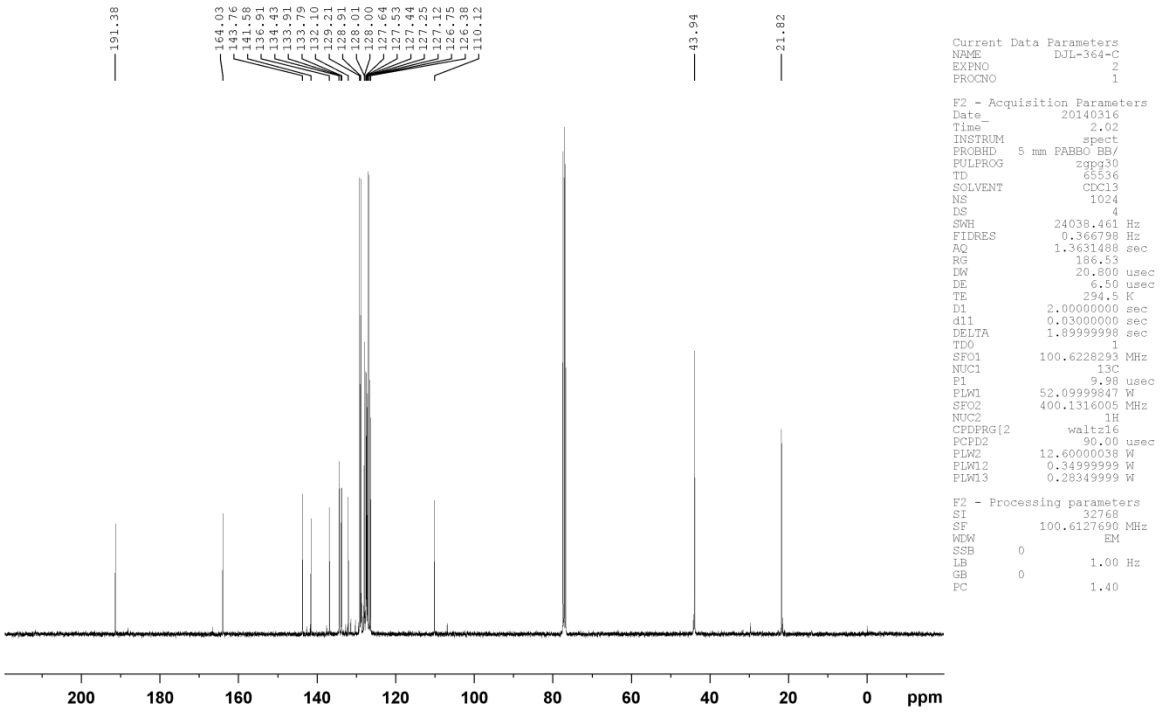

```
Current Data Parameters
NAME                  DJL-362-C
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20140312
Time                      23.27
INSTRUM                   spect
PROBHD     5 mm PABBO BB/
PULPROG                   zg30
TD                       65536
SOLVENT                  CDCl3
NS                          16
DS                           2
SWH                   8223.685 Hz
FIDRES               0.125483 Hz
AQ                    3.9845889 sec
RG                        32.47
DW                       60.800 usec
DE                        6.50 usec
TE                       292.8 K
D1                    1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        1H
P1                       15.00 usec
PLW1                12.60000038 W
SFO1                400.1324710 MHz

F2 - Processing parameters
SI                       65536
SF                  400.1300345 MHz
WDW                         EM
SSB                  0
LB                        0.30 Hz
GB                   0
PC                        1.00
```



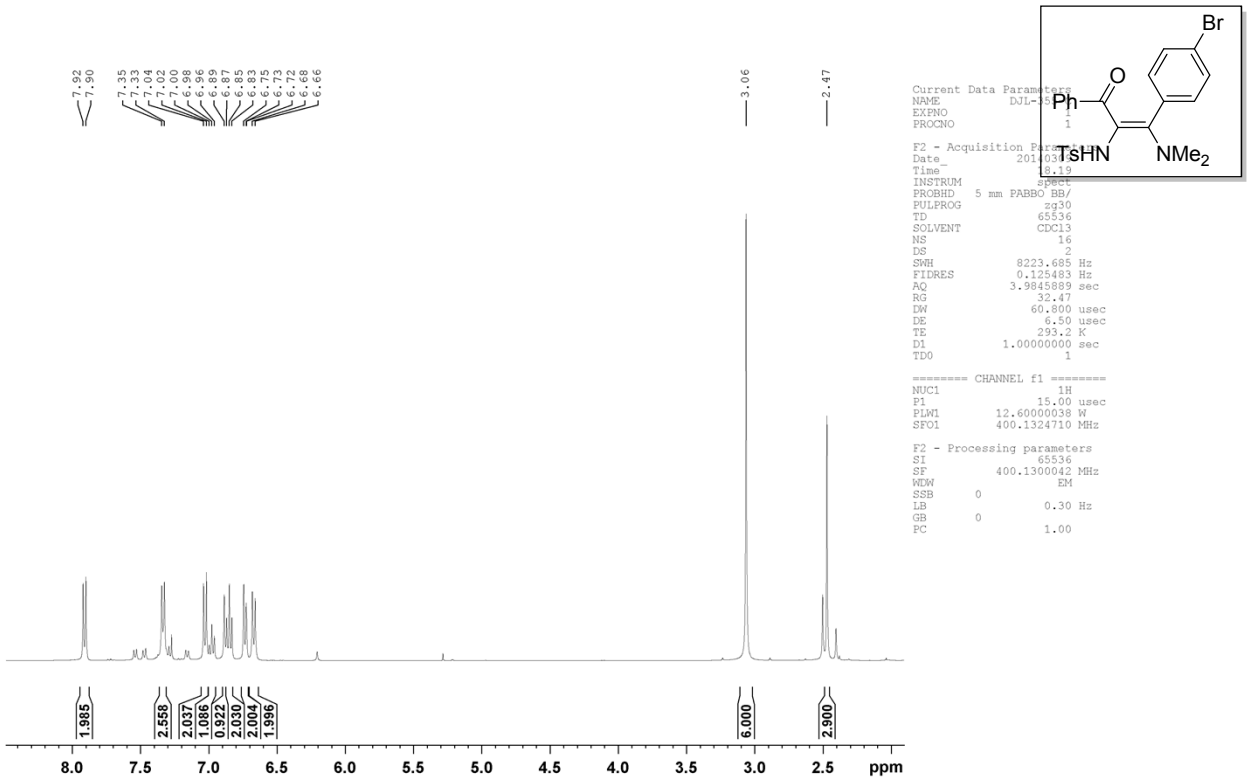

```
Current Data Parameters
NAME                  DJL-362-C
EXPNO                         2
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20140313
Time                       5.02
INSTRUM                   spect
PROBHD     5 mm PABBO BB/
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                        1024
DS                           4
SWH                  24038.461 Hz
FIDRES               0.366798 Hz
AQ                    1.3631488 sec
RG                       186.53
DW                       20.800 usec
DE                        6.50 usec
TE                       294.4 K
D1                    2.00000000 sec
d11                   0.03000000 sec
DELTA                 1.89999998 sec
TD0                          1
SFO1                100.6228293 MHz
NUC1                        13C
P1                        9.98 usec
PLW1                52.09999847 W
SFO2                400.1316005 MHz
NUC2                        1H
CPDPRG[2                waltz16
PCPD2                    90.00 usec
PLW2                12.60000038 W
PLW12                0.34999999 W
PLW13                0.28349999 W

F2 - Processing parameters
SI                       32768
SF                  100.6127690 MHz
WDW                         EM
SSB                  0
LB                        1.00 Hz
GB                   0
PC                        1.40
```

**(Z)-N-(1-(dimethylamino)-1-(naphthalen-2-yl)-3-oxo-3-phenylprop-1-en-2-yl)-4-methylbenzenesulfonamide (3i):**

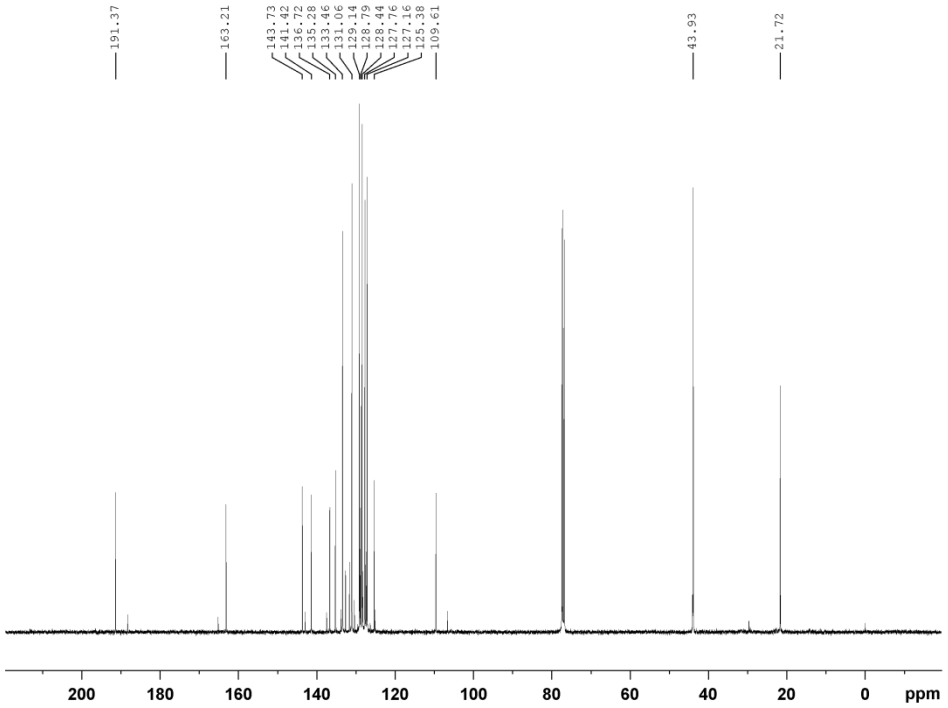


**(Z)-N-(1-(4-bromophenyl)-1-(dimethylamino)-3-oxo-3-phenylprop-1-en-2-yl)-4-methylbenzenesulfonamide (3j):**

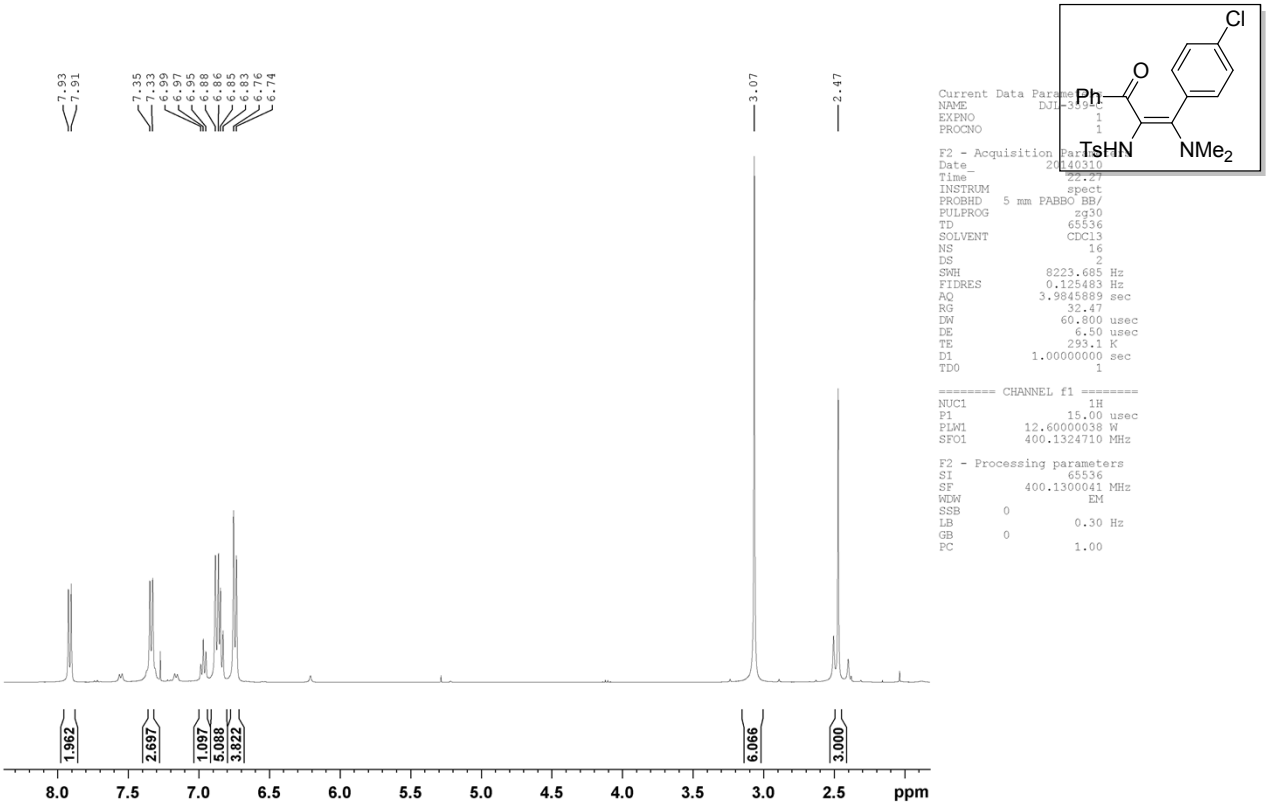



```
Current Data Parameters
NAME                  DJL-355-H
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_               20140310
Time                    8.19
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         2
SWH                 8223.685 Hz
FIDRES              0.125483 Hz
AQ                  3.9845889 sec
RG                      32.47
DW                    60.800 usec
DE                     6.50 usec
TE                     293.2 K
D1                  1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     15.00 usec
PLW1               12.60000038 W
SFO1               400.1324710 MHz

F2 - Processing parameters
SI                        65536
SF                 400.1300042 MHz
WDW                       EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```

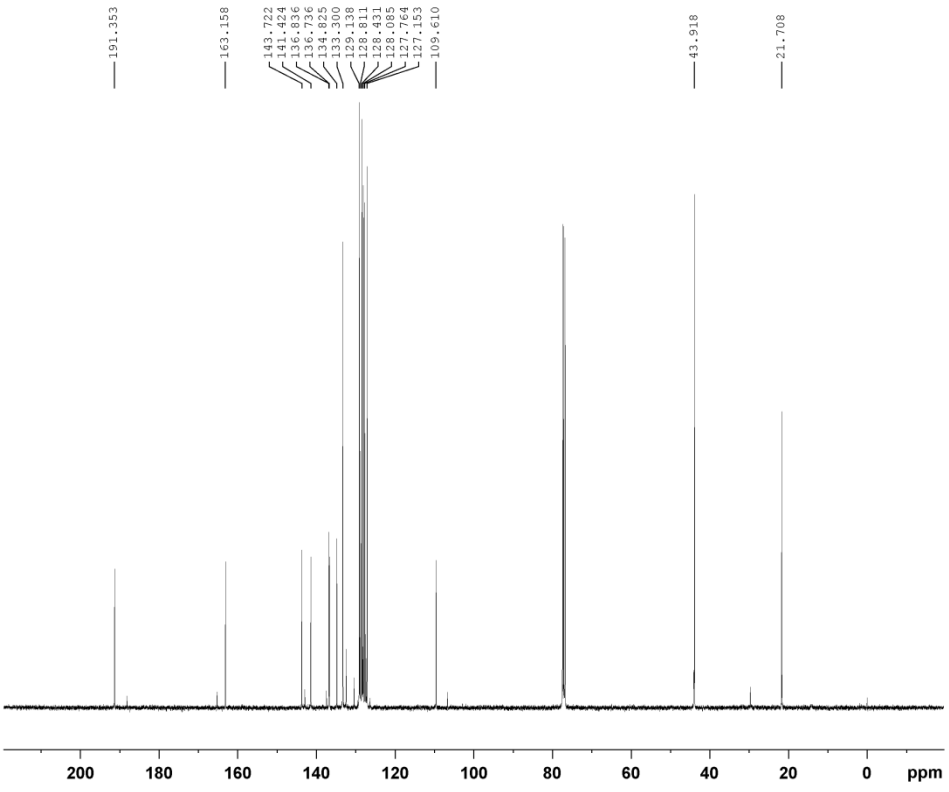



```
Current Data Parameters
NAME                  DJL-355-C
EXPNO                         2
PROCNO                        1

F2 - Acquisition Parameters
Date_               20140310
Time                    3.03
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                     65536
SOLVENT                CDCl3
NS                      1024
DS                         4
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                  1.3631488 sec
RG                     186.53
DW                    20.800 usec
DE                     6.50 usec
TE                     294.7 K
D1                  2.00000000 sec
d11                 0.03000000 sec
DELTA               1.89999998 sec
TD0                        1
SFO1               100.6228293 MHz
NUC1                      13C
P1                     9.98 usec
PLW1               52.09999847 W
SFO2               400.1316005 MHz
NUC2                      1H
CPDPRG[2               waltz16
PCPD2                 90.00 usec
PLW2               12.60000038 W
PLW12               0.34999999 W
PLW13               0.28349999 W

F2 - Processing parameters
SI                        32768
SF                 100.6127690 MHz
WDW                       EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```

**(Z)-N-(1-(4-chlorophenyl)-1-(dimethylamino)-3-oxo-3-phenylprop-1-en-2-yl)-4-methylbenzenesulfonamide (3k):**

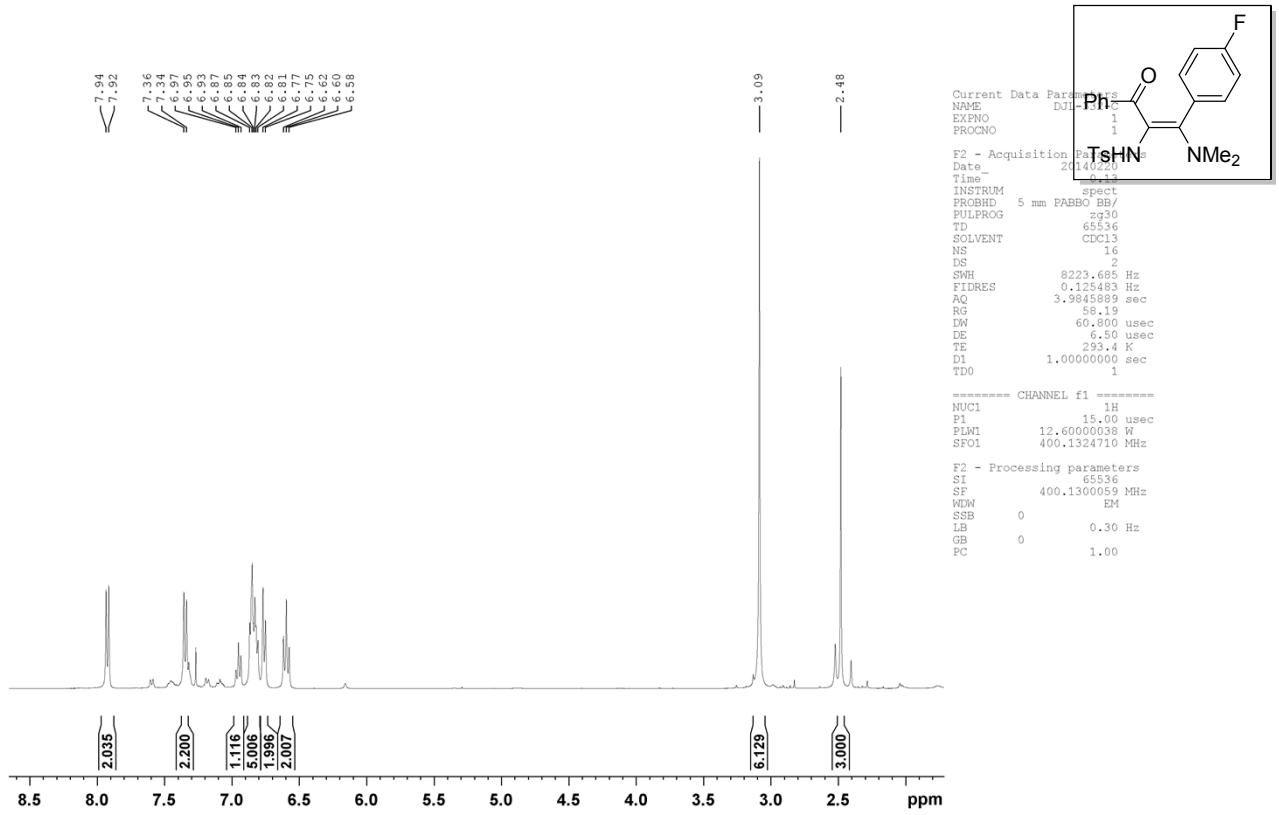



```
Current Data Parameters
NAME                 DJL-359-H
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_               20140310
Time_                   22.27
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8223.685 Hz
FIDRES            0.125483 Hz
AQ                3.9845889 sec
RG                     32.47
DW                  60.800 usec
DE                   6.50 usec
TE                  293.1 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                    15.00 usec
PLW1             12.60000038 W
SFO1            400.1324710 MHz

F2 - Processing parameters
SI                    65536
SF               400.1300041 MHz
WDW                      EM
SSB          0
LB                    0.30 Hz
GB           0
PC                    1.00
```




```
Current Data Parameters
NAME                 DJL-359-C
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_               20140311
Time_                    3.06
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     1024
DS                        4
SWH               24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631488 sec
RG                    186.53
DW                  20.800 usec
DE                   6.50 usec
TE                  294.6 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                       1
SFO1            100.6228293 MHz
NUC1                     13C
P1                    9.98 usec
PLW1             52.09999847 W
SFO2            400.1316005 MHz
NUC2                      1H
CPDPRG[2              waltz16
PCPD2                90.00 usec
PLW2             12.60000038 W
PLW12             0.34999999 W
PLW13             0.28349999 W

F2 - Processing parameters
SI                    32768
SF              100.6127690 MHz
WDW                      EM
SSB          0
LB                    1.00 Hz
GB           0
PC                    1.40
```

**(Z)-N-(1-(dimethylamino)-1-(4-fluorophenyl)-3-oxo-3-phenylprop-1-en-2-yl)-4-methylbenzenesulfonamide (3l):**

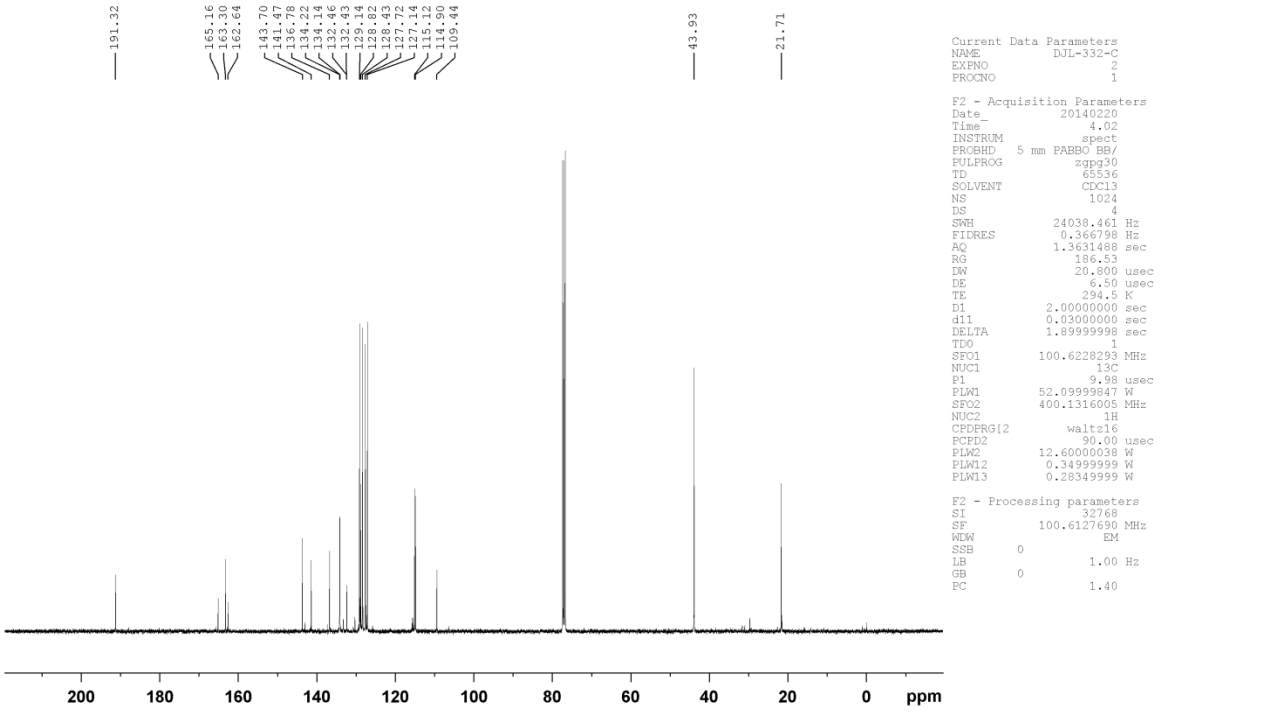



Current Data Parameters
NAME DJL-PH-5
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140220
Time 6.13
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 58.19
DW 60.800 usec
DE 6.50 usec
TE 293.4 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
PLW1 12.60000038 W
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300059 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

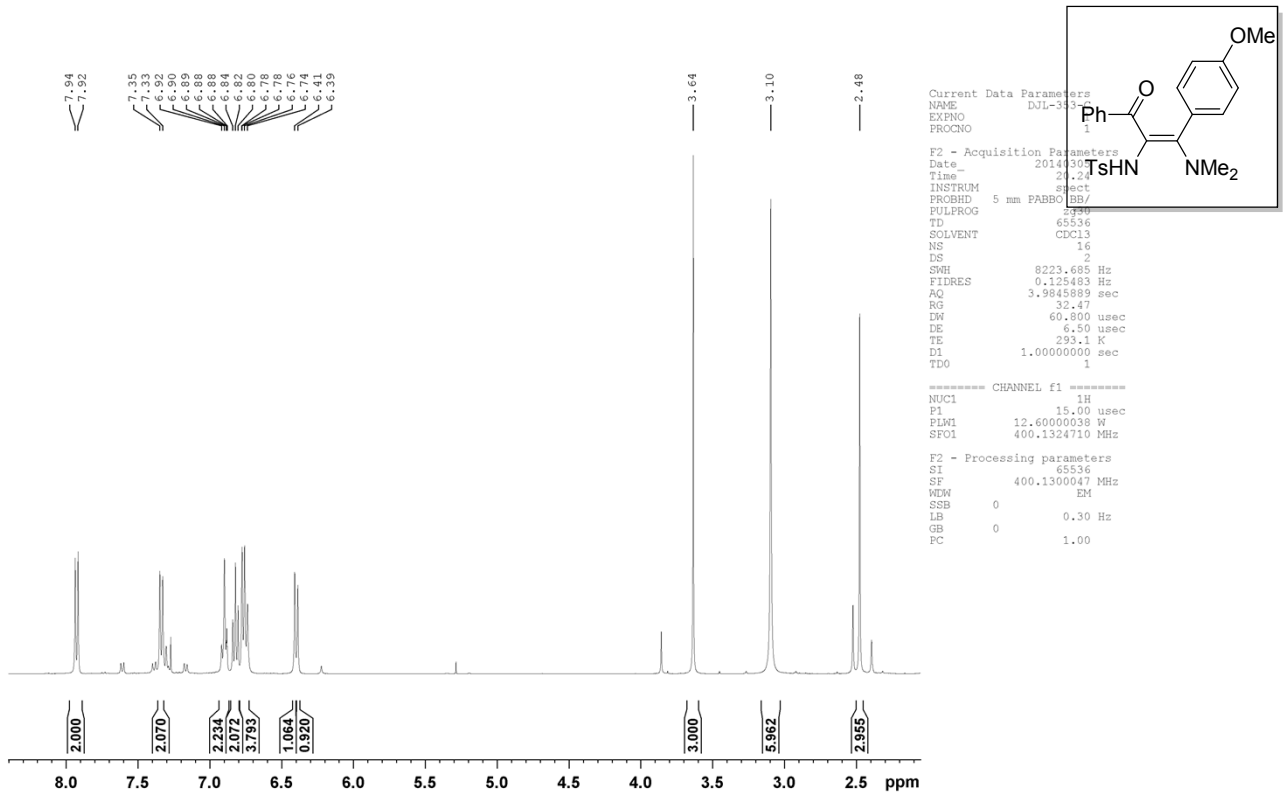



Current Data Parameters
NAME DJL-332-C
EXPNO 2
PROCNO 1

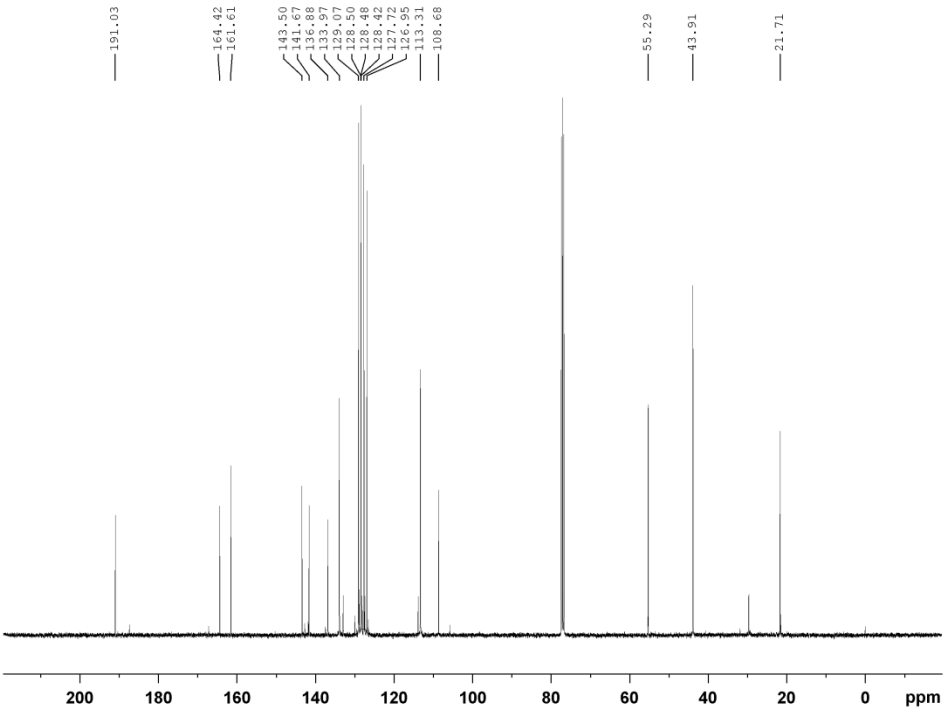
F2 - Acquisition Parameters
Date_ 20140220
Time 4.02
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 186.53
DW 20.800 usec
DE 6.50 usec
TE 294.5 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
SFO1 100.6228293 MHz
NUC1 13C
P1 9.98 usec
PLW1 52.09999847 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 12.60000038 W
PLW12 0.34999999 W
PLW13 0.28349999 W

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

**(Z)-4-methyl-N-(1-(methyl(phenyl)amino)-3-oxo-1,3-diphenylprop-1-en-2-yl)benzenesulfonamide (3m):**

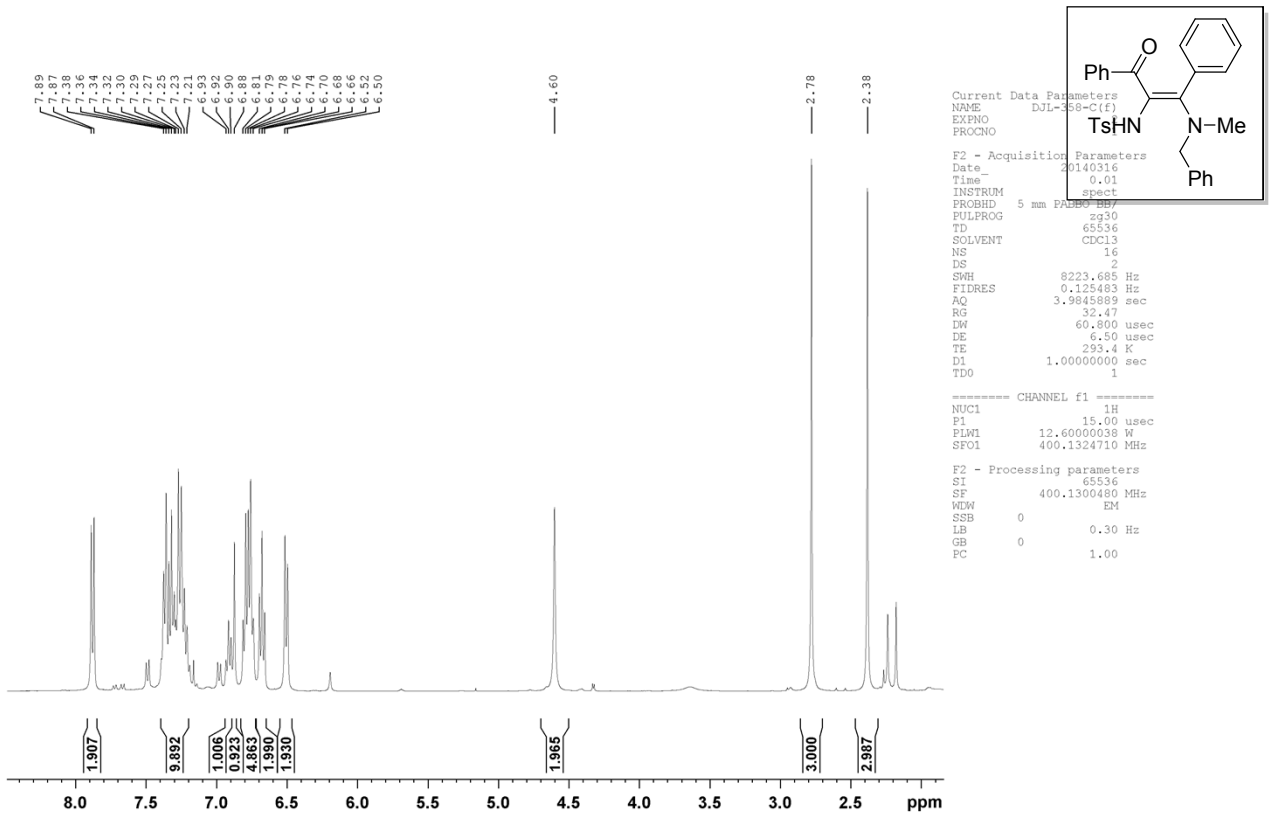


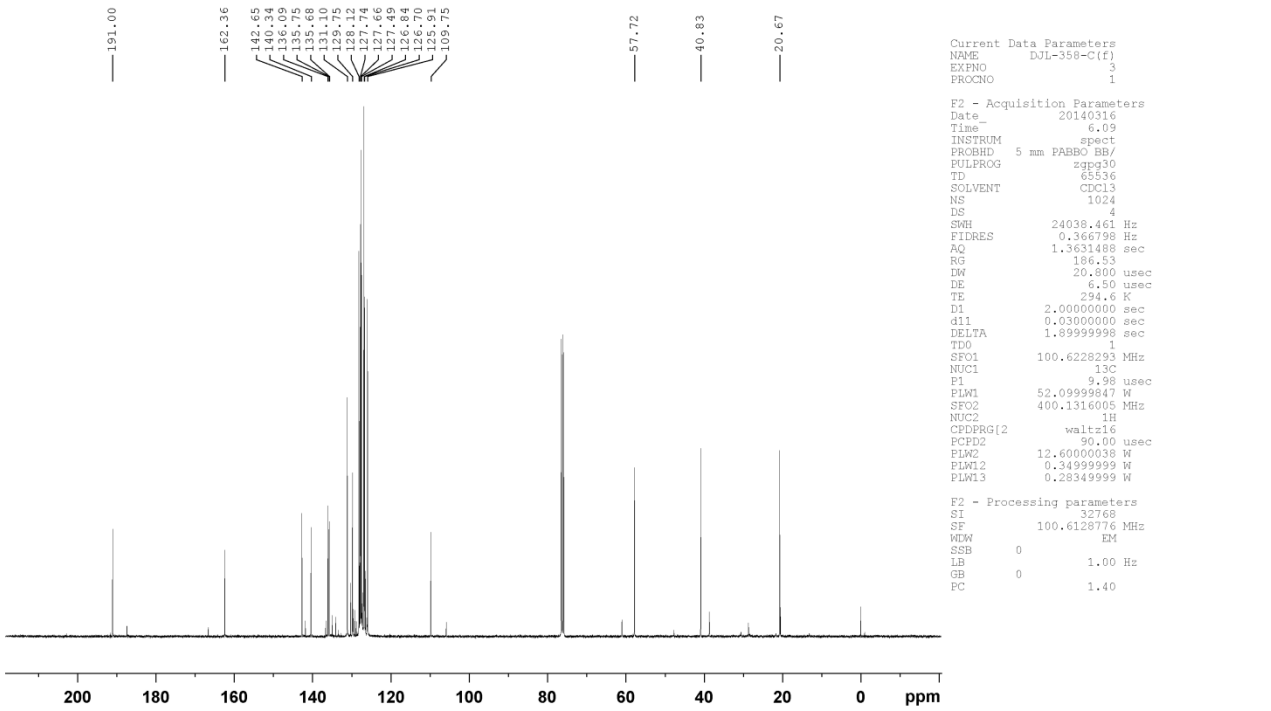

```
Current Data Parameters
NAME                  DJL-353-H
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_               20140305
Time                      21.24
INSTRUM                   spect
PROBHD    5 mm PABBO BB/
PULPROG                   zg30
TD                       65536
SOLVENT                  CDCl3
NS                          16
DS                           2
SWH                   8223.685 Hz
FIDRES                0.125483 Hz
AQ                    3.9845889 sec
RG                       32.47
DW                       60.800 usec
DE                        6.50 usec
TE                      293.1 K
D1                    1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        1H
P1                       15.00 usec
PLW1                12.60000038 W
SFO1                400.1324710 MHz

F2 - Processing parameters
SI                       65536
SF                  400.1300047 MHz
WDW                         EM
SSB                  0
LB                       0.30 Hz
GB                   0
PC                       1.00
```



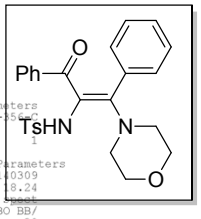

```
Current Data Parameters
NAME                  DJL-353-C
EXPNO                         2
PROCNO                        1

F2 - Acquisition Parameters
Date_               20140306
Time                      3.02
INSTRUM                   spect
PROBHD    5 mm PABBO BB/
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                        1024
DS                           4
SWH                  24038.461 Hz
FIDRES                0.366798 Hz
AQ                    1.3631488 sec
RG                       186.53
DW                       20.800 usec
DE                        6.50 usec
TE                      294.8 K
D1                    2.00000000 sec
d11                   0.03000000 sec
DELTA                 1.89999998 sec
TD0                          1
SFO1                100.6228293 MHz
NUC1                        13C
P1                        9.98 usec
PLW1                52.09999847 W
SFO2                400.1316005 MHz
NUC2                        1H
CPDPRG[2                waltz16
PCPD2                    90.00 usec
PLW2                12.60000038 W
PLW12                0.34999999 W
PLW13                0.28349999 W

F2 - Processing parameters
SI                       32768
SF                  100.6127690 MHz
WDW                         EM
SSB                  0
LB                       1.00 Hz
GB                   0
PC                       1.40
```

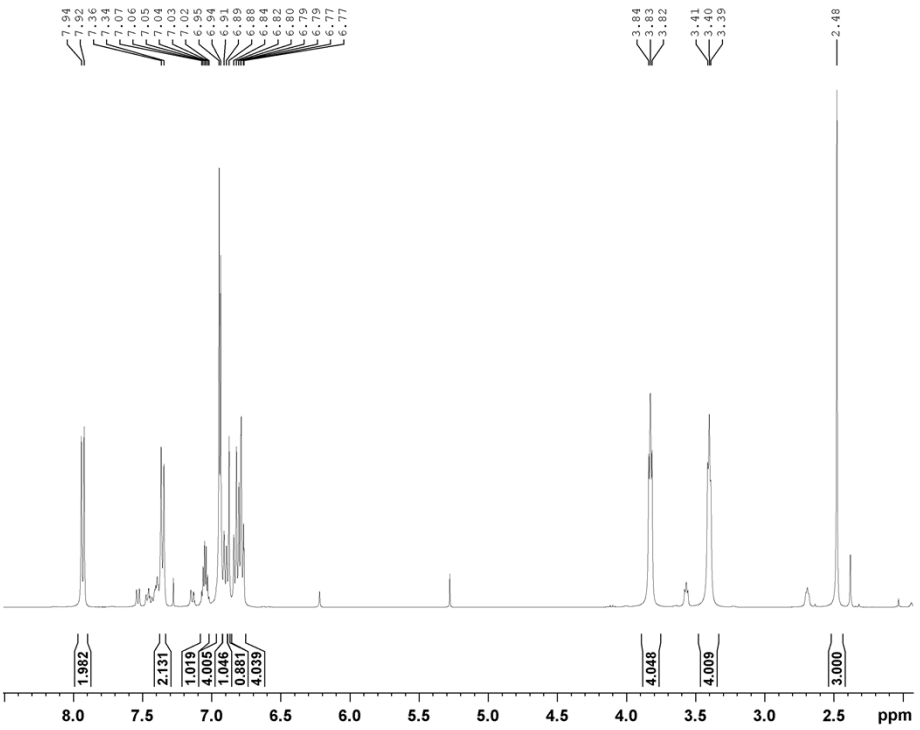
**(Z)-N-(1-(benzyl(methyl)amino)-3-oxo-1,3-diphenylprop-1-en-2-yl)-4-methylbenzenesulfonamide (3n):**



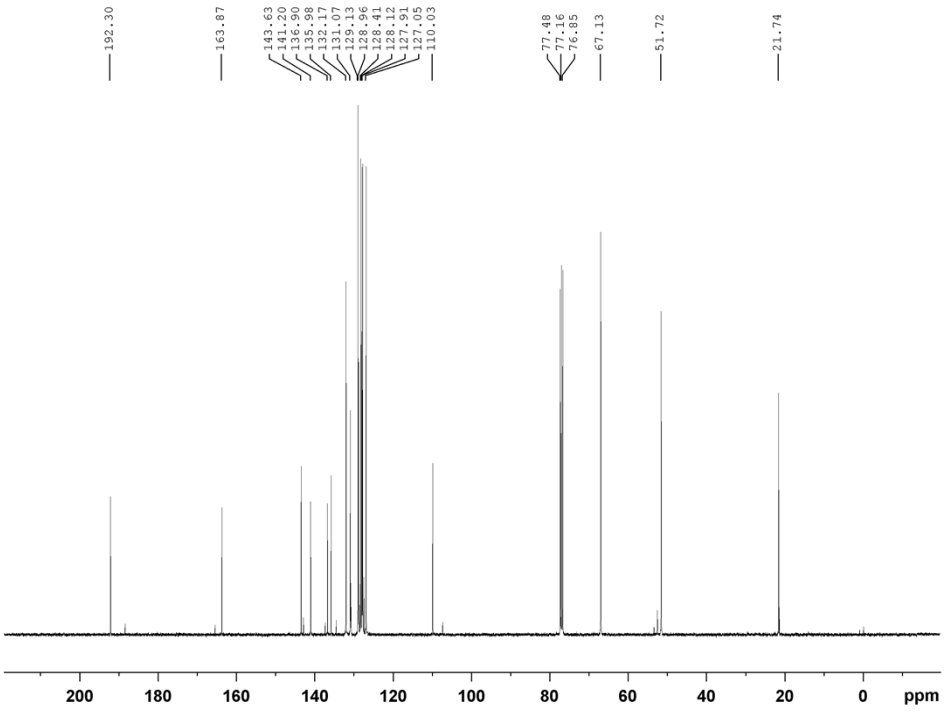



**(Z)-4-methyl-N-(1-morpholino-3-oxo-1,3-diphenylprop-1-en-2-yl)benzenesulfonamide (3o):**



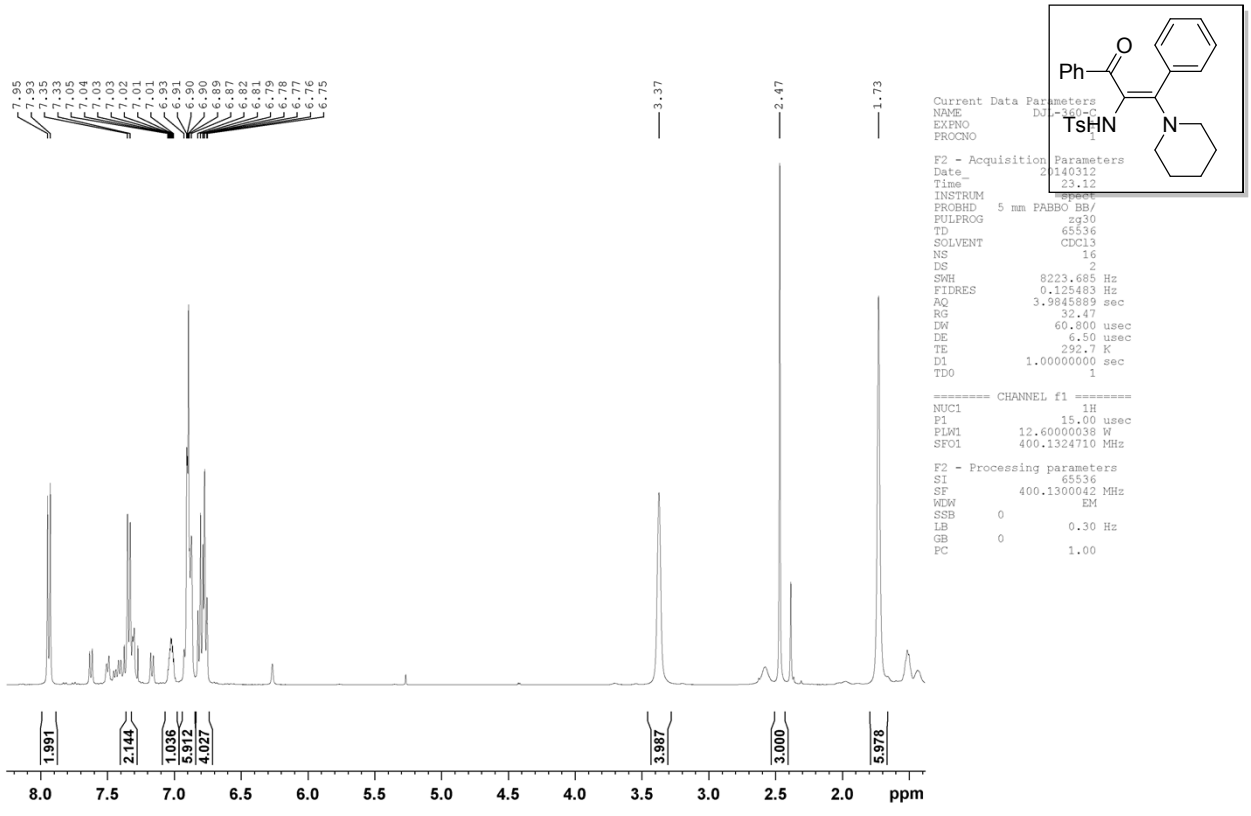



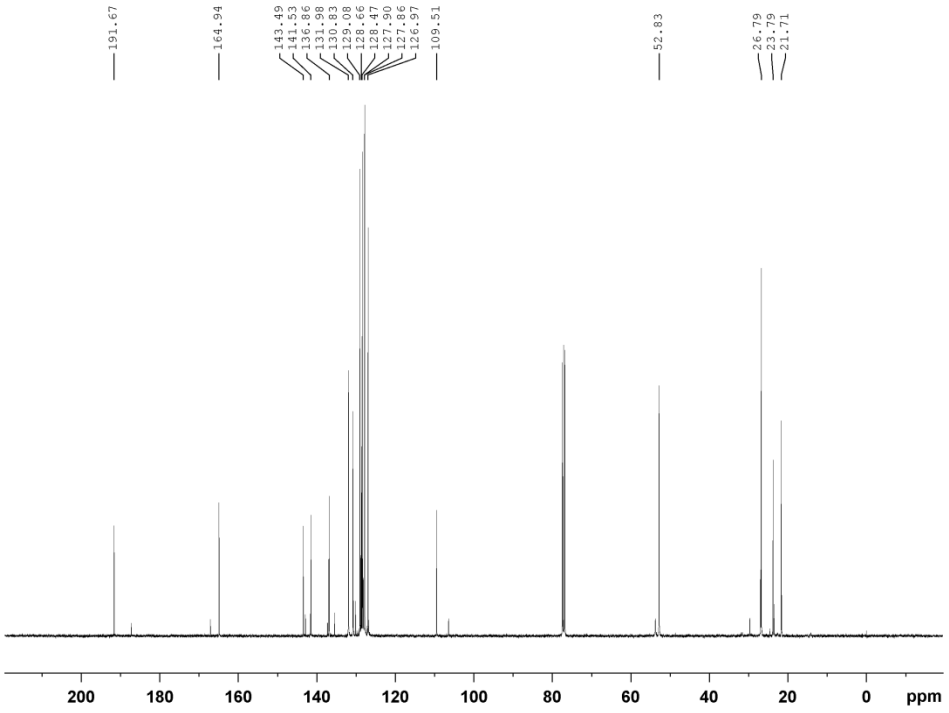

```
Current Data Parameters
NAME                 DJL-356-C
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_               20140309
Time                   18.24
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         2
SWH                 8223.685 Hz
FIDRES              0.125483 Hz
AQ                  3.9845889 sec
RG                      32.47
DW                    60.800 usec
DE                     6.50 usec
TE                    293.3 K
D1                  1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                       1H
P1                    15.00 usec
PLW1               12.60000038 W
SFO1               400.1324710 MHz

F2 - Processing parameters
SI                         65536
SF                 400.1300034 MHz
WDW                           EM
SSB             0
LB                      0.30 Hz
GB              0
PC                      1.00
```



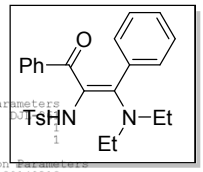

```
Current Data Parameters
NAME                 DJL-356-C
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_               20140310
Time                    4.05
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg30
TD                     65536
SOLVENT                CDCl3
NS                      1024
DS                         4
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                  1.3631488 sec
RG                     186.53
DW                    20.800 usec
DE                     6.50 usec
TE                    294.5 K
D1                  2.00000000 sec
d11                 0.03000000 sec
DELTA               1.89999998 sec
TD0                        1
SFO1               100.6228293 MHz
NUC1                      13C
P1                     9.98 usec
PLW1               52.09999847 W
SFO2               400.1316005 MHz
NUC2                       1H
CPDPRG[2              waltz16
PCPD2                 90.00 usec
PLW2               12.60000038 W
PLW12               0.34999999 W
PLW13               0.28349999 W

F2 - Processing parameters
SI                         32768
SF                 100.6127905 MHz
WDW                           EM
SSB             0
LB                      1.00 Hz
GB              0
PC                      1.40
```

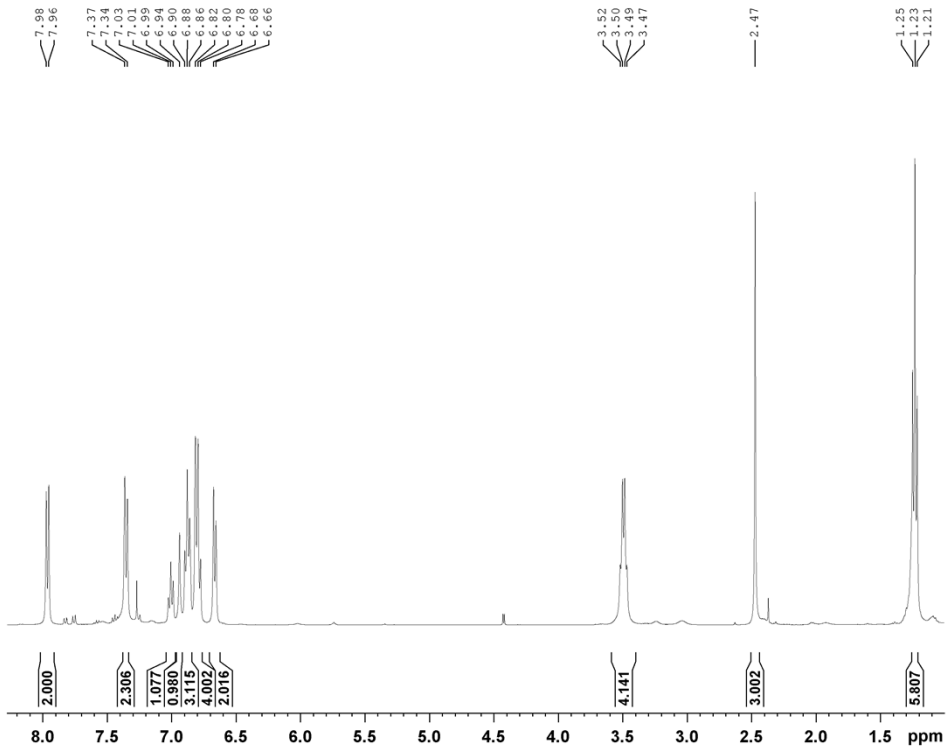
**(Z)-4-methyl-N-(3-oxo-1,3-diphenyl-1-(piperidin-1-yl)prop-1-en-2-yl)benzenesulfonamide (3p):**



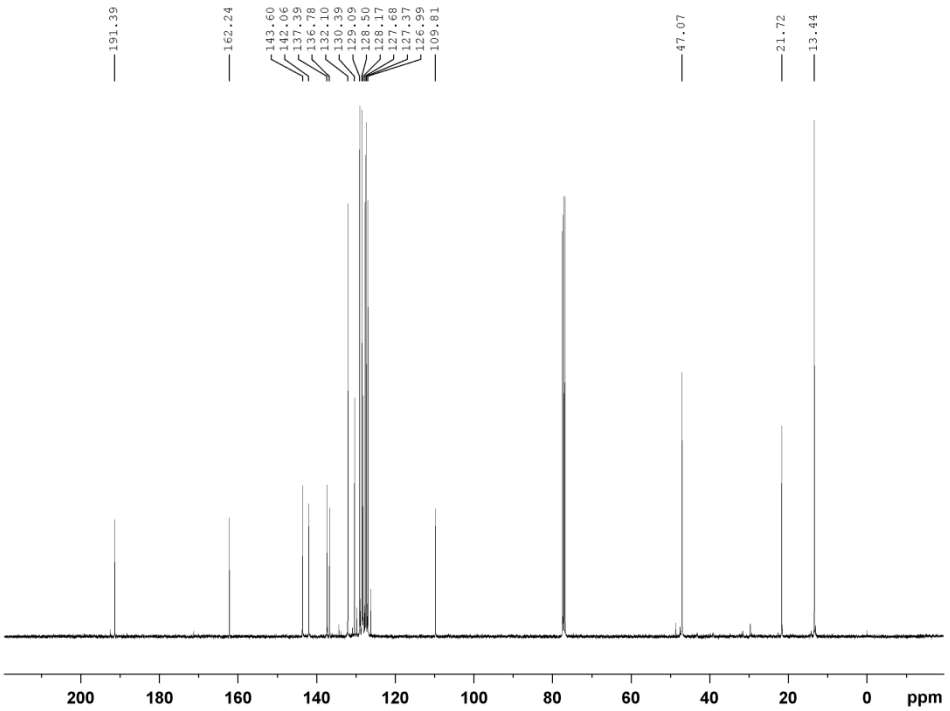



**(Z)-N-(1-(diethylamino)-3-oxo-1,3-diphenylprop-1-en-2-yl)-4-methylbenzenesulfonamide (3q):**



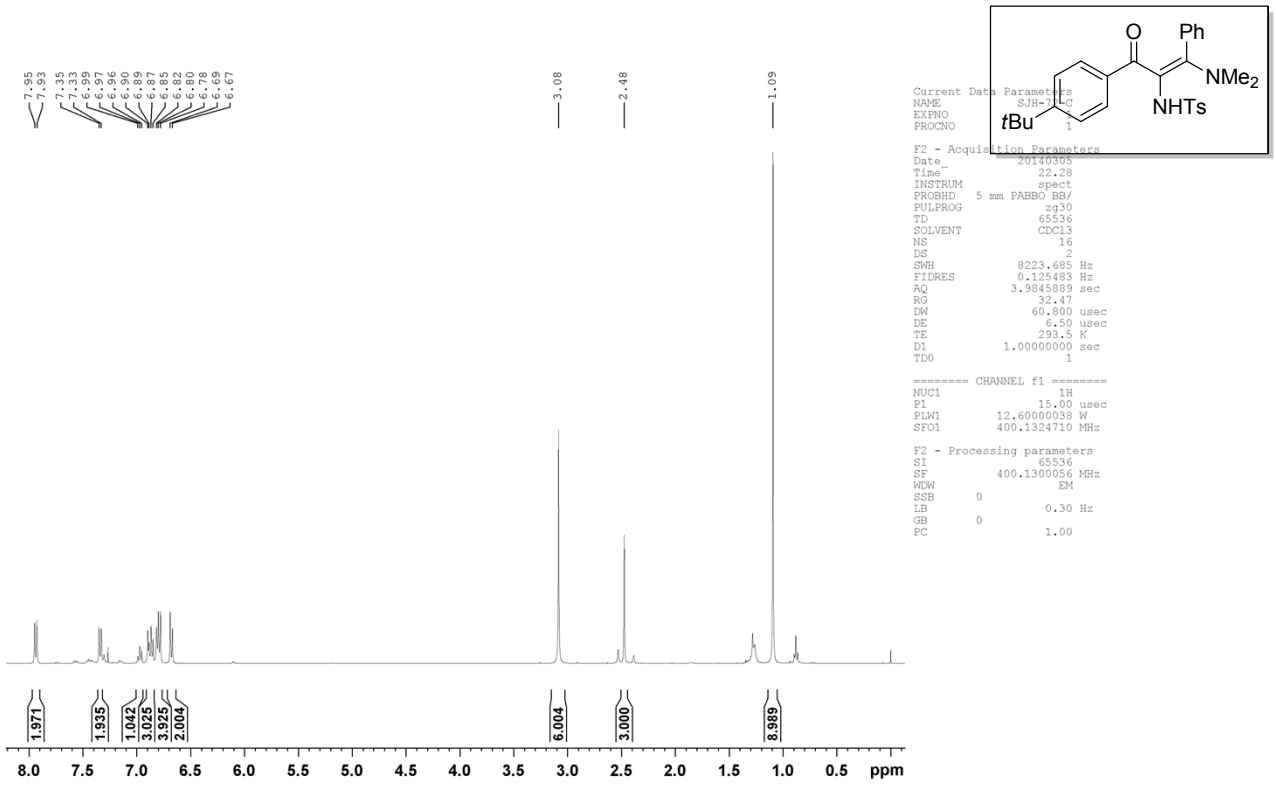




```
Current Data Parameters
NAME                  DJL-361
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20140312
Time                  23.22
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8223.685 Hz
FIDRES            0.125483 Hz
AQ                3.9845889 sec
RG                    32.47
DW                   60.800 usec
DE                    6.50 usec
TE                   292.9 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                    15.00 usec
PLW1             12.60000038 W
SFO1            400.1324710 MHz

F2 - Processing parameters
SI                        65536
SF               400.1300049 MHz
WDW                        EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```

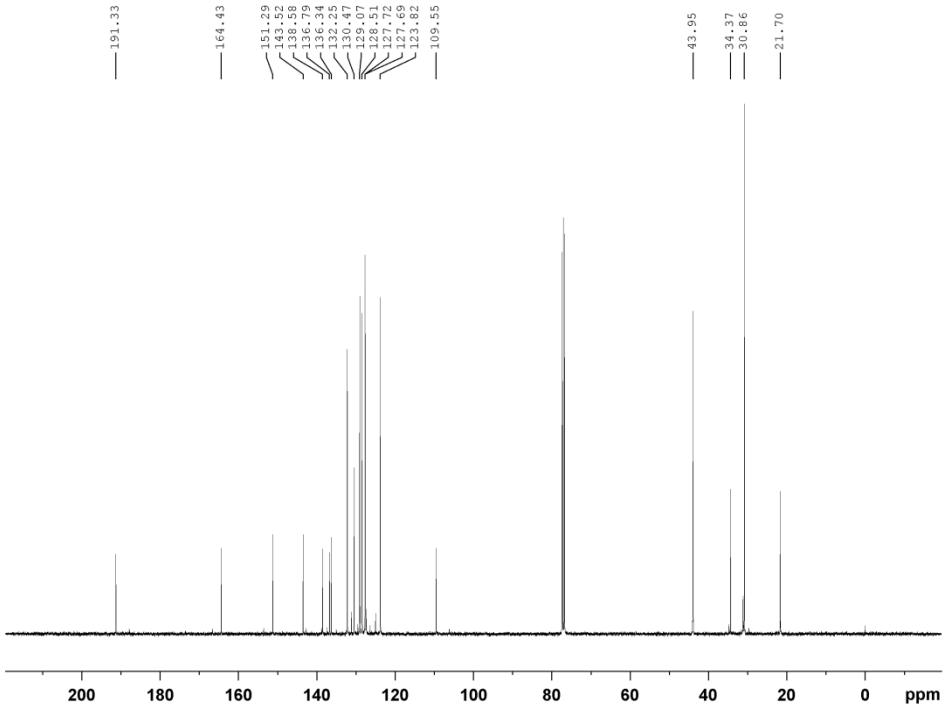



```
Current Data Parameters
NAME                  DJL-361
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_              20140313
Time                   1.01
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     1024
DS                        4
SWH               24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631488 sec
RG                   186.53
DW                   20.800 usec
DE                    6.50 usec
TE                   294.3 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                       1
SFO1            100.6228293 MHz
NUC1                     13C
P1                    9.98 usec
PLW1             52.09999847 W
SFO2            400.1316005 MHz
NUC2                      1H
CPDPRG[2             waltz16
PCPD2                 90.00 usec
PLW2             12.60000038 W
PLW12             0.34999999 W
PLW13             0.28349999 W

F2 - Processing parameters
SI                        32768
SF              100.6127690 MHz
WDW                        EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```

**(Z)-N-(3-(4-(tert-butyl)phenyl)-1-(dimethylamino)-3-oxo-1-phenylprop-1-en-2-yl)-4-methylbenzenesulfonamide (3r):**

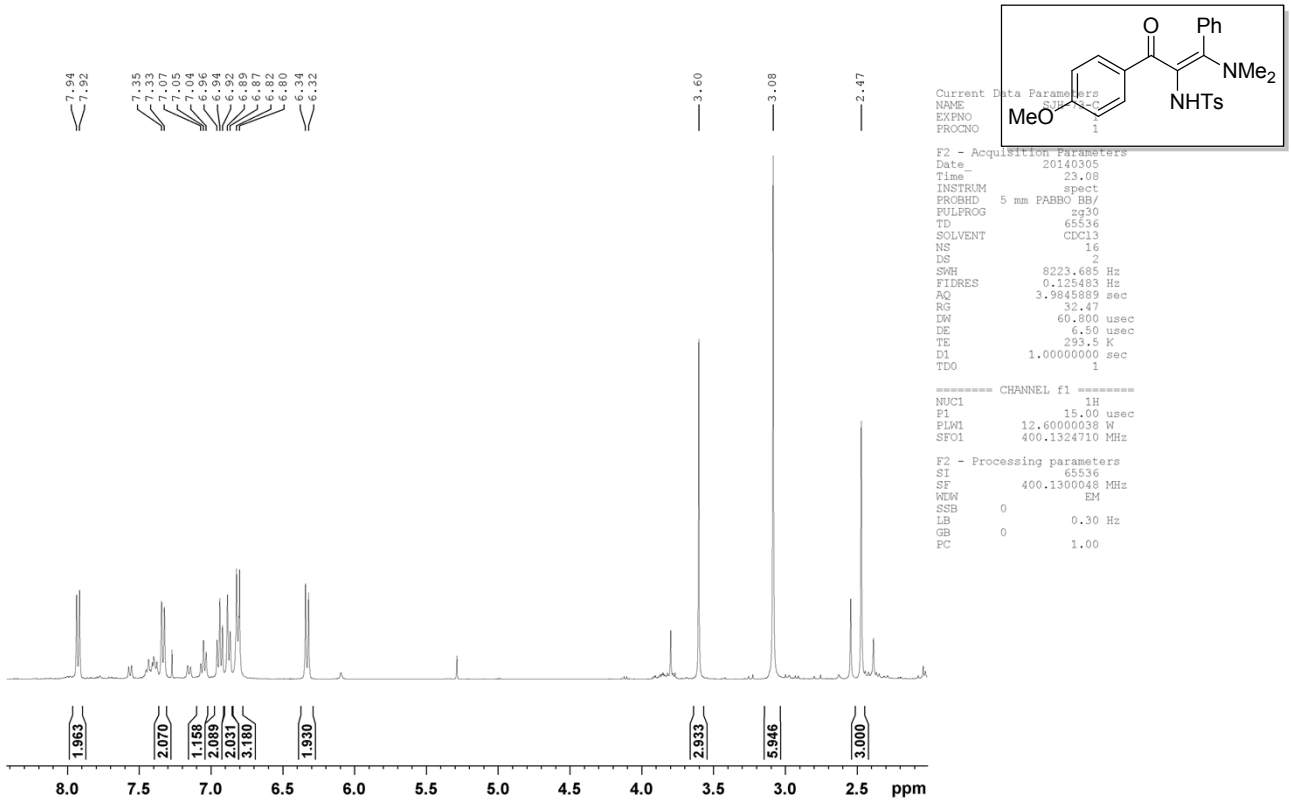


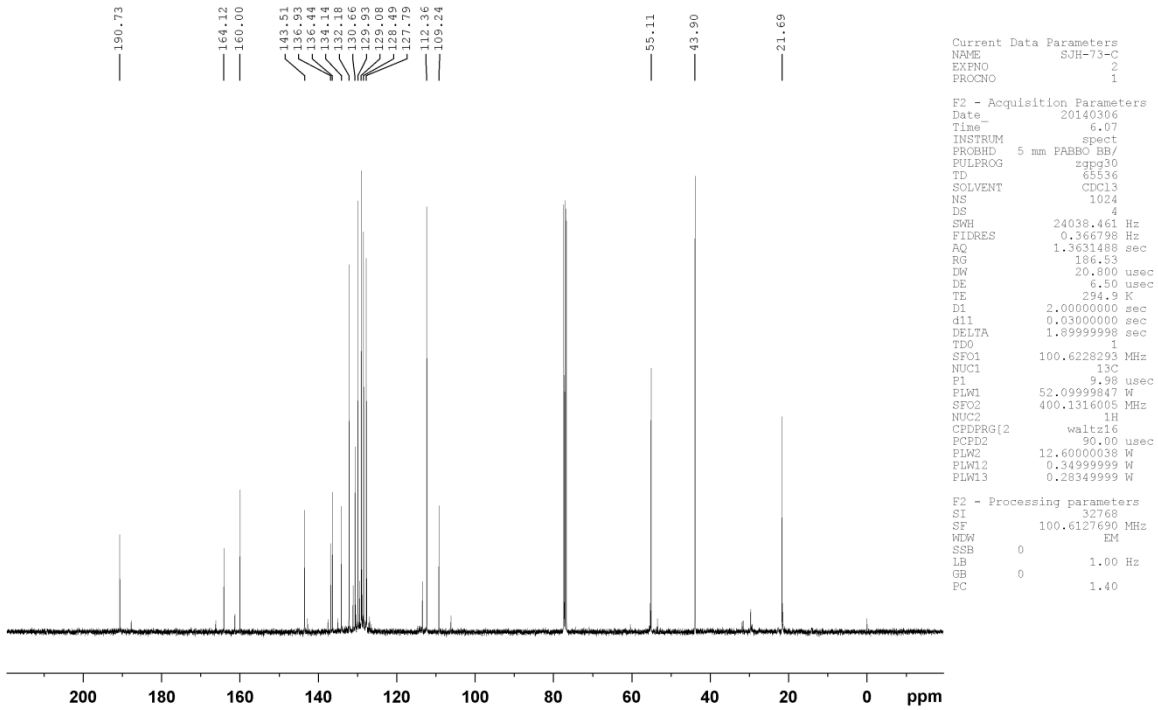

```
Current Data Parameters
NAME                 SJH-72-C
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_               20140305
Time                   22.28
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8223.685 Hz
FIDRES            0.125483 Hz
AQ                3.9845889 sec
RG                     32.47
DW                  60.800 usec
DE                   6.50 usec
TE                   293.5 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                     15.00 usec
PLW1            12.60000038 W
SFO1           400.1324710 MHz

F2 - Processing parameters
SI                    65536
SF               400.1300056 MHz
WDW                      EM
SSB          0
LB                    0.30 Hz
GB           0
PC                    1.00
```



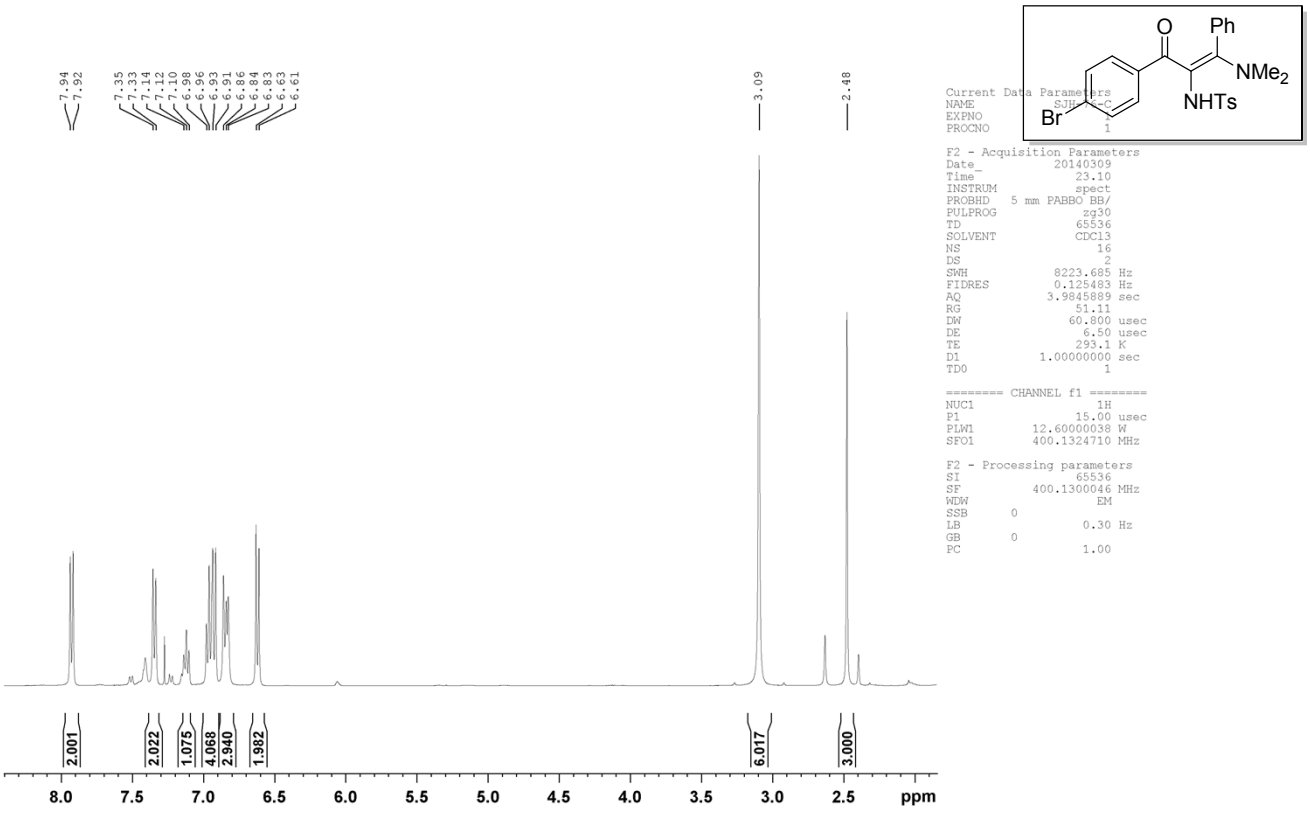

```
Current Data Parameters
NAME                 SJH-72-C
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_               20140306
Time                    5.05
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     1024
DS                        4
SWH               24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631488 sec
RG                    186.53
DW                  20.800 usec
DE                   6.50 usec
TE                   294.7 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                       1
SFO1           100.6228293 MHz
NUC1                    13C
P1                     9.98 usec
PLW1            52.09999847 W
SFO2           400.1316005 MHz
NUC2                      1H
CPDPRG[2          waltz16
PCPD2                90.00 usec
PLW2            12.60000038 W
PLW12            0.34999999 W
PLW13            0.28349999 W

F2 - Processing parameters
SI                    32768
SF               100.6127690 MHz
WDW                      EM
SSB          0
LB                    1.00 Hz
GB           0
PC                    1.40
```

**(Z)-N-(1-(dimethylamino)-3-(4-methoxyphenyl)-3-oxo-1-phenylprop-1-en-2-yl)-4-methylbenzenesulfonamide (3s):**

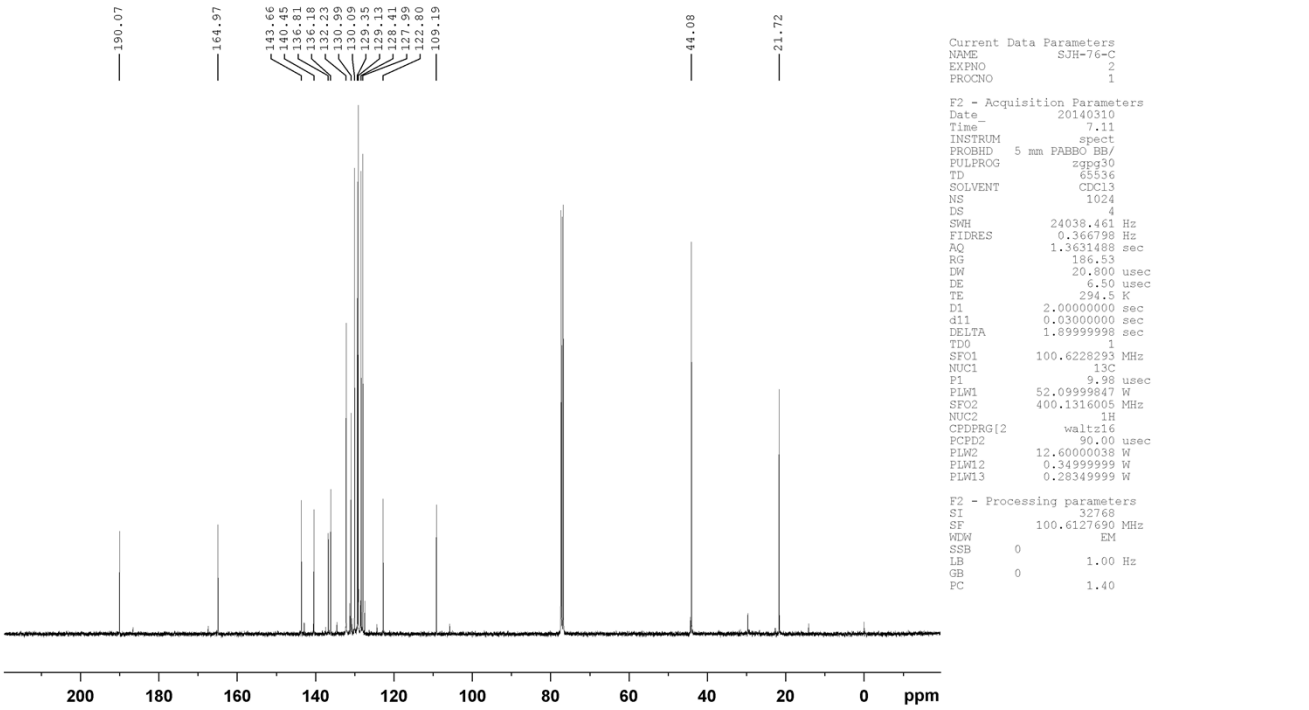


**(Z)-N-(3-(4-bromophenyl)-1-(dimethylamino)-3-oxo-1-phenylprop-1-en-2-yl)-4-methylbenzenesulfonamide (3t):**

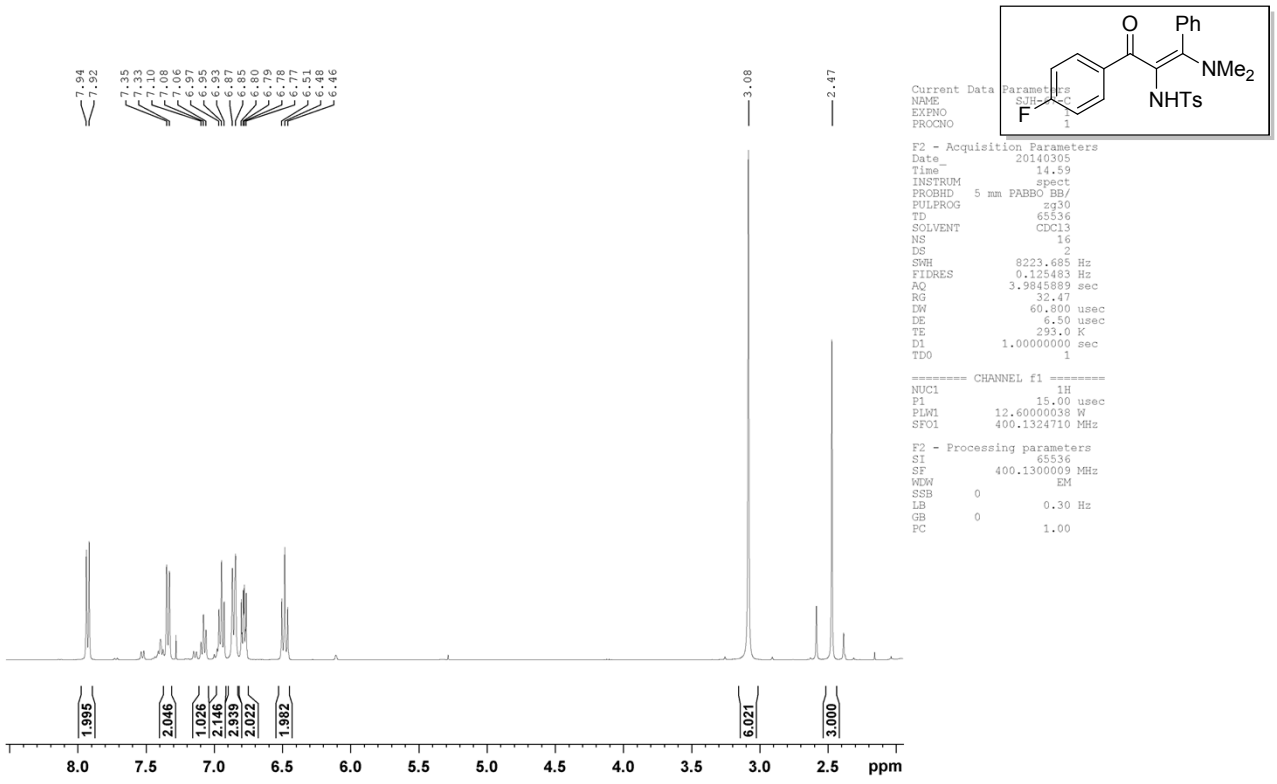



```
Current Data Parameters
NAME                 SJH-76-C
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_               20140309
Time                   23.10
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8223.685 Hz
FIDRES            0.125483 Hz
AQ                3.9845889 sec
RG                     51.11
DW                    60.800 usec
DE                     6.50 usec
TE                   293.1 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                     15.00 usec
PLW1             12.60000038 W
SFO1            400.1324710 MHz

F2 - Processing parameters
SI                    65536
SF               400.1300046 MHz
WDW                      EM
SSB          0
LB                    0.30 Hz
GB           0
PC                    1.00
```




```
Current Data Parameters
NAME                 SJH-76-C
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_               20140310
Time                    7.11
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     1024
DS                        4
SWH               24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631488 sec
RG                    186.53
DW                    20.800 usec
DE                     6.50 usec
TE                   294.5 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                       1
SFO1            100.6228293 MHz
NUC1                     13C
P1                     9.98 usec
PLW1             52.09999847 W
SFO2            400.1316005 MHz
NUC2                      1H
CPDPRG[2             waltz16
PCPD2                 90.00 usec
PLW2             12.60000038 W
PLW12             0.34999999 W
PLW13             0.28349999 W

F2 - Processing parameters
SI                    32768
SF               100.6127690 MHz
WDW                      EM
SSB          0
LB                    1.00 Hz
GB           0
PC                    1.40
```

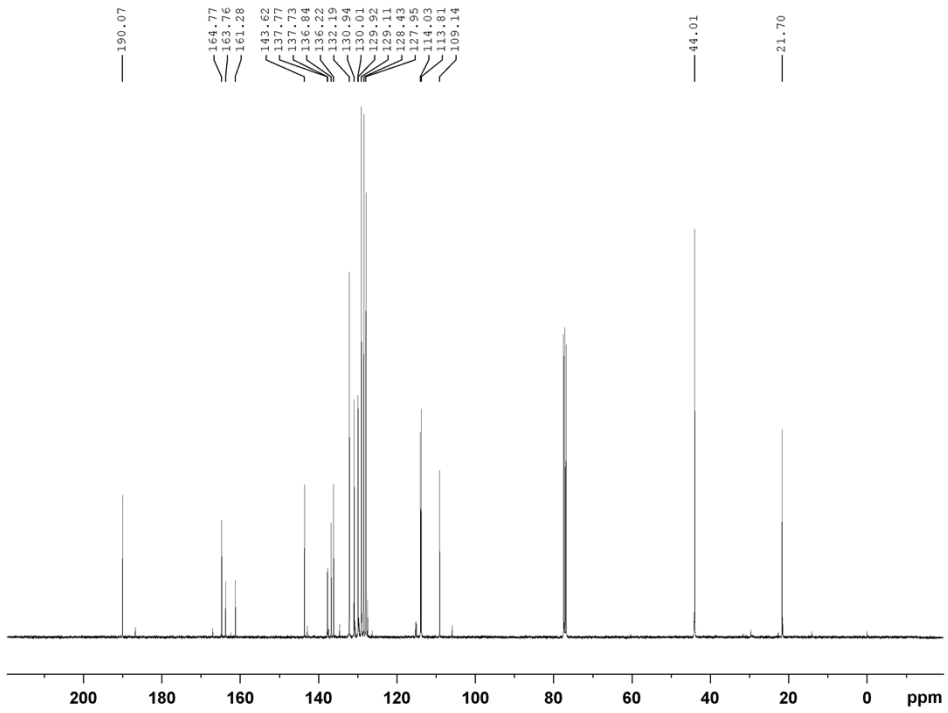
**(Z)-N-(1-(dimethylamino)-3-(4-fluorophenyl)-3-oxo-1-phenylprop-1-en-2-yl)-4-methylbenzenesulfonamide (3u):**





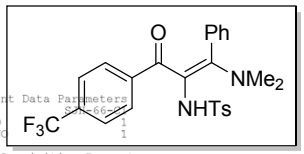


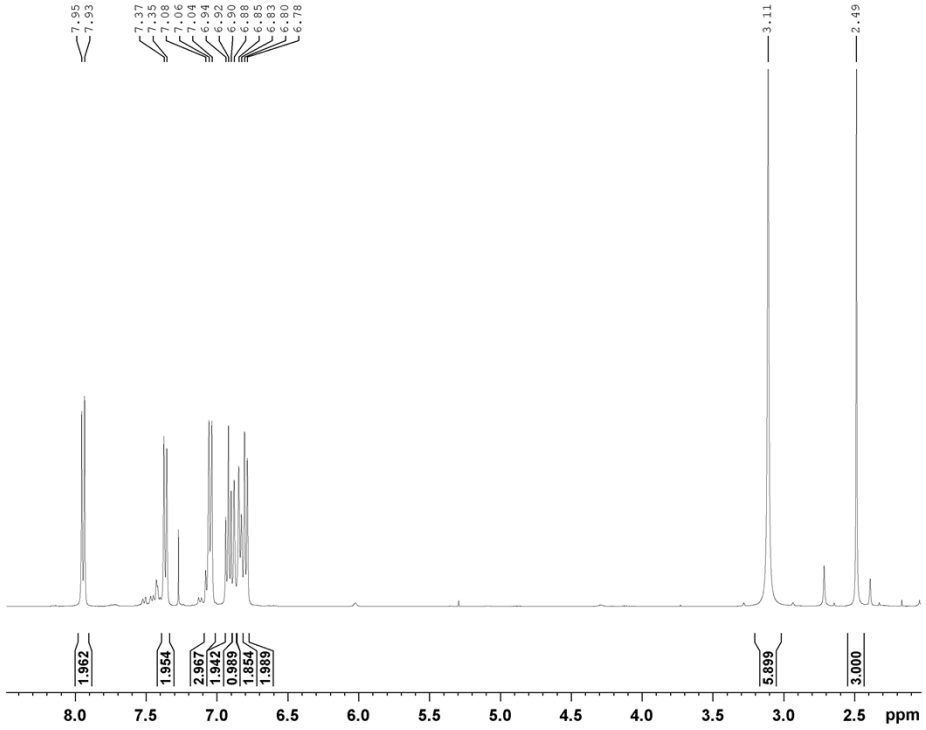
```
Current Data Parameters
NAME                  SJH-67-C
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_               20140305
Time                   14.59
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         2
SWH                 8223.685 Hz
FIDRES              0.125483 Hz
AQ                  3.9845889 sec
RG                      32.47
DW                     60.800 usec
DE                      6.50 usec
TE                     293.0 K
D1                  1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     15.00 usec
PLW1               12.60000038 W
SFO1               400.1324710 MHz

F2 - Processing parameters
SI                        65536
SF                 400.1300009 MHz
WDW                        EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```



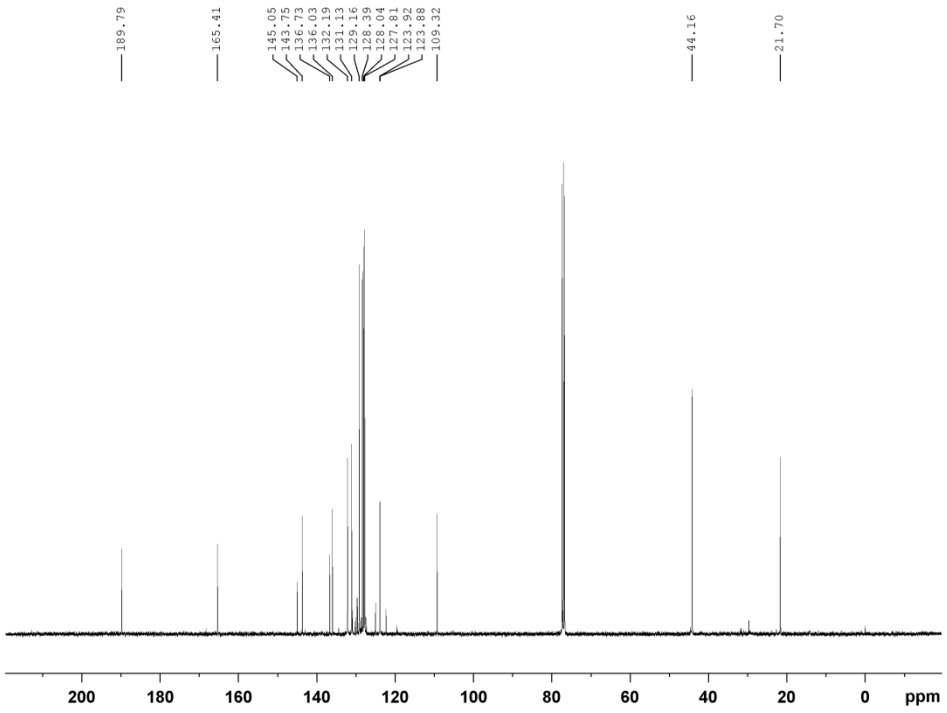

```
Current Data Parameters
NAME                  SJH-67-C
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_               20140305
Time                    6.01
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG               zgpg30
TD                     65536
SOLVENT                CDCl3
NS                      1024
DS                         4
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                  1.3631488 sec
RG                     186.53
DW                     20.800 usec
DE                      6.50 usec
TE                     294.2 K
D1                  2.00000000 sec
d11                 0.03000000 sec
DELTA               1.89999998 sec
TD0                        1
SFO1               100.6228293 MHz
NUC1                      13C
P1                      9.98 usec
PLW1               52.09999847 W
SFO2               400.1316005 MHz
NUC2                      1H
CPDPRG[2              waltz16
PCPD2                  90.00 usec
PLW2               12.60000038 W
PLW12               0.34999999 W
PLW13               0.28349999 W

F2 - Processing parameters
SI                        32768
SF                 100.6127690 MHz
WDW                        EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```

**(Z)-N-(1-(dimethylamino)-3-oxo-1-phenyl-3-(4-(trifluoromethyl)phenyl)prop-1-en-2-yl)-4-methylbenzenesulfonamide (3v):**



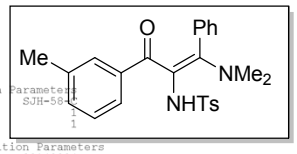



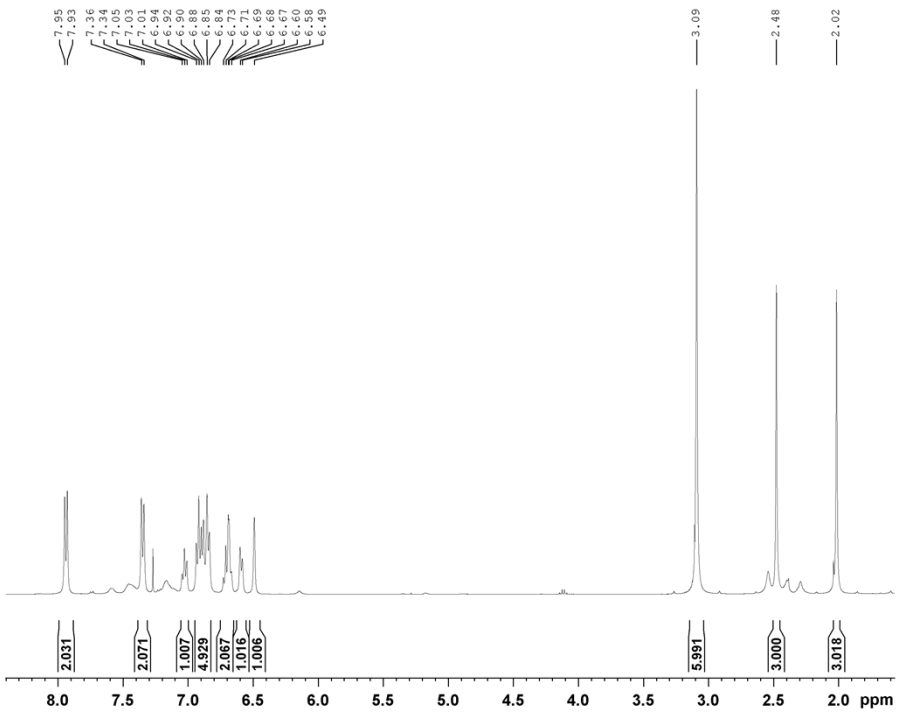

```
Current Data Parameters
NAME                  SJH-66-H1
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_               20140227
Time                   22.36
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                 8223.685 Hz
FIDRES              0.125483 Hz
AQ                  3.9845889 sec
RG                     54.15
DW                   60.800 usec
DE                    6.50 usec
TE                   293.0 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                     15.00 usec
PLW1             12.60000038 W
SFO1            400.1324710 MHz

F2 - Processing parameters
SI                    65536
SF               400.1300053 MHz
WDW                      EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```



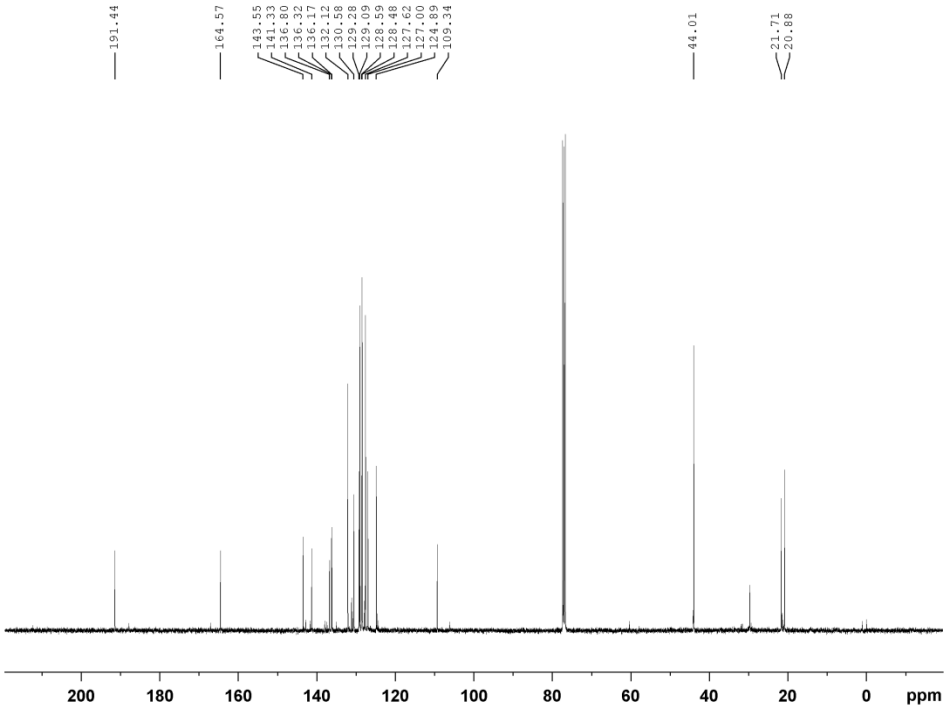

```
Current Data Parameters
NAME                  SJH-66-C1
EXPNO                         2
PROCNO                        1

F2 - Acquisition Parameters
Date_               20140228
Time                    4.03
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     1024
DS                        4
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                  1.3631488 sec
RG                     186.53
DW                   20.800 usec
DE                    6.50 usec
TE                   294.3 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
TD0                       1
SFO1            100.6228293 MHz
NUC1                     13C
P1                     9.98 usec
PLW1            52.09999847 W
SFO2            400.1316005 MHz
NUC2                      1H
CPDPRG[2             waltz16
PCPD2                 90.00 usec
PLW2             12.60000038 W
PLW12             0.34999999 W
PLW13             0.28349999 W

F2 - Processing parameters
SI                    32768
SF               100.6127690 MHz
WDW                      EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```

**(Z)-N-(1-(dimethylamino)-3-oxo-1-phenyl-3-(m-tolyl)prop-1-en-2-yl)-4-methylbenzenesulfonamide (3w):**



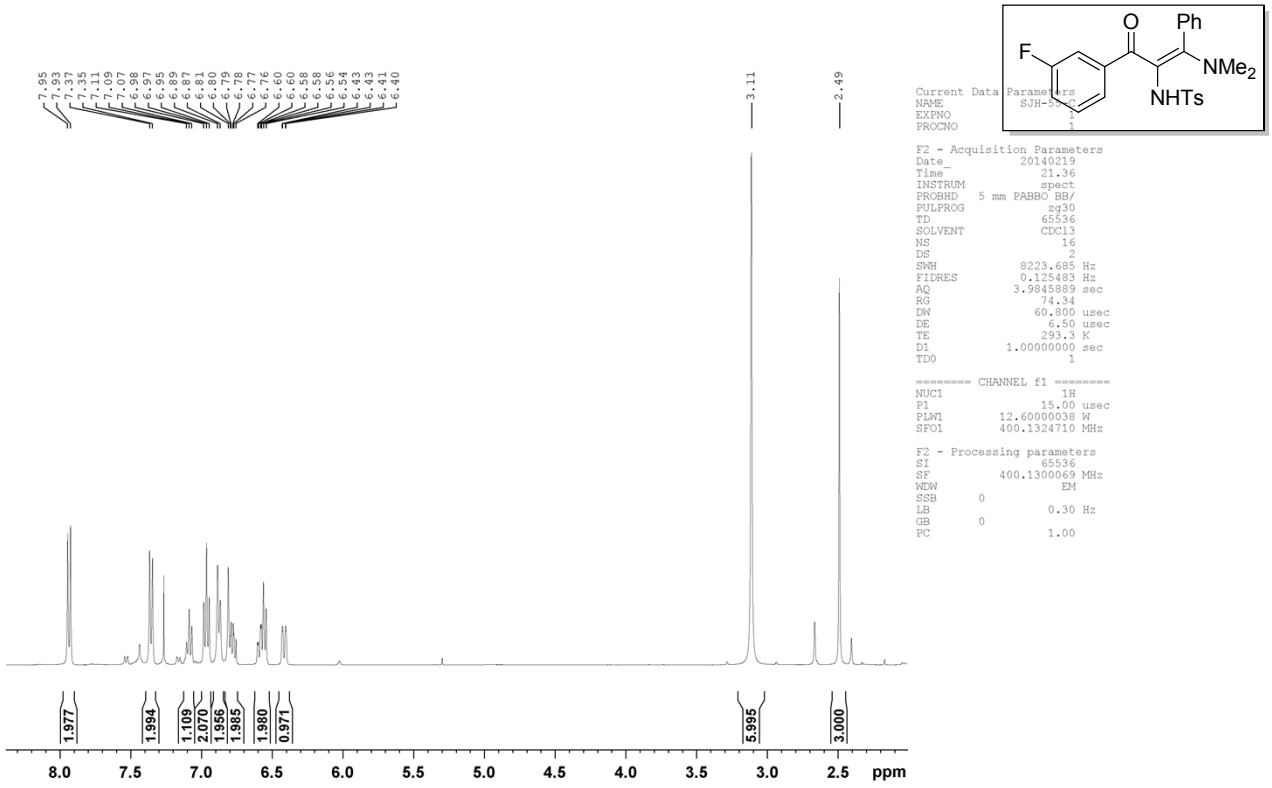



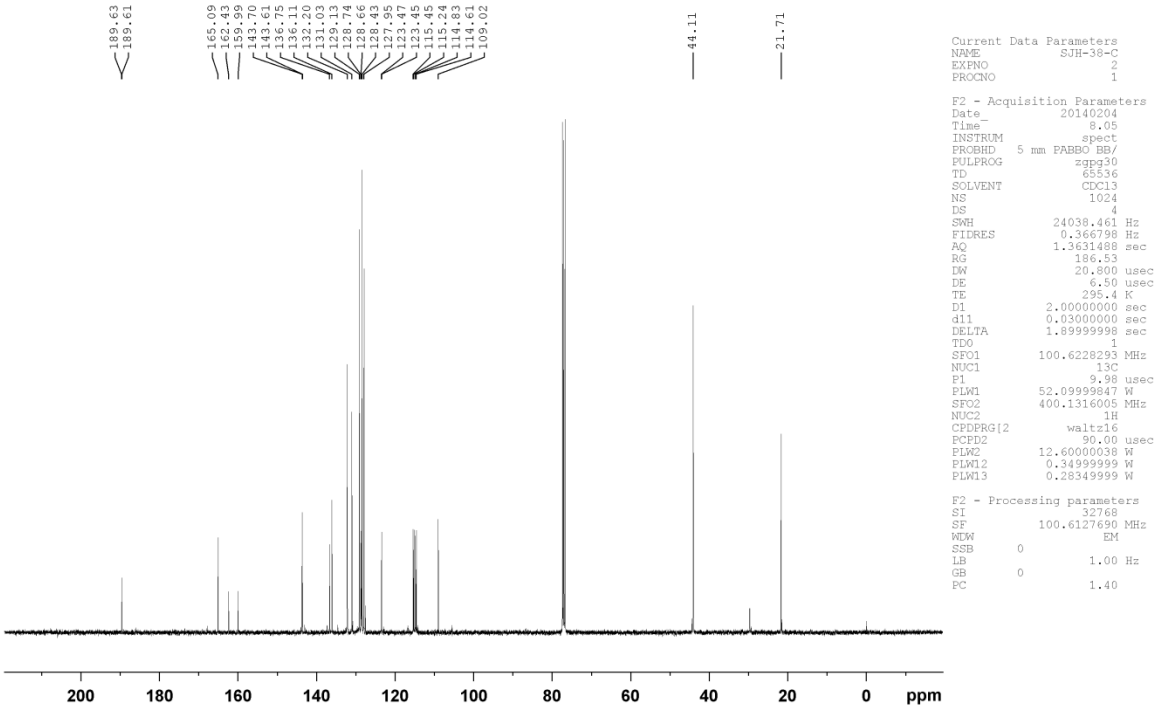

```
Current Data Parameters
NAME                  SJH-58-H
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_               20140224
Time                   22.14
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8223.685 Hz
FIDRES             0.125483 Hz
AQ                 3.9845889 sec
RG                     32.47
DW                   60.800 usec
DE                    6.50 usec
TE                   293.3 K
D1                 1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                     15.00 usec
PLW1              12.60000038 W
SFO1             400.1324710 MHz

F2 - Processing parameters
SI                        65536
SF                 400.1300058 MHz
WDW                       EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```



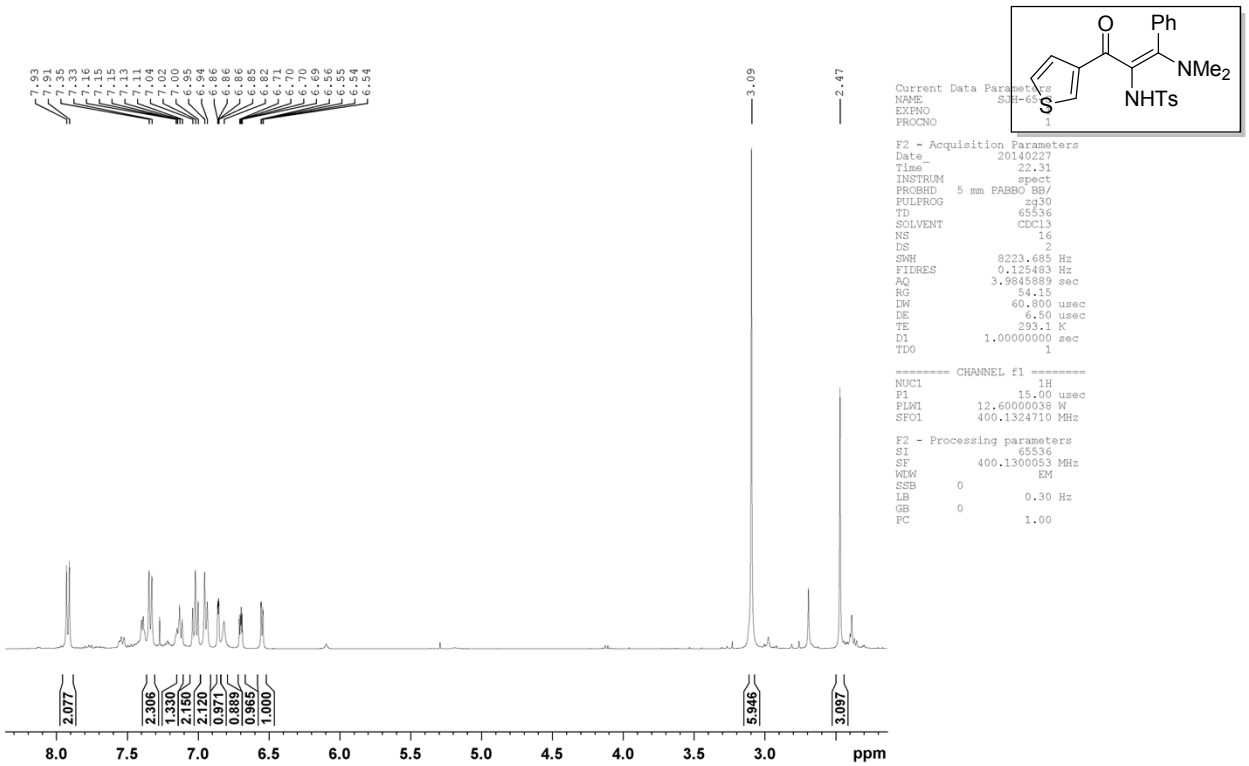

```
Current Data Parameters
NAME                  SJH-39-C
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_               20140204
Time                    4.05
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     1024
DS                        4
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631488 sec
RG                    186.53
DW                   20.800 usec
DE                    6.50 usec
TE                   295.5 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
TD0                       1
SFO1             100.6228293 MHz
NUC1                     13C
P1                     9.98 usec
PLW1              52.09999847 W
SFO2             400.1316005 MHz
NUC2                      1H
CPDPRG[2             waltz16
PCPD2                 90.00 usec
PLW2              12.60000038 W
PLW12              0.34999999 W
PLW13              0.28349999 W

F2 - Processing parameters
SI                        32768
SF                 100.6127690 MHz
WDW                       EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```

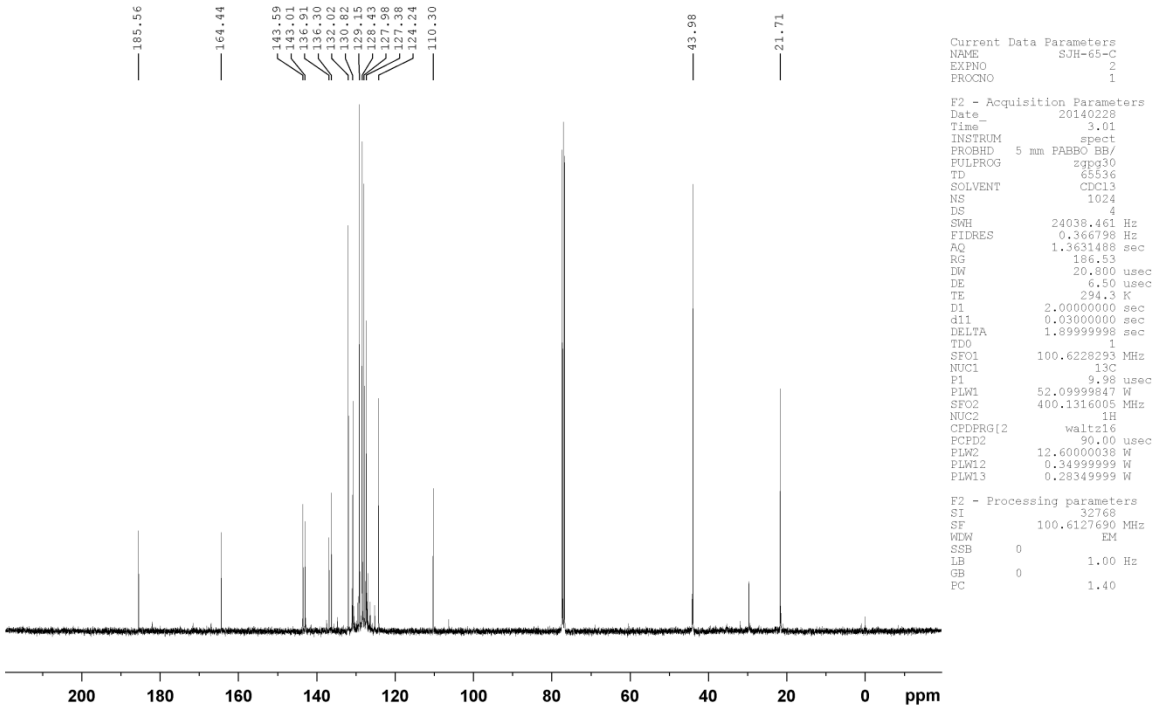
**(Z)-N-(1-(dimethylamino)-3-(3-fluorophenyl)-3-oxo-1-phenylprop-1-en-2-yl)-4-methylbenzenesulfonamide (3x):**



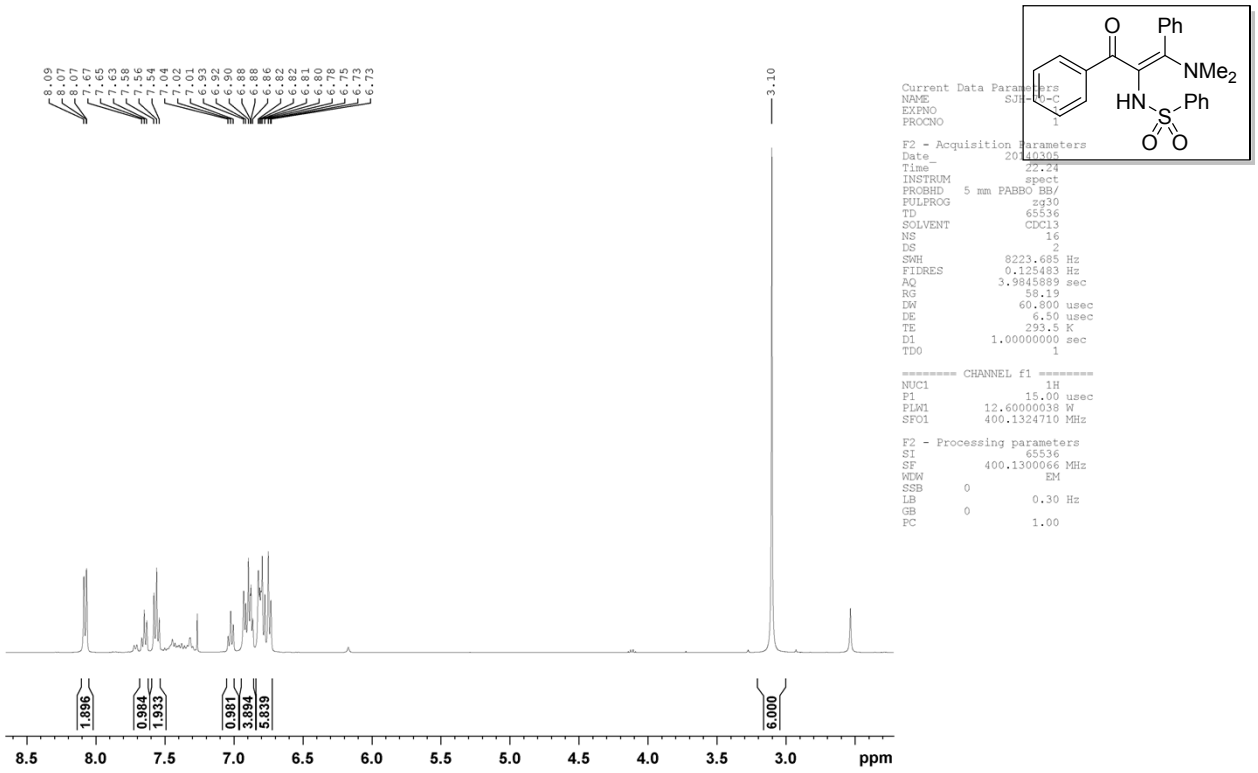



**(Z)-N-(1-(dimethylamino)-3-oxo-1-phenyl-3-(thiophen-3-yl)prop-1-en-2-yl)-4-methylbenzenesulfonamide (3y):**

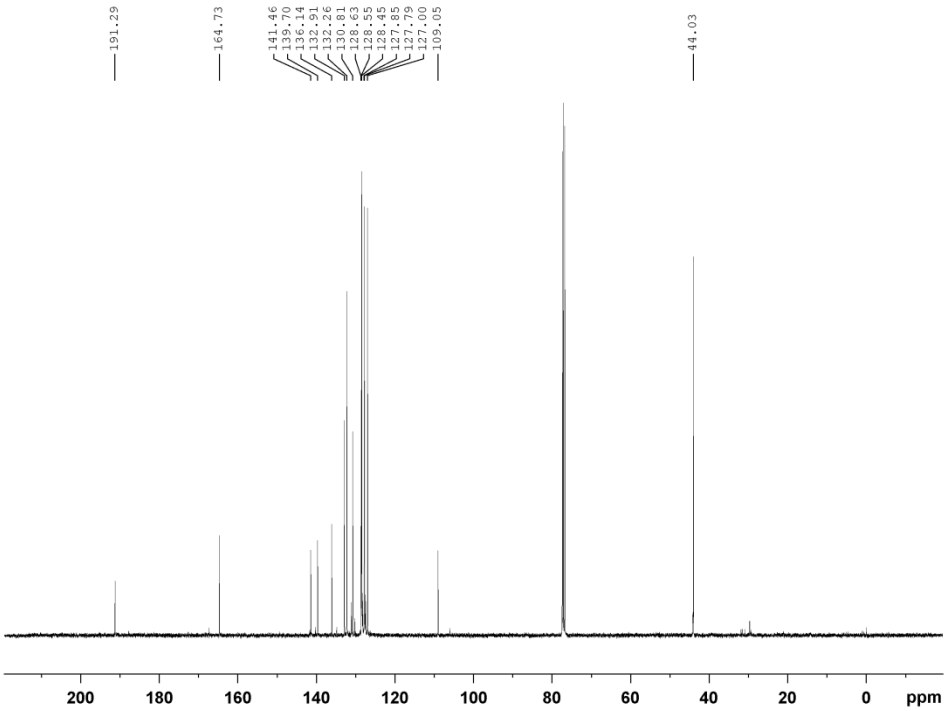


**(Z)-N-(1-(dimethylamino)-3-oxo-1,3-diphenylprop-1-en-2-yl)benzenesulfonamide (3z):**

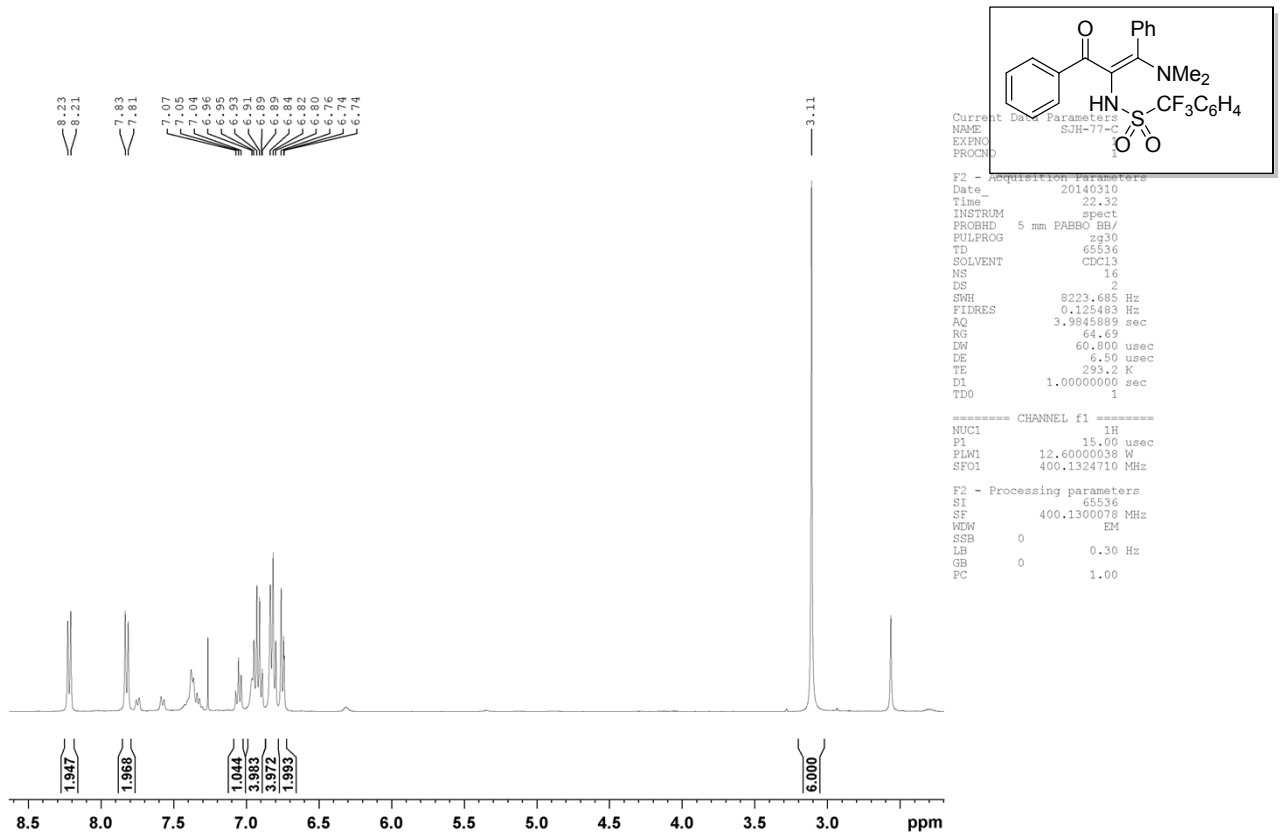



```
Current Data Parameters
NAME                  SJH-32-C
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_               20140305
Time                   22.24
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8223.685 Hz
FIDRES             0.125483 Hz
AQ                 3.9845889 sec
RG                     58.19
DW                   60.800 usec
DE                    6.50 usec
TE                   293.5 K
D1                 1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     1H
P1                    15.00 usec
PLW1           12.60000038 W
SFO1           400.1324710 MHz

F2 - Processing parameters
SI                    65536
SF               400.1300066 MHz
WDW                      EM
SSB          0
LB                    0.30 Hz
GB           0
PC                    1.00
```




```
Current Data Parameters
NAME                  SJH-32-C
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_               20140122
Time                    7.08
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     1024
DS                        4
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631488 sec
RG                    186.53
DW                   20.800 usec
DE                    6.50 usec
TE                   295.0 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
TD0                       1
SFO1           100.6228293 MHz
NUC1                     13C
P1                    9.98 usec
PLW1           52.09999847 W
SFO2           400.1316005 MHz
NUC2                     1H
CPDPRG[2          waltz16
PCPD2                90.00 usec
PLW2           12.60000038 W
PLW12           0.34999999 W
PLW13           0.28349999 W

F2 - Processing parameters
SI                    32768
SF               100.6127690 MHz
WDW                      EM
SSB          0
LB                    1.00 Hz
GB           0
PC                    1.40
```

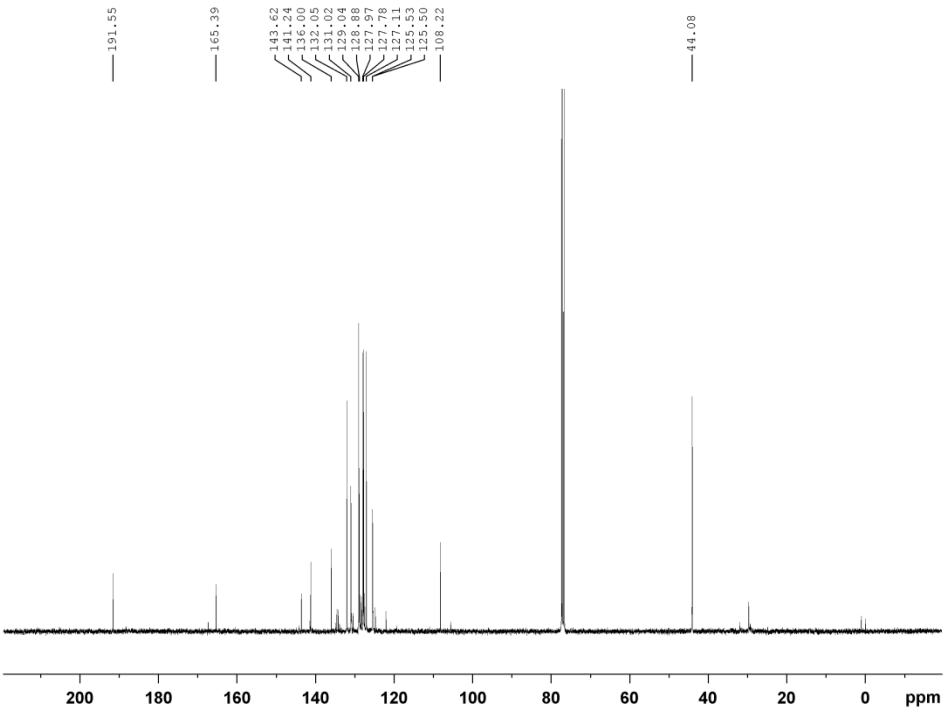
**(Z)-N-(1-(dimethylamino)-3-oxo-1,3-diphenylprop-1-en-2-yl)-4-(trifluoromethyl)benzenesulfonamide (3aa):**





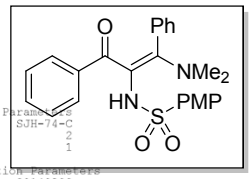


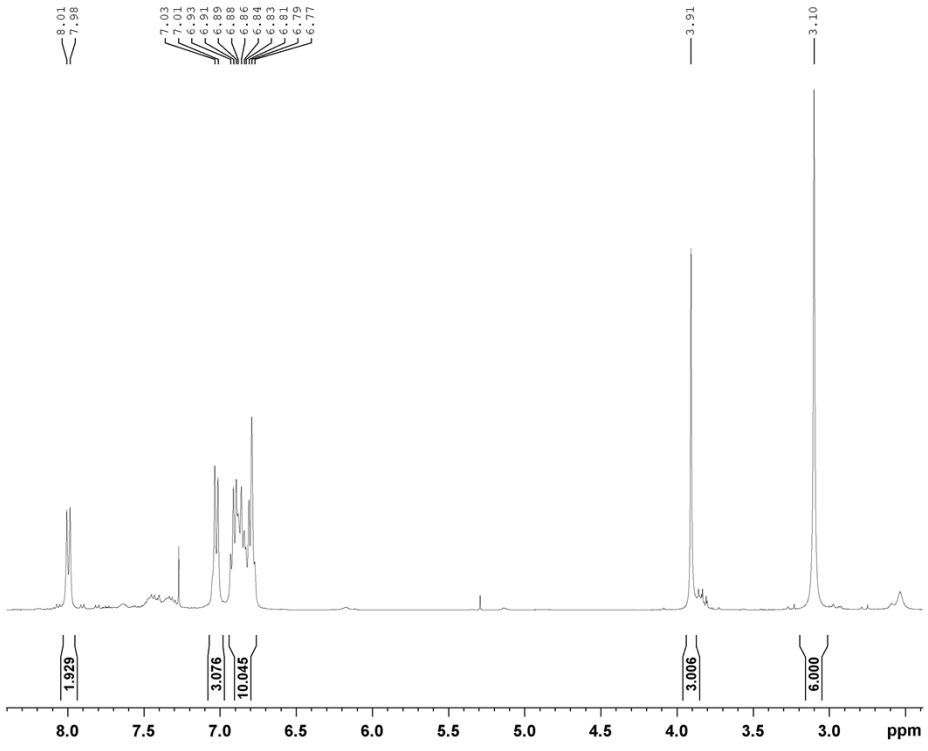
```
Current Data Parameters
NAME                  SJH-77-C
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_              20140310
Time                 22.32
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG              zg30
TD                  65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH                8223.685 Hz
FIDRES            0.125483 Hz
AQ                3.9845889 sec
RG                   64.69
DW                  60.800 usec
DE                   6.50 usec
TE                  293.2 K
D1                1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   15.00 usec
PLW1           12.60000038 W
SFO1           400.1324710 MHz

F2 - Processing parameters
SI                   65536
SF              400.1300078 MHz
WDW                     EM
SSB          0
LB                    0.30 Hz
GB           0
PC                    1.00
```



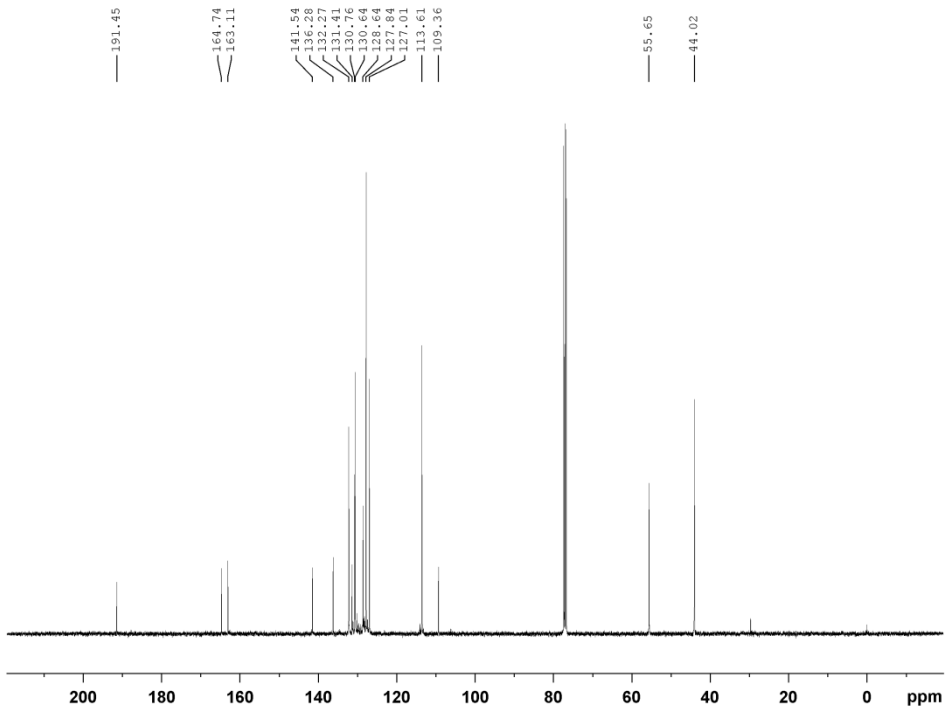

```
Current Data Parameters
NAME                  SJH-77-C
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_              20140311
Time                  4.08
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG           zgpg30
TD                  65536
SOLVENT              CDCl3
NS                    1024
DS                       4
SWH               24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631488 sec
RG                   186.53
DW                  20.800 usec
DE                   6.50 usec
TE                  294.6 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                      1
SFO1           100.6228293 MHz
NUC1                    13C
P1                   9.98 usec
PLW1           52.09999847 W
SFO2           400.1316005 MHz
NUC2                    1H
CPDPRG[2            waltz16
PCPD2                90.00 usec
PLW2           12.60000038 W
PLW12           0.34999999 W
PLW13           0.28349999 W

F2 - Processing parameters
SI                   32768
SF              100.6127690 MHz
WDW                     EM
SSB          0
LB                    1.00 Hz
GB           0
PC                    1.40
```

**(Z)-N-(1-(dimethylamino)-3-oxo-1,3-diphenylprop-1-en-2-yl)-4-methoxybenzenesulfonamide (3ab):**



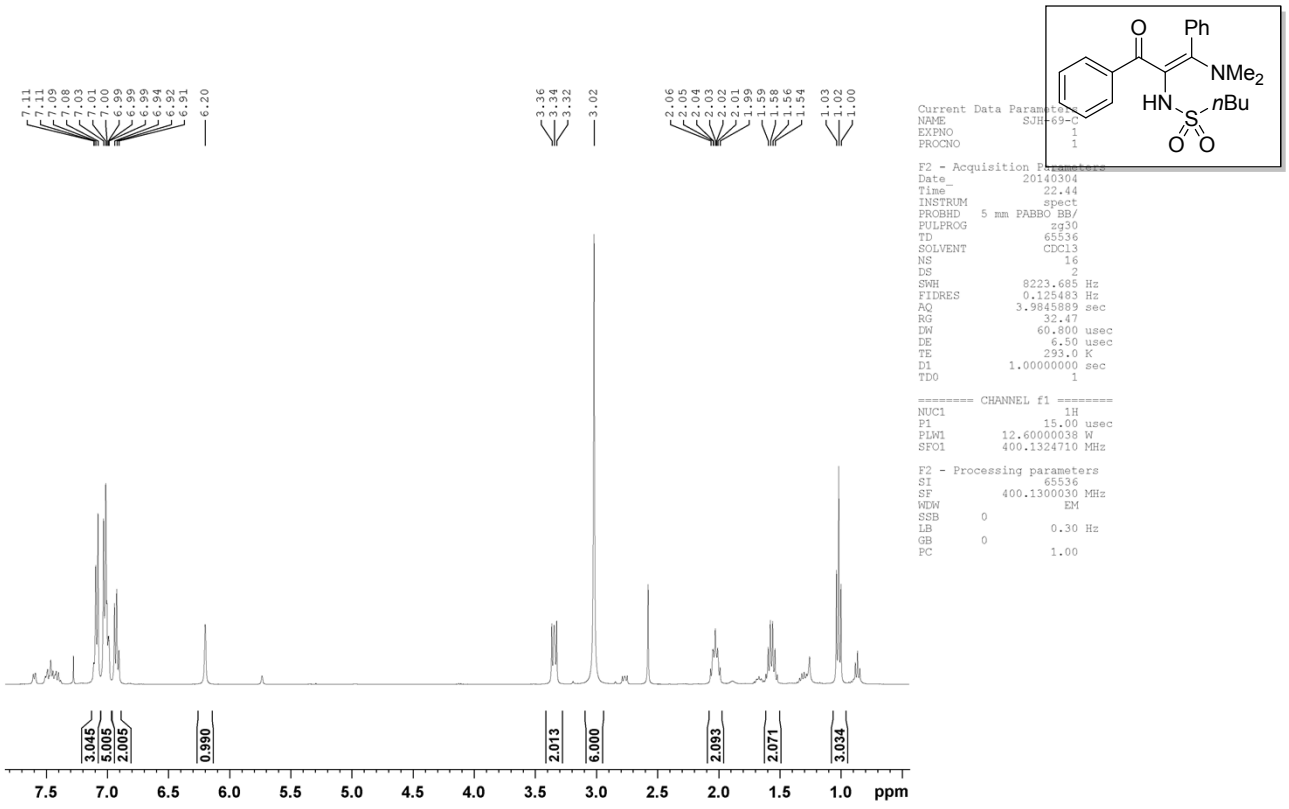




```
Current Data Parameters
NAME                  SJH-74-C
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_               20140309
Time                   23.01
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8223.685 Hz
FIDRES             0.125483 Hz
AQ                 3.9845889 sec
RG                     54.15
DW                   60.800 usec
DE                    6.50 usec
TE                   293.5 K
D1                 1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                      1H
P1                     15.00 usec
PLW1              12.60000038 W
SFO1              400.1324710 MHz

F2 - Processing parameters
SI                    65536
SF                400.1300058 MHz
WDW                      EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```

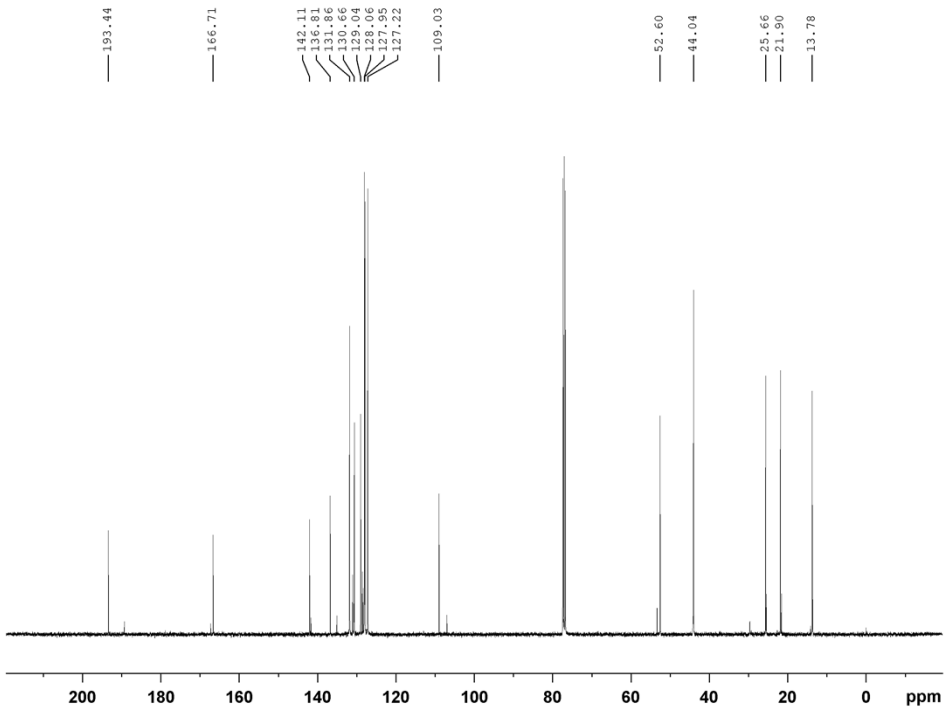



```
Current Data Parameters
NAME                  SJH-74-C
EXPNO                        3
PROCNO                       1

F2 - Acquisition Parameters
Date_               20140310
Time                    5.08
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     1024
DS                        4
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631488 sec
RG                    186.53
DW                   20.800 usec
DE                    6.50 usec
TE                   294.7 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
TD0                          1
SFO1              100.6228293 MHz
NUC1                      13C
P1                     9.98 usec
PLW1              52.09999847 W
SFO2              400.1316005 MHz
NUC2                      1H
CPDPRG[2             waltz16
PCPD2                 90.00 usec
PLW2              12.60000038 W
PLW12              0.34999999 W
PLW13              0.28349999 W

F2 - Processing parameters
SI                    32768
SF                100.6127690 MHz
WDW                      EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```

**(Z)-N-(1-(dimethylamino)-3-oxo-1,3-diphenylprop-1-en-2-yl)butane-1-sulfonamide (3ac):**

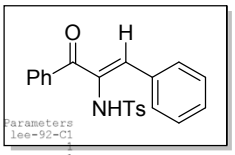


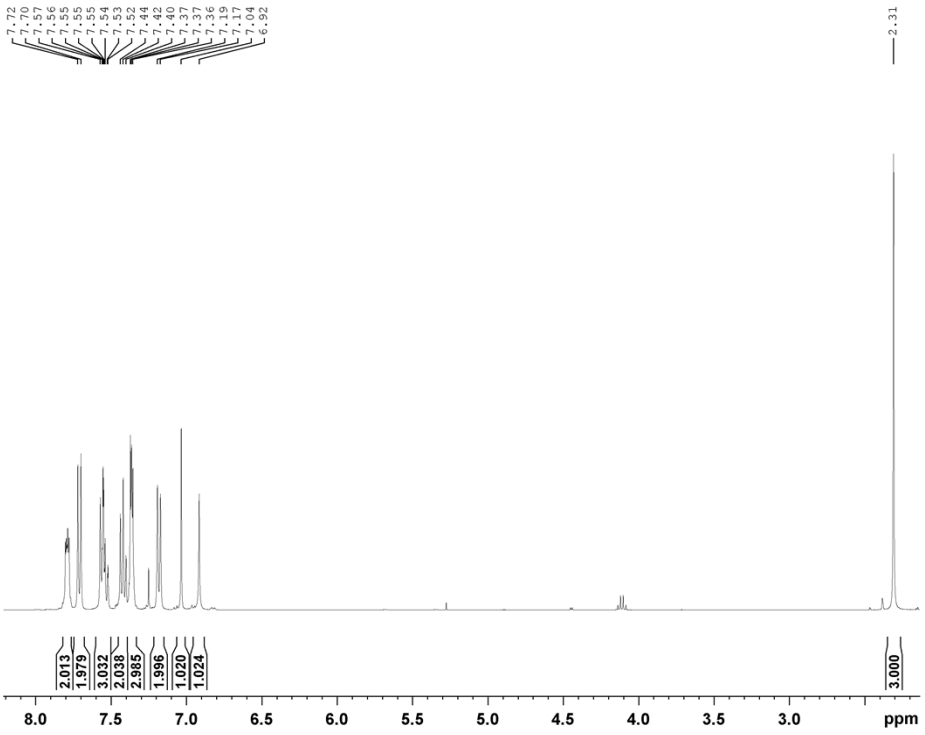

```
Current Data Parameters
NAME                 SJH-69-C
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_               20140304
Time_                  22.44
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8223.685 Hz
FIDRES             0.125483 Hz
AQ                 3.9845889 sec
RG                     32.47
DW                   60.800 usec
DE                    6.50 usec
TE                   293.0 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                     15.00 usec
PLW1             12.60000038 W
SFO1            400.1324710 MHz

F2 - Processing parameters
SI                    65536
SF               400.1300030 MHz
WDW                      EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```



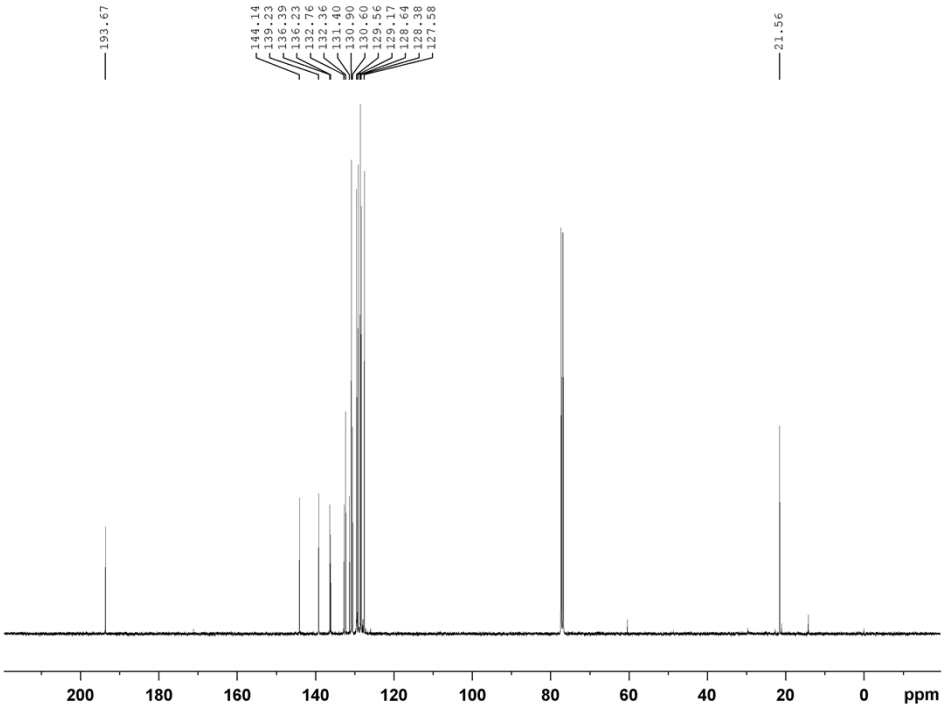

```
Current Data Parameters
NAME                 SJH-69-C
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_               20140305
Time_                   3.01
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     1024
DS                        4
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631488 sec
RG                    186.53
DW                   20.800 usec
DE                    6.50 usec
TE                   293.9 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                       1
SFO1            100.6228293 MHz
NUC1                     13C
P1                     9.98 usec
PLW1             52.09999847 W
SFO2            400.1316005 MHz
NUC2                      1H
CPDPRG[2              waltz16
PCPD2                 90.00 usec
PLW2             12.60000038 W
PLW12             0.34999999 W
PLW13             0.28349999 W

F2 - Processing parameters
SI                    32768
SF               100.6127690 MHz
WDW                      EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```

**(Z)-4-methyl-N-(3-oxo-1,3-diphenylprop-1-en-2-yl)benzenesulfonamide (4a):**



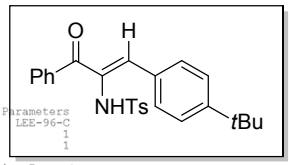



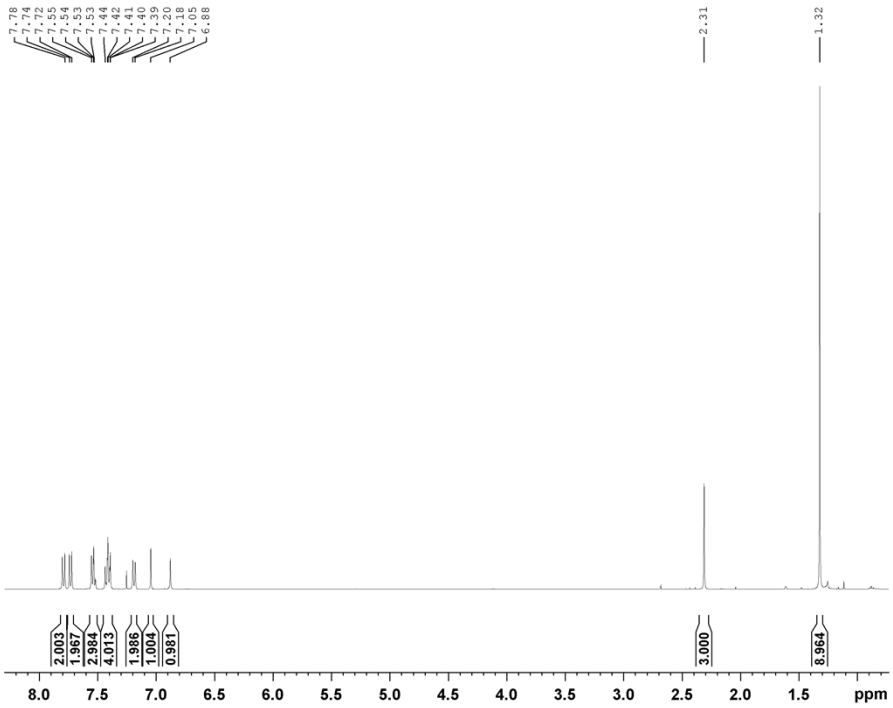

```
Current Data Parameters
NAME                  lee-92-C1
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_               20140305
Time                   19.22
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                        8
DS                        2
SWH                8223.685 Hz
FIDRES            0.125483 Hz
AQ                3.9845889 sec
RG                     54.15
DW                   60.800 usec
DE                    6.50 usec
TE                   293.3 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                    1H
P1                   15.00 usec
PLW1           12.60000038 W
SFO1          400.1324710 MHz

F2 - Processing parameters
SI                    65536
SF            400.1300130 MHz
WDW                     EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
```



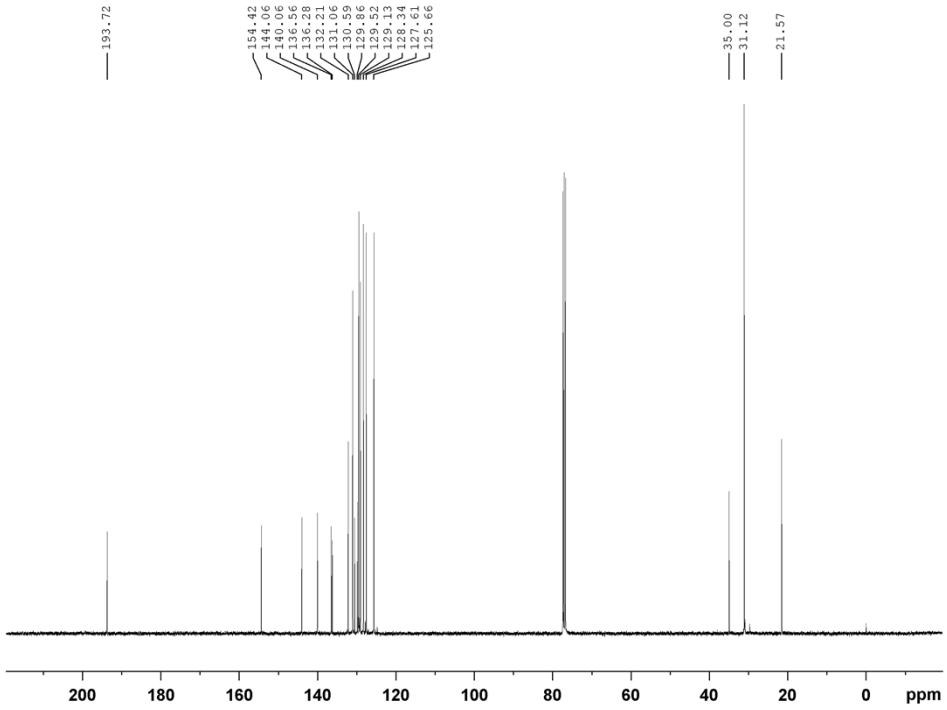

```
Current Data Parameters
NAME                  lee-92-C1
EXPNO                         2
PROCNO                        1

F2 - Acquisition Parameters
Date_               20140306
Time                    1.01
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     1024
DS                        4
SWH               24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631488 sec
RG                    186.53
DW                   20.800 usec
DE                    6.50 usec
TE                   294.7 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                       1
SFO1          100.6228293 MHz
NUC1                   13C
P1                    9.98 usec
PLW1           52.09999847 W
SFO2          400.1316005 MHz
NUC2                   1H
CPDPRG[2         waltz16
PCPD2                90.00 usec
PLW2           12.60000038 W
PLW12           0.34999999 W
PLW13           0.28349999 W

F2 - Processing parameters
SI                    32768
SF            100.6127690 MHz
WDW                     EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```

**(Z)-N-(1-(4-(tert-butyl)phenyl)-3-oxo-3-phenylprop-1-en-2-yl)-4-methylbenzenesulfonamide (4b):**



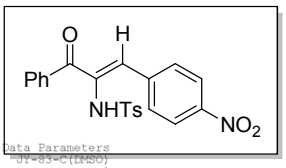



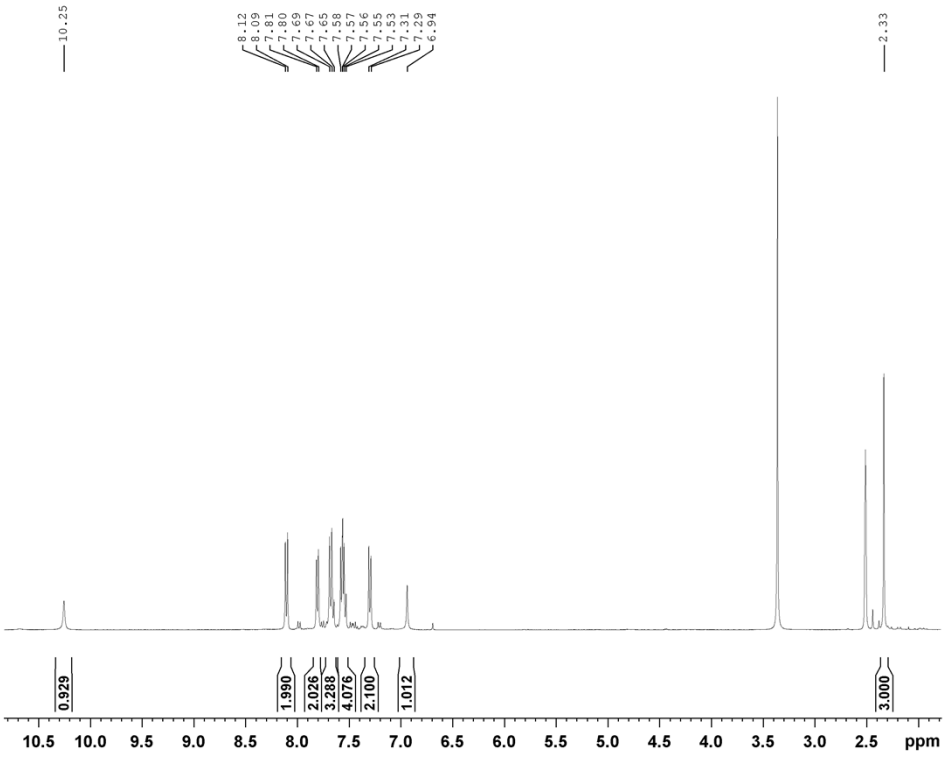

```
Current Data Parameters
NAME                 LEE-96-C
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_               20140314
Time                   19.10
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8223.685 Hz
FIDRES             0.125483 Hz
AQ                 3.9845889 sec
RG                      64.69
DW                    60.800 usec
DE                     6.50 usec
TE                    293.7 K
D1                 1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                     15.00 usec
PLW1              12.60000038 W
SFO1             400.1324710 MHz

F2 - Processing parameters
SI                        65536
SF                400.1300120 MHz
WDW                        EM
SSB           0
LB                     0.30 Hz
GB            0
PC                     1.00
```



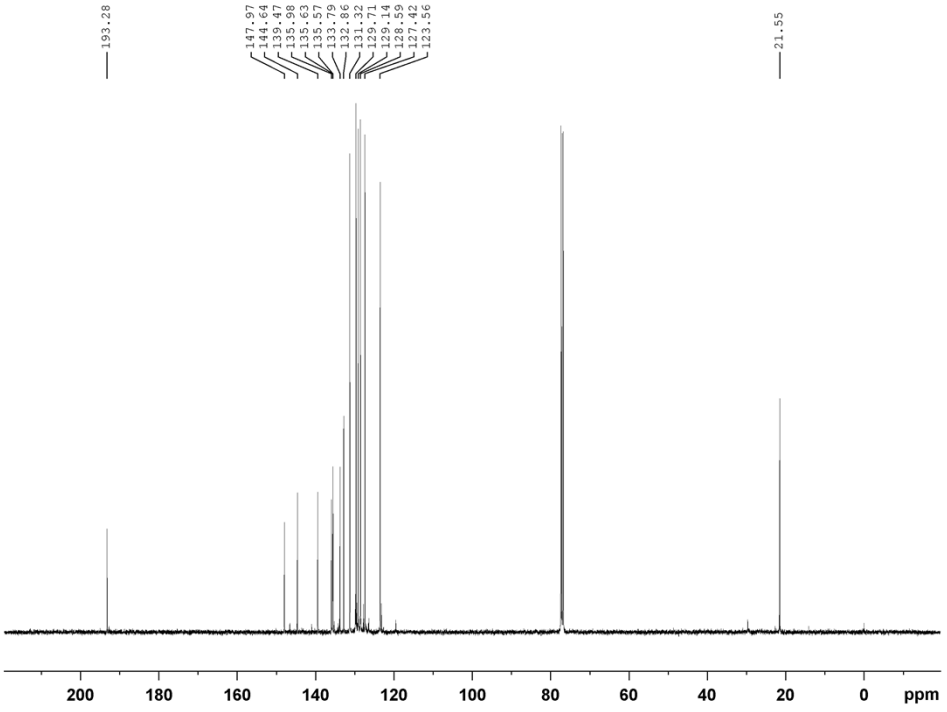

```
Current Data Parameters
NAME              lee-96-C(2)
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_               20140316
Time                    8.02
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     1024
DS                        4
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631488 sec
RG                    186.53
DW                    20.800 usec
DE                     6.50 usec
TE                    294.6 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
TD0                       1
SFO1             100.6228293 MHz
NUC1                     13C
P1                     9.98 usec
PLW1              52.09999847 W
SFO2             400.1316005 MHz
NUC2                      1H
CPDPRG[2             waltz16
PCPD2                 90.00 usec
PLW2              12.60000038 W
PLW12              0.34999999 W
PLW13              0.28349999 W

F2 - Processing parameters
SI                        32768
SF               100.6127690 MHz
WDW                        EM
SSB           0
LB                     1.00 Hz
GB            0
PC                     1.40
```

**(Z)-4-methyl-N-(1-(4-nitrophenyl)-3-oxo-3-phenylprop-1-en-2-yl)benzenesulfonamide (4c):**



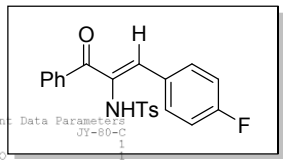



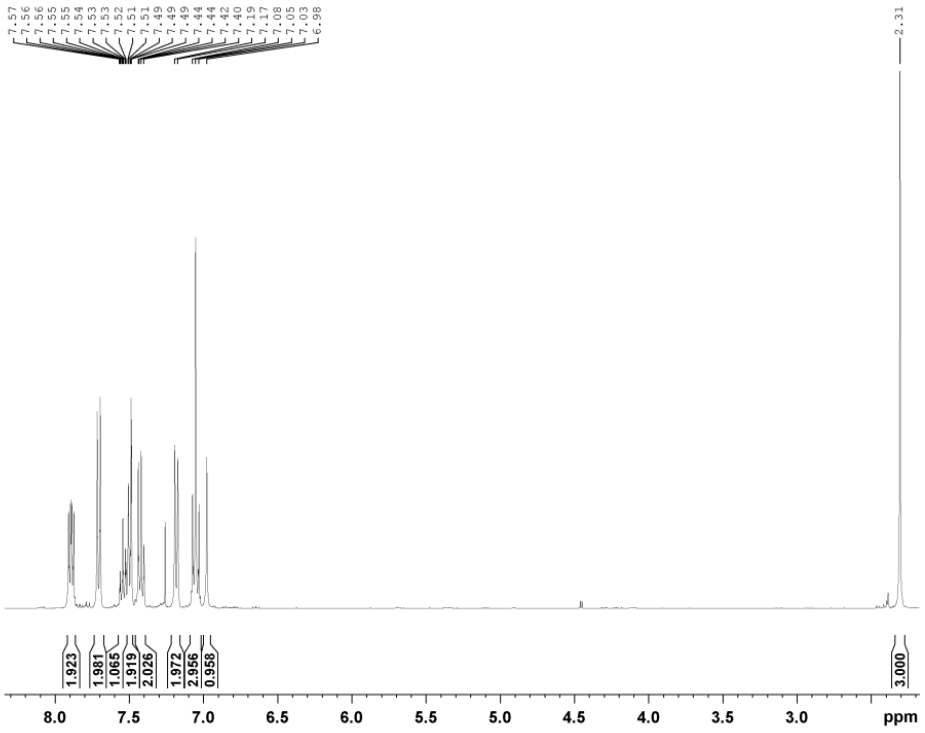

```
Current Data Parameters
NAME                  JY-83-C(DMSO)
EXPNO                             1
PROCNO                            1

F2 - Acquisition Parameters
Date_                      20140316
Time                          22.43
INSTRUM                       spect
PROBHD    5 mm PABBO BB/
PULPROG                       zg30
TD                           65536
SOLVENT                       DMSO
NS                              16
DS                               2
SWH                       8223.685 Hz
FIDRES                    0.125483 Hz
AQ                        3.9845889 sec
RG                           127.32
DW                           60.800 usec
DE                            6.50 usec
TE                           293.0 K
D1                        1.00000000 sec
TD0                               1

======== CHANNEL f1 ========
NUC1                             1H
P1                            15.00 usec
PLW1                   12.60000038 W
SFO1                  400.1324710 MHz

F2 - Processing parameters
SI                           65536
SF                    400.1300000 MHz
WDW                             EM
SSB                0
LB                            0.30 Hz
GB                 0
PC                            1.00
```



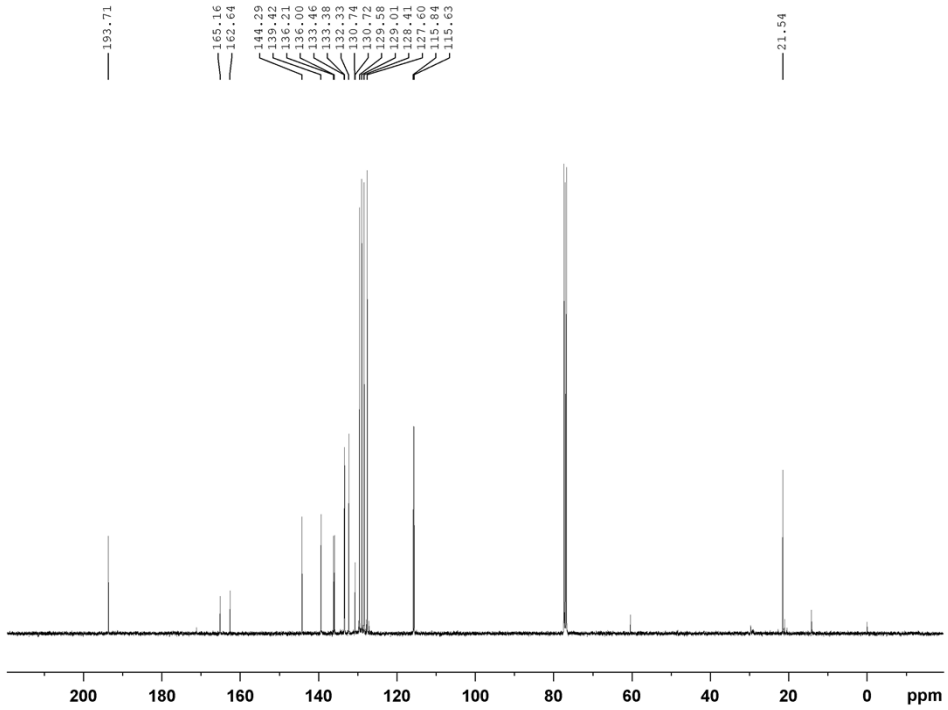

```
Current Data Parameters
NAME                     JY-83-C
EXPNO                          3
PROCNO                         1

F2 - Acquisition Parameters
Date_                      20140316
Time                           5.07
INSTRUM                       spect
PROBHD    5 mm PABBO BB/
PULPROG                     zgpg30
TD                           65536
SOLVENT                      CDCl3
NS                            1024
DS                               4
SWH                      24038.461 Hz
FIDRES                    0.366798 Hz
AQ                        1.3631488 sec
RG                           186.53
DW                           20.800 usec
DE                            6.50 usec
TE                           294.5 K
D1                        2.00000000 sec
d11                       0.03000000 sec
DELTA                     1.89999998 sec
TD0                               1
SFO1                  100.6228293 MHz
NUC1                             13C
P1                            9.98 usec
PLW1                  52.09999847 W
SFO2                  400.1316005 MHz
NUC2                             1H
CPDPRG[2                  waltz16
PCPD2                        90.00 usec
PLW2                   12.60000038 W
PLW12                   0.34999999 W
PLW13                   0.28349999 W

F2 - Processing parameters
SI                           32768
SF                    100.6127690 MHz
WDW                             EM
SSB                0
LB                            1.00 Hz
GB                 0
PC                            1.40
```

**(Z)-N-(1-(4-fluorophenyl)-3-oxo-3-phenylprop-1-en-2-yl)-4-methylbenzenesulfonamide (4d):**



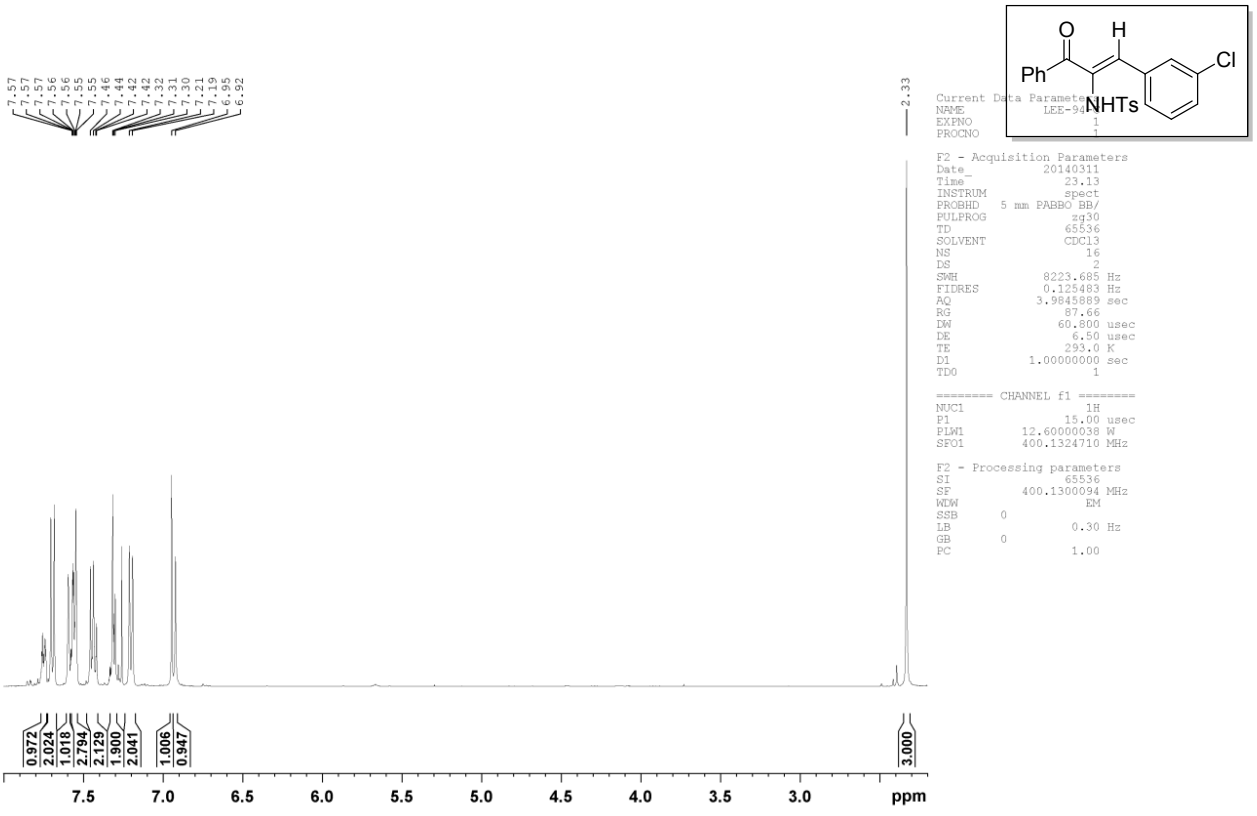




```
Current Data Parameters
NAME                  JY-80-C
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20140310
Time                 22.41
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8223.685 Hz
FIDRES             0.125483 Hz
AQ                 3.9845889 sec
RG                     64.69
DW                   60.800 usec
DE                    6.50 usec
TE                   293.2 K
D1                 1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                     15.00 usec
PLW1             12.60000038 W
SFO1             400.1324710 MHz

F2 - Processing parameters
SI                        65536
SF               400.1300098 MHz
WDW                       EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```




```
Current Data Parameters
NAME                  JY-80-C
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_              20140311
Time                  7.01
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     1024
DS                        4
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631488 sec
RG                    186.53
DW                   20.800 usec
DE                    6.50 usec
TE                   294.6 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
TD0                       1
SFO1             100.6228293 MHz
NUC1                      13C
P1                     9.98 usec
PLW1             52.09999847 W
SFO2             400.1316005 MHz
NUC2                      1H
CPDPRG[2          waltz16
PCPD2                90.00 usec
PLW2             12.60000038 W
PLW12             0.34999999 W
PLW13             0.28349999 W

F2 - Processing parameters
SI                        32768
SF               100.6127690 MHz
WDW                       EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```

**(Z)-N-(1-(3-chlorophenyl)-3-oxo-3-phenylprop-1-en-2-yl)-4-methylbenzenesulfonamide (4e):**

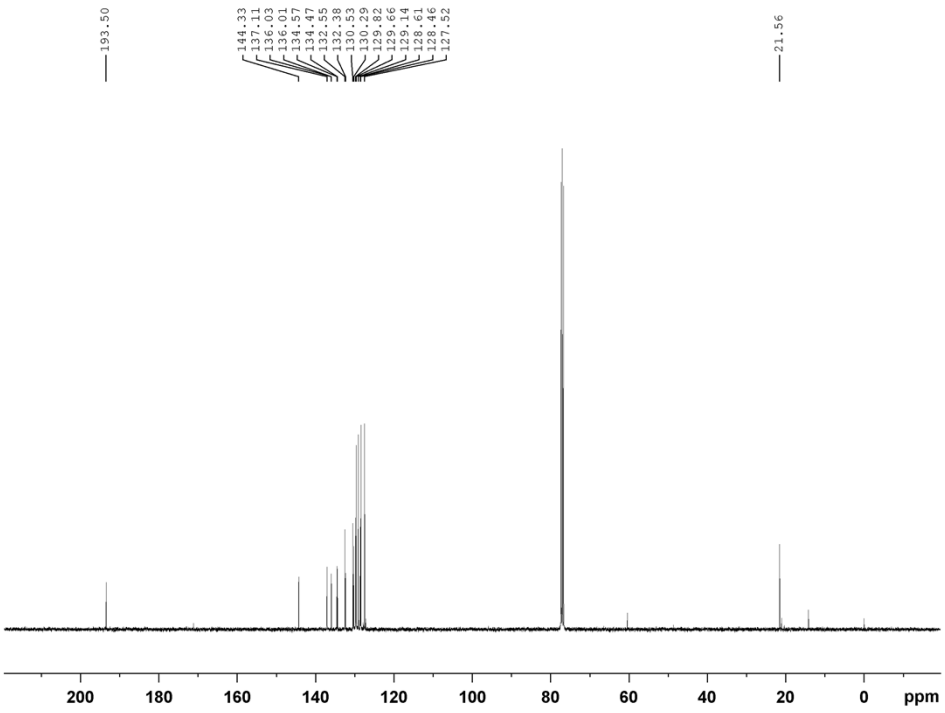



Current Data Parameters
NAME LEE-94-H
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140311
Time 23.13
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 87.66
DW 60.800 usec
DE 6.50 usec
TE 293.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
PLW1 12.60000038 W
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00




Current Data Parameters
NAME LEE-94-C
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140312
Time 8.01
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 186.53
DW 20.800 usec
DE 6.50 usec
TE 294.5 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
SFO1 100.6228293 MHz
NUC1 13C
P1 9.98 usec
PLW1 52.09999847 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 12.60000038 W
PLW12 0.34999999 W
PLW13 0.28349999 W

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

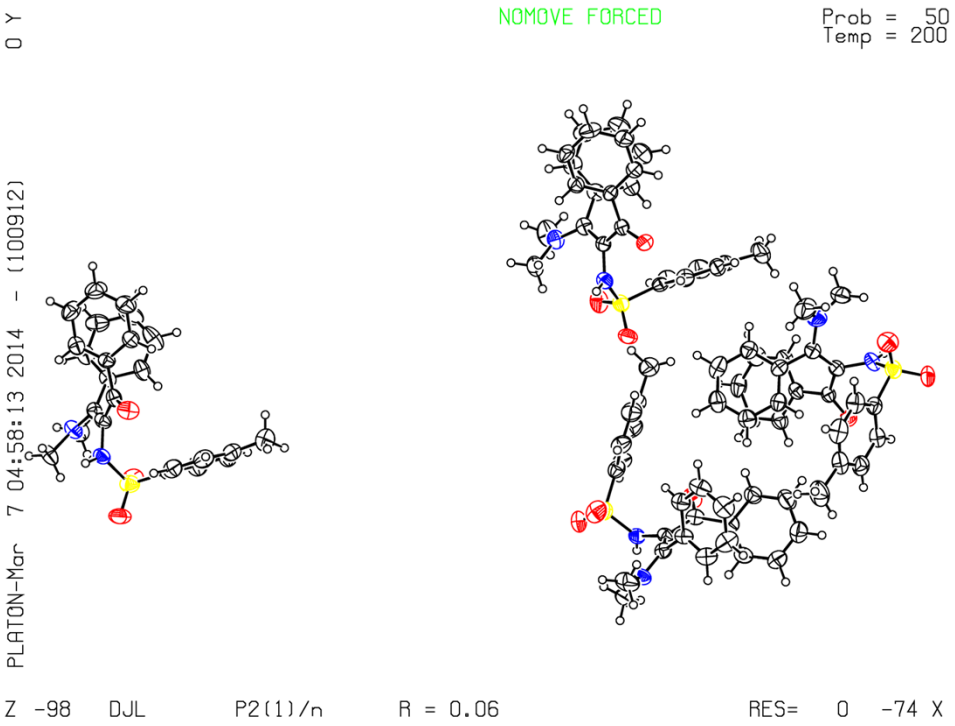



Table 1. Crystal data and structure refinement for DJL.

| | | |
|---|---|---|
| Identification code | DJL | |
| Empirical formula | $C_{24}$ $H_{24}$ $N_2$ $O_3$ S | |
| Formula weight | 420.51 | |
| Temperature | 200(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Monoclinic | |
| Space group | P2(1)/n | |
| Unit cell dimensions | a = 24.1033(9) Å | α= 90°. |
| | b = 13.6845(5) Å | β= 94.8790(10)°. |
| | c = 26.7566(9) Å | γ = 90°. |
| Volume | 8793.5(5) $Å^3$ | |
| Z | 16 | |
| Density (calculated) | 1.271 $Mg/m^3$ | |
| Absorption coefficient | 0.175 $mm^{-1}$ | |
| F(000) | 3552 | |
| Crystal size | 0.22 x 0.12 x 0.05 $mm^3$ | |
| Theta range for data collection | 1.09 to 26.01°. | |
| Index ranges | -27<=h<=29, -16<=k<=16, -32<=l<=23 | |
| Reflections collected | 54302 | |
| Independent reflections | 17276 [R(int) = 0.1025] | |

| | |
|---|---|
| Completeness to theta = 26.01° | 99.9 % |
| Absorption correction | None |
| Refinement method | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters | 17276 / 0 / 1093 |
| Goodness-of-fit on $F^2$ | 0.867 |
| Final R indices [I>2sigma(I)] | R1 = 0.0578, wR2 = 0.1149 |
| R indices (all data) | R1 = 0.1605, wR2 = 0.1588 |
| Largest diff. peak and hole | 0.300 and -0.320 e.$Å^{-3}$ |

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

| | x | y | z | U(eq) |
|---|---|---|---|---|
| C(1) | 2865(2) | 7295(3) | 310(1) | 40(1) |
| O(1) | 2661(1) | 7900(2) | 587(1) | 54(1) |
| C(2) | 2494(2) | 6650(3) | 3(1) | 40(1) |
| C(3) | 2644(2) | 5801(3) | -231(1) | 40(1) |
| C(4) | 3478(2) | 7321(3) | 284(2) | 39(1) |
| C(5) | 3740(2) | 7228(3) | -155(2) | 45(1) |
| C(6) | 4308(2) | 7293(3) | -151(2) | 57(1) |
| C(7) | 4626(2) | 7449(4) | 290(2) | 68(2) |
| C(8) | 4371(2) | 7568(4) | 727(2) | 67(2) |
| C(9) | 3805(2) | 7517(3) | 722(2) | 48(1) |
| N(1) | 1923(1) | 6975(2) | -44(1) | 44(1) |
| S(1) | 1443(1) | 6407(1) | 235(1) | 53(1) |
| O(2) | 1488(1) | 5380(2) | 135(1) | 65(1) |
| O(3) | 936(1) | 6914(2) | 94(1) | 68(1) |
| C(10) | 1608(2) | 6566(3) | 885(2) | 49(1) |
| C(11) | 1671(2) | 5777(3) | 1204(2) | 61(1) |
| C(12) | 1803(2) | 5933(4) | 1710(2) | 66(1) |
| C(13) | 1879(2) | 6856(4) | 1907(2) | 60(1) |
| C(14) | 1807(2) | 7644(3) | 1583(2) | 57(1) |
| C(15) | 1673(2) | 7510(3) | 1078(2) | 52(1) |
| C(16) | 2055(2) | 7010(4) | 2457(2) | 81(2) |
| N(2) | 2354(1) | 5421(2) | -641(1) | 47(1) |
| C(17) | 2301(2) | 4367(3) | -721(2) | 61(1) |
| C(18) | 1972(2) | 6009(3) | -973(2) | 60(1) |
| C(19) | 3149(2) | 5249(3) | -42(2) | 38(1) |
| C(20) | 3546(2) | 4983(3) | -360(2) | 50(1) |
| C(21) | 4044(2) | 4574(3) | -179(2) | 62(1) |
| C(22) | 4149(2) | 4420(3) | 322(2) | 70(2) |
| C(23) | 3756(2) | 4649(3) | 640(2) | 68(2) |
| C(24) | 3254(2) | 5061(3) | 465(2) | 49(1) |
| C(25) | 5151(2) | 3474(3) | 7768(1) | 35(1) |
| O(4) | 4888(1) | 3751(2) | 8122(1) | 41(1) |

| | | | | |
|---|---|---|---|---|
| C(26) | 4886(2) | 2880(3) | 7366(1) | 35(1) |
| C(27) | 5175(2) | 2334(3) | 7035(2) | 41(1) |
| C(28) | 5721(2) | 3870(3) | 7727(1) | 34(1) |
| C(29) | 5891(2) | 4206(3) | 7275(2) | 42(1) |
| C(30) | 6408(2) | 4625(3) | 7248(2) | 52(1) |
| C(31) | 6767(2) | 4692(3) | 7672(2) | 58(1) |
| C(32) | 6603(2) | 4367(4) | 8124(2) | 62(1) |
| C(33) | 6082(2) | 3970(3) | 8152(2) | 52(1) |
| N(3) | 4290(1) | 2942(2) | 7318(1) | 40(1) |
| S(2) | 3894(1) | 1998(1) | 7375(1) | 43(1) |
| O(5) | 3932(1) | 1357(2) | 6957(1) | 59(1) |
| O(6) | 3360(1) | 2390(2) | 7468(1) | 52(1) |
| C(34) | 4157(2) | 1341(3) | 7912(1) | 36(1) |
| C(35) | 4250(2) | 1801(3) | 8372(2) | 47(1) |
| C(36) | 4388(2) | 1244(4) | 8797(2) | 54(1) |
| C(37) | 4431(2) | 247(4) | 8777(2) | 58(1) |
| C(38) | 4351(2) | -201(3) | 8314(2) | 64(1) |
| C(39) | 4218(2) | 337(3) | 7881(2) | 52(1) |
| C(40) | 4557(2) | -355(4) | 9245(2) | 92(2) |
| N(4) | 4983(1) | 2156(2) | 6551(1) | 47(1) |
| C(41) | 5072(2) | 1217(3) | 6310(2) | 80(2) |
| C(42) | 4578(2) | 2797(3) | 6279(2) | 58(1) |
| C(43) | 5713(2) | 1894(3) | 7220(2) | 42(1) |
| C(44) | 6175(2) | 1950(3) | 6938(2) | 53(1) |
| C(45) | 6685(2) | 1615(3) | 7137(2) | 65(1) |
| C(46) | 6742(2) | 1203(3) | 7609(2) | 64(1) |
| C(47) | 6290(2) | 1122(3) | 7886(2) | 58(1) |
| C(48) | 5779(2) | 1462(3) | 7695(2) | 48(1) |
| C(49) | 2205(2) | -448(3) | 9954(1) | 35(1) |
| O(7) | 1801(1) | -766(2) | 10157(1) | 45(1) |
| C(50) | 2636(2) | 146(3) | 10219(1) | 37(1) |
| C(51) | 2952(2) | 826(3) | 9994(1) | 40(1) |
| C(52) | 2286(2) | -771(3) | 9430(1) | 37(1) |
| C(53) | 2807(2) | -1003(3) | 9285(2) | 45(1) |
| C(54) | 2868(2) | -1354(3) | 8810(2) | 57(1) |
| C(55) | 2406(2) | -1468(3) | 8470(2) | 58(1) |
| C(56) | 1883(2) | -1244(3) | 8614(2) | 58(1) |

| | | | | |
|---|---|---|---|---|
| C(57) | 1817(2) | -918(3) | 9096(1) | 45(1) |
| N(5) | 2707(1) | -42(2) | 10745(1) | 42(1) |
| S(3) | 2581(1) | 774(1) | 11162(1) | 47(1) |
| O(8) | 3037(1) | 1439(2) | 11235(1) | 60(1) |
| O(9) | 2432(1) | 219(2) | 11586(1) | 58(1) |
| C(58) | 2017(2) | 1466(3) | 10898(1) | 43(1) |
| C(59) | 2100(2) | 2420(3) | 10761(2) | 58(1) |
| C(60) | 1661(2) | 2943(3) | 10523(2) | 64(1) |
| C(61) | 1139(2) | 2518(3) | 10419(2) | 58(1) |
| C(62) | 1061(2) | 1568(3) | 10584(2) | 54(1) |
| C(63) | 1500(2) | 1035(3) | 10817(1) | 47(1) |
| C(64) | 668(2) | 3048(4) | 10118(2) | 84(2) |
| N(6) | 3473(2) | 1102(3) | 10169(1) | 52(1) |
| C(65) | 3656(2) | 2112(3) | 10163(2) | 75(2) |
| C(66) | 3824(2) | 453(4) | 10489(2) | 68(2) |
| C(67) | 2706(2) | 1291(3) | 9525(2) | 40(1) |
| C(68) | 3022(2) | 1390(3) | 9117(2) | 53(1) |
| C(69) | 2775(2) | 1753(3) | 8669(2) | 63(1) |
| C(70) | 2224(2) | 2035(3) | 8627(2) | 60(1) |
| C(71) | 1917(2) | 1962(3) | 9032(2) | 52(1) |
| C(72) | 2158(2) | 1594(3) | 9481(2) | 43(1) |
| C(73) | 350(2) | 728(3) | 7857(2) | 39(1) |
| O(10) | 651(1) | 30(2) | 7756(1) | 50(1) |
| C(74) | 82(2) | 1322(3) | 7458(1) | 38(1) |
| C(75) | -142(2) | 2241(3) | 7524(1) | 40(1) |
| C(76) | 225(2) | 823(3) | 8396(2) | 39(1) |
| C(77) | -305(2) | 986(3) | 8542(2) | 44(1) |
| C(78) | -403(2) | 993(3) | 9042(2) | 54(1) |
| C(79) | 24(2) | 850(3) | 9404(2) | 62(1) |
| C(80) | 555(2) | 681(4) | 9270(2) | 65(1) |
| C(81) | 657(2) | 658(3) | 8767(2) | 50(1) |
| N(7) | 92(1) | 921(2) | 6965(1) | 40(1) |
| S(4) | 533(1) | 1313(1) | 6585(1) | 49(1) |
| O(11) | 543(1) | 2358(2) | 6615(1) | 64(1) |
| O(12) | 372(1) | 851(2) | 6111(1) | 61(1) |
| C(82) | 1191(2) | 874(3) | 6795(2) | 45(1) |
| C(83) | 1596(2) | 1496(3) | 7009(2) | 58(1) |

| | | | | |
|---|---|---|---|---|
| C(84) | 2109(2) | 1128(4) | 7179(2) | 63(1) |
| C(85) | 2233(2) | 142(4) | 7146(2) | 55(1) |
| C(86) | 1820(2) | -472(3) | 6925(2) | 58(1) |
| C(87) | 1303(2) | -104(3) | 6754(2) | 50(1) |
| C(88) | 2802(2) | -255(4) | 7336(2) | 77(2) |
| N(8) | -542(1) | 2651(2) | 7205(1) | 48(1) |
| C(89) | -596(2) | 3702(3) | 7131(2) | 73(2) |
| C(90) | -879(2) | 2082(3) | 6827(2) | 60(1) |
| C(91) | 83(2) | 2854(3) | 7958(2) | 39(1) |
| C(92) | -257(2) | 3215(3) | 8307(2) | 52(1) |
| C(93) | -26(2) | 3724(3) | 8720(2) | 63(1) |
| C(94) | 539(2) | 3919(3) | 8774(2) | 61(1) |
| C(95) | 872(2) | 3594(3) | 8418(2) | 55(1) |
| C(96) | 647(2) | 3047(3) | 8013(2) | 48(1) |

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

| | |
|---|---|
| C(1)-O(1) | 1.239(4) |
| C(1)-C(2) | 1.459(5) |
| C(1)-C(4) | 1.486(5) |
| C(2)-C(3) | 1.383(5) |
| C(2)-N(1) | 1.440(5) |
| C(3)-N(2) | 1.354(4) |
| C(3)-C(19) | 1.484(5) |
| C(4)-C(9) | 1.382(5) |
| C(4)-C(5) | 1.384(5) |
| C(5)-C(6) | 1.371(5) |
| C(5)-H(5) | 0.9500 |
| C(6)-C(7) | 1.368(5) |
| C(6)-H(6) | 0.9500 |
| C(7)-C(8) | 1.374(6) |
| C(7)-H(7) | 0.9500 |
| C(8)-C(9) | 1.367(6) |
| C(8)-H(8) | 0.9500 |
| C(9)-H(9) | 0.9500 |
| N(1)-S(1) | 1.629(3) |
| N(1)-H(1A) | 0.8800 |
| S(1)-O(3) | 1.427(3) |
| S(1)-O(2) | 1.436(3) |
| S(1)-C(10) | 1.764(4) |
| C(10)-C(11) | 1.376(5) |
| C(10)-C(15) | 1.394(5) |
| C(11)-C(12) | 1.380(6) |
| C(11)-H(11) | 0.9500 |
| C(12)-C(13) | 1.376(6) |
| C(12)-H(12) | 0.9500 |
| C(13)-C(14) | 1.385(6) |
| C(13)-C(16) | 1.511(6) |
| C(14)-C(15) | 1.375(5) |
| C(14)-H(14) | 0.9500 |
| C(15)-H(15) | 0.9500 |
| C(16)-H(16A) | 0.9800 |

| | |
|---|---|
| C(16)-H(16B) | 0.9800 |
| C(16)-H(16C) | 0.9800 |
| N(2)-C(17) | 1.462(5) |
| N(2)-C(18) | 1.465(4) |
| C(17)-H(17A) | 0.9800 |
| C(17)-H(17B) | 0.9800 |
| C(17)-H(17C) | 0.9800 |
| C(18)-H(18A) | 0.9800 |
| C(18)-H(18B) | 0.9800 |
| C(18)-H(18C) | 0.9800 |
| C(19)-C(24) | 1.382(5) |
| C(19)-C(20) | 1.383(6) |
| C(20)-C(21) | 1.376(5) |
| C(20)-H(20) | 0.9500 |
| C(21)-C(22) | 1.361(6) |
| C(21)-H(21) | 0.9500 |
| C(22)-C(23) | 1.363(7) |
| C(22)-H(22) | 0.9500 |
| C(23)-C(24) | 1.380(6) |
| C(23)-H(23) | 0.9500 |
| C(24)-H(24) | 0.9500 |
| C(25)-O(4) | 1.242(4) |
| C(25)-C(26) | 1.451(5) |
| C(25)-C(28) | 1.491(5) |
| C(26)-C(27) | 1.391(5) |
| C(26)-N(3) | 1.433(5) |
| C(27)-N(4) | 1.358(4) |
| C(27)-C(43) | 1.477(5) |
| C(28)-C(33) | 1.379(5) |
| C(28)-C(29) | 1.388(5) |
| C(29)-C(30) | 1.378(5) |
| C(29)-H(29) | 0.9500 |
| C(30)-C(31) | 1.372(5) |
| C(30)-H(30) | 0.9500 |
| C(31)-C(32) | 1.376(6) |
| C(31)-H(31) | 0.9500 |
| C(32)-C(33) | 1.375(6) |

| | |
|---|---|
| C(32)-H(32) | 0.9500 |
| C(33)-H(33) | 0.9500 |
| N(3)-S(2) | 1.622(3) |
| N(3)-H(3A) | 0.8800 |
| S(2)-O(5) | 1.429(3) |
| S(2)-O(6) | 1.435(3) |
| S(2)-C(34) | 1.767(4) |
| C(34)-C(35) | 1.383(5) |
| C(34)-C(39) | 1.384(5) |
| C(35)-C(36) | 1.387(5) |
| C(35)-H(35) | 0.9500 |
| C(36)-C(37) | 1.370(6) |
| C(36)-H(36) | 0.9500 |
| C(37)-C(38) | 1.381(6) |
| C(37)-C(40) | 1.509(6) |
| C(38)-C(39) | 1.386(5) |
| C(38)-H(38) | 0.9500 |
| C(39)-H(39) | 0.9500 |
| C(40)-H(40A) | 0.9800 |
| C(40)-H(40B) | 0.9800 |
| C(40)-H(40C) | 0.9800 |
| N(4)-C(42) | 1.459(5) |
| N(4)-C(41) | 1.464(5) |
| C(41)-H(41A) | 0.9800 |
| C(41)-H(41B) | 0.9800 |
| C(41)-H(41C) | 0.9800 |
| C(42)-H(42A) | 0.9800 |
| C(42)-H(42B) | 0.9800 |
| C(42)-H(42C) | 0.9800 |
| C(43)-C(44) | 1.399(6) |
| C(43)-C(48) | 1.399(5) |
| C(44)-C(45) | 1.377(5) |
| C(44)-H(44) | 0.9500 |
| C(45)-C(46) | 1.379(6) |
| C(45)-H(45) | 0.9500 |
| C(46)-C(47) | 1.376(6) |
| C(46)-H(46) | 0.9500 |

| | |
|---|---|
| C(47)-C(48) | 1.375(5) |
| C(47)-H(47) | 0.9500 |
| C(48)-H(48) | 0.9500 |
| C(49)-O(7) | 1.234(4) |
| C(49)-C(50) | 1.453(5) |
| C(49)-C(52) | 1.497(5) |
| C(50)-C(51) | 1.373(5) |
| C(50)-N(5) | 1.427(4) |
| C(51)-N(6) | 1.355(5) |
| C(51)-C(67) | 1.484(5) |
| C(52)-C(53) | 1.383(5) |
| C(52)-C(57) | 1.394(5) |
| C(53)-C(54) | 1.378(5) |
| C(53)-H(53) | 0.9500 |
| C(54)-C(55) | 1.384(5) |
| C(54)-H(54) | 0.9500 |
| C(55)-C(56) | 1.383(6) |
| C(55)-H(55) | 0.9500 |
| C(56)-C(57) | 1.385(6) |
| C(56)-H(56) | 0.9500 |
| C(57)-H(57) | 0.9500 |
| N(5)-S(3) | 1.626(3) |
| N(5)-H(5A) | 0.8800 |
| S(3)-O(8) | 1.427(3) |
| S(3)-O(9) | 1.437(3) |
| S(3)-C(58) | 1.757(4) |
| C(58)-C(59) | 1.375(5) |
| C(58)-C(63) | 1.378(5) |
| C(59)-C(60) | 1.386(6) |
| C(59)-H(59) | 0.9500 |
| C(60)-C(61) | 1.393(6) |
| C(60)-H(60) | 0.9500 |
| C(61)-C(62) | 1.391(6) |
| C(61)-C(64) | 1.519(6) |
| C(62)-C(63) | 1.389(5) |
| C(62)-H(62) | 0.9500 |
| C(63)-H(63) | 0.9500 |

| | |
|---|---|
| C(64)-H(64A) | 0.9800 |
| C(64)-H(64B) | 0.9800 |
| C(64)-H(64C) | 0.9800 |
| N(6)-C(65) | 1.452(5) |
| N(6)-C(66) | 1.455(5) |
| C(65)-H(65A) | 0.9800 |
| C(65)-H(65B) | 0.9800 |
| C(65)-H(65C) | 0.9800 |
| C(66)-H(66A) | 0.9800 |
| C(66)-H(66B) | 0.9800 |
| C(66)-H(66C) | 0.9800 |
| C(67)-C(72) | 1.380(5) |
| C(67)-C(68) | 1.392(6) |
| C(68)-C(69) | 1.383(5) |
| C(68)-H(68) | 0.9500 |
| C(69)-C(70) | 1.378(6) |
| C(69)-H(69) | 0.9500 |
| C(70)-C(71) | 1.367(6) |
| C(70)-H(70) | 0.9500 |
| C(71)-C(72) | 1.384(5) |
| C(71)-H(71) | 0.9500 |
| C(72)-H(72) | 0.9500 |
| C(73)-O(10) | 1.242(4) |
| C(73)-C(74) | 1.451(5) |
| C(73)-C(76) | 1.505(5) |
| C(74)-C(75) | 1.387(5) |
| C(74)-N(7) | 1.429(5) |
| C(75)-N(8) | 1.353(4) |
| C(75)-C(91) | 1.496(5) |
| C(76)-C(77) | 1.386(5) |
| C(76)-C(81) | 1.394(5) |
| C(77)-C(78) | 1.379(6) |
| C(77)-H(77) | 0.9500 |
| C(78)-C(79) | 1.366(5) |
| C(78)-H(78) | 0.9500 |
| C(79)-C(80) | 1.378(6) |
| C(79)-H(79) | 0.9500 |

| | |
|---|---|
| C(80)-C(81) | 1.389(6) |
| C(80)-H(80) | 0.9500 |
| C(81)-H(81) | 0.9500 |
| N(7)-S(4) | 1.624(3) |
| N(7)-H(7A) | 0.8800 |
| S(4)-O(11) | 1.432(3) |
| S(4)-O(12) | 1.441(3) |
| S(4)-C(82) | 1.742(4) |
| C(82)-C(87) | 1.372(5) |
| C(82)-C(83) | 1.382(5) |
| C(83)-C(84) | 1.377(6) |
| C(83)-H(83) | 0.9500 |
| C(84)-C(85) | 1.387(6) |
| C(84)-H(84) | 0.9500 |
| C(85)-C(86) | 1.394(6) |
| C(85)-C(88) | 1.522(6) |
| C(86)-C(87) | 1.385(5) |
| C(86)-H(86) | 0.9500 |
| C(87)-H(87) | 0.9500 |
| C(88)-H(88A) | 0.9800 |
| C(88)-H(88B) | 0.9800 |
| C(88)-H(88C) | 0.9800 |
| N(8)-C(89) | 1.457(5) |
| N(8)-C(90) | 1.465(5) |
| C(89)-H(89A) | 0.9800 |
| C(89)-H(89B) | 0.9800 |
| C(89)-H(89C) | 0.9800 |
| C(90)-H(90A) | 0.9800 |
| C(90)-H(90B) | 0.9800 |
| C(90)-H(90C) | 0.9800 |
| C(91)-C(96) | 1.381(5) |
| C(91)-C(92) | 1.385(6) |
| C(92)-C(93) | 1.382(5) |
| C(92)-H(92) | 0.9500 |
| C(93)-C(94) | 1.385(6) |
| C(93)-H(93) | 0.9500 |
| C(94)-C(95) | 1.371(6) |

| | |
|---|---|
| C(94)-H(94) | 0.9500 |
| C(95)-C(96) | 1.387(5) |
| C(95)-H(95) | 0.9500 |
| C(96)-H(96) | 0.9500 |

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| O(1)-C(1)-C(2) | 119.0(4) |
| O(1)-C(1)-C(4) | 117.3(4) |
| C(2)-C(1)-C(4) | 123.5(4) |
| C(3)-C(2)-N(1) | 120.3(3) |
| C(3)-C(2)-C(1) | 126.3(4) |
| N(1)-C(2)-C(1) | 113.5(3) |
| N(2)-C(3)-C(2) | 123.6(4) |
| N(2)-C(3)-C(19) | 115.6(4) |
| C(2)-C(3)-C(19) | 120.8(3) |
| C(9)-C(4)-C(5) | 118.0(4) |
| C(9)-C(4)-C(1) | 117.4(4) |
| C(5)-C(4)-C(1) | 124.4(4) |
| C(6)-C(5)-C(4) | 121.0(4) |
| C(6)-C(5)-H(5) | 119.5 |
| C(4)-C(5)-H(5) | 119.5 |
| C(7)-C(6)-C(5) | 120.1(4) |
| C(7)-C(6)-H(6) | 119.9 |
| C(5)-C(6)-H(6) | 119.9 |
| C(6)-C(7)-C(8) | 119.6(5) |
| C(6)-C(7)-H(7) | 120.2 |
| C(8)-C(7)-H(7) | 120.2 |
| C(9)-C(8)-C(7) | 120.3(4) |
| C(9)-C(8)-H(8) | 119.8 |
| C(7)-C(8)-H(8) | 119.8 |
| C(8)-C(9)-C(4) | 120.9(4) |
| C(8)-C(9)-H(9) | 119.6 |
| C(4)-C(9)-H(9) | 119.6 |
| C(2)-N(1)-S(1) | 121.5(3) |
| C(2)-N(1)-H(1A) | 119.3 |
| S(1)-N(1)-H(1A) | 119.3 |
| O(3)-S(1)-O(2) | 120.13(19) |
| O(3)-S(1)-N(1) | 105.78(18) |

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| O(2)-S(1)-N(1) | 108.23(19) |
| O(3)-S(1)-C(10) | 108.5(2) |
| O(2)-S(1)-C(10) | 106.9(2) |
| N(1)-S(1)-C(10) | 106.52(18) |
| C(11)-C(10)-C(15) | 119.7(4) |
| C(11)-C(10)-S(1) | 121.2(4) |
| C(15)-C(10)-S(1) | 119.2(3) |
| C(10)-C(11)-C(12) | 119.4(4) |
| C(10)-C(11)-H(11) | 120.3 |
| C(12)-C(11)-H(11) | 120.3 |
| C(13)-C(12)-C(11) | 122.1(4) |
| C(13)-C(12)-H(12) | 119.0 |
| C(11)-C(12)-H(12) | 119.0 |
| C(12)-C(13)-C(14) | 117.9(4) |
| C(12)-C(13)-C(16) | 121.3(5) |
| C(14)-C(13)-C(16) | 120.8(5) |
| C(15)-C(14)-C(13) | 121.3(4) |
| C(15)-C(14)-H(14) | 119.4 |
| C(13)-C(14)-H(14) | 119.4 |
| C(14)-C(15)-C(10) | 119.7(4) |
| C(14)-C(15)-H(15) | 120.1 |
| C(10)-C(15)-H(15) | 120.1 |
| C(13)-C(16)-H(16A) | 109.5 |
| C(13)-C(16)-H(16B) | 109.5 |
| H(16A)-C(16)-H(16B) | 109.5 |
| C(13)-C(16)-H(16C) | 109.5 |
| H(16A)-C(16)-H(16C) | 109.5 |
| H(16B)-C(16)-H(16C) | 109.5 |
| C(3)-N(2)-C(17) | 121.9(3) |
| C(3)-N(2)-C(18) | 122.4(3) |
| C(17)-N(2)-C(18) | 114.2(3) |
| N(2)-C(17)-H(17A) | 109.5 |
| N(2)-C(17)-H(17B) | 109.5 |
| H(17A)-C(17)-H(17B) | 109.5 |
| N(2)-C(17)-H(17C) | 109.5 |
| H(17A)-C(17)-H(17C) | 109.5 |
| H(17B)-C(17)-H(17C) | 109.5 |

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| N(2)-C(18)-H(18A) | 109.5 |
| N(2)-C(18)-H(18B) | 109.5 |
| H(18A)-C(18)-H(18B) | 109.5 |
| N(2)-C(18)-H(18C) | 109.5 |
| H(18A)-C(18)-H(18C) | 109.5 |
| H(18B)-C(18)-H(18C) | 109.5 |
| C(24)-C(19)-C(20) | 118.5(4) |
| C(24)-C(19)-C(3) | 120.4(4) |
| C(20)-C(19)-C(3) | 120.9(4) |
| C(21)-C(20)-C(19) | 121.3(4) |
| C(21)-C(20)-H(20) | 119.4 |
| C(19)-C(20)-H(20) | 119.4 |
| C(22)-C(21)-C(20) | 119.6(5) |
| C(22)-C(21)-H(21) | 120.2 |
| C(20)-C(21)-H(21) | 120.2 |
| C(21)-C(22)-C(23) | 119.9(5) |
| C(21)-C(22)-H(22) | 120.1 |
| C(23)-C(22)-H(22) | 120.1 |
| C(22)-C(23)-C(24) | 121.2(5) |
| C(22)-C(23)-H(23) | 119.4 |
| C(24)-C(23)-H(23) | 119.4 |
| C(23)-C(24)-C(19) | 119.5(5) |
| C(23)-C(24)-H(24) | 120.3 |
| C(19)-C(24)-H(24) | 120.3 |
| O(4)-C(25)-C(26) | 121.0(4) |
| O(4)-C(25)-C(28) | 118.6(3) |
| C(26)-C(25)-C(28) | 119.9(4) |
| C(27)-C(26)-N(3) | 121.7(3) |
| C(27)-C(26)-C(25) | 124.2(4) |
| N(3)-C(26)-C(25) | 114.1(3) |
| N(4)-C(27)-C(26) | 123.8(4) |
| N(4)-C(27)-C(43) | 117.7(4) |
| C(26)-C(27)-C(43) | 118.5(3) |
| C(33)-C(28)-C(29) | 118.3(4) |
| C(33)-C(28)-C(25) | 119.7(4) |
| C(29)-C(28)-C(25) | 121.9(3) |
| C(30)-C(29)-C(28) | 121.3(4) |

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| C(30)-C(29)-H(29) | 119.4 |
| C(28)-C(29)-H(29) | 119.4 |
| C(31)-C(30)-C(29) | 119.6(4) |
| C(31)-C(30)-H(30) | 120.2 |
| C(29)-C(30)-H(30) | 120.2 |
| C(30)-C(31)-C(32) | 119.8(4) |
| C(30)-C(31)-H(31) | 120.1 |
| C(32)-C(31)-H(31) | 120.1 |
| C(33)-C(32)-C(31) | 120.5(4) |
| C(33)-C(32)-H(32) | 119.8 |
| C(31)-C(32)-H(32) | 119.8 |
| C(32)-C(33)-C(28) | 120.6(4) |
| C(32)-C(33)-H(33) | 119.7 |
| C(28)-C(33)-H(33) | 119.7 |
| C(26)-N(3)-S(2) | 122.6(3) |
| C(26)-N(3)-H(3A) | 118.7 |
| S(2)-N(3)-H(3A) | 118.7 |
| O(5)-S(2)-O(6) | 118.94(17) |
| O(5)-S(2)-N(3) | 109.75(17) |
| O(6)-S(2)-N(3) | 105.19(17) |
| O(5)-S(2)-C(34) | 106.31(18) |
| O(6)-S(2)-C(34) | 108.31(18) |
| N(3)-S(2)-C(34) | 107.93(16) |
| C(35)-C(34)-C(39) | 119.7(4) |
| C(35)-C(34)-S(2) | 120.8(3) |
| C(39)-C(34)-S(2) | 119.3(3) |
| C(34)-C(35)-C(36) | 119.3(4) |
| C(34)-C(35)-H(35) | 120.3 |
| C(36)-C(35)-H(35) | 120.3 |
| C(37)-C(36)-C(35) | 121.9(4) |
| C(37)-C(36)-H(36) | 119.0 |
| C(35)-C(36)-H(36) | 119.0 |
| C(36)-C(37)-C(38) | 118.1(4) |
| C(36)-C(37)-C(40) | 121.4(5) |
| C(38)-C(37)-C(40) | 120.4(5) |
| C(37)-C(38)-C(39) | 121.3(4) |
| C(37)-C(38)-H(38) | 119.4 |

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| C(39)-C(38)-H(38) | 119.4 |
| C(34)-C(39)-C(38) | 119.7(4) |
| C(34)-C(39)-H(39) | 120.2 |
| C(38)-C(39)-H(39) | 120.2 |
| C(37)-C(40)-H(40A) | 109.5 |
| C(37)-C(40)-H(40B) | 109.5 |
| H(40A)-C(40)-H(40B) | 109.5 |
| C(37)-C(40)-H(40C) | 109.5 |
| H(40A)-C(40)-H(40C) | 109.5 |
| H(40B)-C(40)-H(40C) | 109.5 |
| C(27)-N(4)-C(42) | 121.7(3) |
| C(27)-N(4)-C(41) | 121.8(3) |
| C(42)-N(4)-C(41) | 115.2(3) |
| N(4)-C(41)-H(41A) | 109.5 |
| N(4)-C(41)-H(41B) | 109.5 |
| H(41A)-C(41)-H(41B) | 109.5 |
| N(4)-C(41)-H(41C) | 109.5 |
| H(41A)-C(41)-H(41C) | 109.5 |
| H(41B)-C(41)-H(41C) | 109.5 |
| N(4)-C(42)-H(42A) | 109.5 |
| N(4)-C(42)-H(42B) | 109.5 |
| H(42A)-C(42)-H(42B) | 109.5 |
| N(4)-C(42)-H(42C) | 109.5 |
| H(42A)-C(42)-H(42C) | 109.5 |
| H(42B)-C(42)-H(42C) | 109.5 |
| C(44)-C(43)-C(48) | 118.7(4) |
| C(44)-C(43)-C(27) | 120.9(4) |
| C(48)-C(43)-C(27) | 120.3(4) |
| C(45)-C(44)-C(43) | 120.0(4) |
| C(45)-C(44)-H(44) | 120.0 |
| C(43)-C(44)-H(44) | 120.0 |
| C(44)-C(45)-C(46) | 120.4(5) |
| C(44)-C(45)-H(45) | 119.8 |
| C(46)-C(45)-H(45) | 119.8 |
| C(47)-C(46)-C(45) | 120.4(5) |
| C(47)-C(46)-H(46) | 119.8 |
| C(45)-C(46)-H(46) | 119.8 |

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| C(48)-C(47)-C(46) | 119.9(5) |
| C(48)-C(47)-H(47) | 120.1 |
| C(46)-C(47)-H(47) | 120.1 |
| C(47)-C(48)-C(43) | 120.6(4) |
| C(47)-C(48)-H(48) | 119.7 |
| C(43)-C(48)-H(48) | 119.7 |
| O(7)-C(49)-C(50) | 122.7(4) |
| O(7)-C(49)-C(52) | 118.5(3) |
| C(50)-C(49)-C(52) | 118.5(4) |
| C(51)-C(50)-N(5) | 121.9(3) |
| C(51)-C(50)-C(49) | 124.4(4) |
| N(5)-C(50)-C(49) | 113.7(3) |
| N(6)-C(51)-C(50) | 124.8(4) |
| N(6)-C(51)-C(67) | 117.6(4) |
| C(50)-C(51)-C(67) | 117.6(4) |
| C(53)-C(52)-C(57) | 119.4(4) |
| C(53)-C(52)-C(49) | 121.6(3) |
| C(57)-C(52)-C(49) | 118.7(4) |
| C(54)-C(53)-C(52) | 120.7(4) |
| C(54)-C(53)-H(53) | 119.6 |
| C(52)-C(53)-H(53) | 119.6 |
| C(53)-C(54)-C(55) | 120.0(5) |
| C(53)-C(54)-H(54) | 120.0 |
| C(55)-C(54)-H(54) | 120.0 |
| C(56)-C(55)-C(54) | 119.6(4) |
| C(56)-C(55)-H(55) | 120.2 |
| C(54)-C(55)-H(55) | 120.2 |
| C(55)-C(56)-C(57) | 120.6(4) |
| C(55)-C(56)-H(56) | 119.7 |
| C(57)-C(56)-H(56) | 119.7 |
| C(56)-C(57)-C(52) | 119.5(4) |
| C(56)-C(57)-H(57) | 120.2 |
| C(52)-C(57)-H(57) | 120.2 |
| C(50)-N(5)-S(3) | 122.7(3) |
| C(50)-N(5)-H(5A) | 118.6 |
| S(3)-N(5)-H(5A) | 118.6 |
| O(8)-S(3)-O(9) | 118.17(17) |

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| O(8)-S(3)-N(5) | 110.18(18) |
| O(9)-S(3)-N(5) | 104.70(18) |
| O(8)-S(3)-C(58) | 105.8(2) |
| O(9)-S(3)-C(58) | 111.3(2) |
| N(5)-S(3)-C(58) | 106.11(17) |
| C(59)-C(58)-C(63) | 120.9(4) |
| C(59)-C(58)-S(3) | 119.6(4) |
| C(63)-C(58)-S(3) | 119.5(3) |
| C(58)-C(59)-C(60) | 119.4(5) |
| C(58)-C(59)-H(59) | 120.3 |
| C(60)-C(59)-H(59) | 120.3 |
| C(59)-C(60)-C(61) | 121.1(5) |
| C(59)-C(60)-H(60) | 119.4 |
| C(61)-C(60)-H(60) | 119.4 |
| C(62)-C(61)-C(60) | 118.2(4) |
| C(62)-C(61)-C(64) | 119.9(5) |
| C(60)-C(61)-C(64) | 121.9(5) |
| C(63)-C(62)-C(61) | 120.9(5) |
| C(63)-C(62)-H(62) | 119.5 |
| C(61)-C(62)-H(62) | 119.5 |
| C(58)-C(63)-C(62) | 119.4(4) |
| C(58)-C(63)-H(63) | 120.3 |
| C(62)-C(63)-H(63) | 120.3 |
| C(61)-C(64)-H(64A) | 109.5 |
| C(61)-C(64)-H(64B) | 109.5 |
| H(64A)-C(64)-H(64B) | 109.5 |
| C(61)-C(64)-H(64C) | 109.5 |
| H(64A)-C(64)-H(64C) | 109.5 |
| H(64B)-C(64)-H(64C) | 109.5 |
| C(51)-N(6)-C(65) | 122.5(4) |
| C(51)-N(6)-C(66) | 120.6(4) |
| C(65)-N(6)-C(66) | 115.0(3) |
| N(6)-C(65)-H(65A) | 109.5 |
| N(6)-C(65)-H(65B) | 109.5 |
| H(65A)-C(65)-H(65B) | 109.5 |
| N(6)-C(65)-H(65C) | 109.5 |
| H(65A)-C(65)-H(65C) | 109.5 |

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| H(65B)-C(65)-H(65C) | 109.5 |
| N(6)-C(66)-H(66A) | 109.5 |
| N(6)-C(66)-H(66B) | 109.5 |
| H(66A)-C(66)-H(66B) | 109.5 |
| N(6)-C(66)-H(66C) | 109.5 |
| H(66A)-C(66)-H(66C) | 109.5 |
| H(66B)-C(66)-H(66C) | 109.5 |
| C(72)-C(67)-C(68) | 119.1(4) |
| C(72)-C(67)-C(51) | 120.8(4) |
| C(68)-C(67)-C(51) | 120.0(4) |
| C(69)-C(68)-C(67) | 119.5(4) |
| C(69)-C(68)-H(68) | 120.3 |
| C(67)-C(68)-H(68) | 120.3 |
| C(70)-C(69)-C(68) | 120.7(4) |
| C(70)-C(69)-H(69) | 119.6 |
| C(68)-C(69)-H(69) | 119.6 |
| C(71)-C(70)-C(69) | 119.9(4) |
| C(71)-C(70)-H(70) | 120.1 |
| C(69)-C(70)-H(70) | 120.1 |
| C(70)-C(71)-C(72) | 119.9(4) |
| C(70)-C(71)-H(71) | 120.0 |
| C(72)-C(71)-H(71) | 120.0 |
| C(67)-C(72)-C(71) | 120.8(4) |
| C(67)-C(72)-H(72) | 119.6 |
| C(71)-C(72)-H(72) | 119.6 |
| O(10)-C(73)-C(74) | 120.1(4) |
| O(10)-C(73)-C(76) | 116.4(3) |
| C(74)-C(73)-C(76) | 123.0(4) |
| C(75)-C(74)-N(7) | 120.2(3) |
| C(75)-C(74)-C(73) | 124.6(4) |
| N(7)-C(74)-C(73) | 115.0(3) |
| N(8)-C(75)-C(74) | 124.1(4) |
| N(8)-C(75)-C(91) | 116.7(3) |
| C(74)-C(75)-C(91) | 119.2(3) |
| C(77)-C(76)-C(81) | 118.5(4) |
| C(77)-C(76)-C(73) | 123.3(4) |
| C(81)-C(76)-C(73) | 118.0(4) |

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| C(78)-C(77)-C(76) | 120.8(4) |
| C(78)-C(77)-H(77) | 119.6 |
| C(76)-C(77)-H(77) | 119.6 |
| C(79)-C(78)-C(77) | 120.5(4) |
| C(79)-C(78)-H(78) | 119.8 |
| C(77)-C(78)-H(78) | 119.8 |
| C(78)-C(79)-C(80) | 120.0(5) |
| C(78)-C(79)-H(79) | 120.0 |
| C(80)-C(79)-H(79) | 120.0 |
| C(79)-C(80)-C(81) | 120.1(4) |
| C(79)-C(80)-H(80) | 120.0 |
| C(81)-C(80)-H(80) | 120.0 |
| C(80)-C(81)-C(76) | 120.2(4) |
| C(80)-C(81)-H(81) | 119.9 |
| C(76)-C(81)-H(81) | 119.9 |
| C(74)-N(7)-S(4) | 120.9(3) |
| C(74)-N(7)-H(7A) | 119.5 |
| S(4)-N(7)-H(7A) | 119.5 |
| O(11)-S(4)-O(12) | 119.31(18) |
| O(11)-S(4)-N(7) | 107.64(19) |
| O(12)-S(4)-N(7) | 105.41(17) |
| O(11)-S(4)-C(82) | 108.4(2) |
| O(12)-S(4)-C(82) | 107.56(19) |
| N(7)-S(4)-C(82) | 108.06(18) |
| C(87)-C(82)-C(83) | 119.8(4) |
| C(87)-C(82)-S(4) | 119.4(3) |
| C(83)-C(82)-S(4) | 120.8(4) |
| C(84)-C(83)-C(82) | 119.7(5) |
| C(84)-C(83)-H(83) | 120.2 |
| C(82)-C(83)-H(83) | 120.2 |
| C(83)-C(84)-C(85) | 121.8(4) |
| C(83)-C(84)-H(84) | 119.1 |
| C(85)-C(84)-H(84) | 119.1 |
| C(84)-C(85)-C(86) | 117.6(4) |
| C(84)-C(85)-C(88) | 121.3(4) |
| C(86)-C(85)-C(88) | 121.1(5) |
| C(87)-C(86)-C(85) | 120.7(4) |

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| C(87)-C(86)-H(86) | 119.6 |
| C(85)-C(86)-H(86) | 119.6 |
| C(82)-C(87)-C(86) | 120.4(4) |
| C(82)-C(87)-H(87) | 119.8 |
| C(86)-C(87)-H(87) | 119.8 |
| C(85)-C(88)-H(88A) | 109.5 |
| C(85)-C(88)-H(88B) | 109.5 |
| H(88A)-C(88)-H(88B) | 109.5 |
| C(85)-C(88)-H(88C) | 109.5 |
| H(88A)-C(88)-H(88C) | 109.5 |
| H(88B)-C(88)-H(88C) | 109.5 |
| C(75)-N(8)-C(89) | 123.0(3) |
| C(75)-N(8)-C(90) | 122.5(3) |
| C(89)-N(8)-C(90) | 113.2(3) |
| N(8)-C(89)-H(89A) | 109.5 |
| N(8)-C(89)-H(89B) | 109.5 |
| H(89A)-C(89)-H(89B) | 109.5 |
| N(8)-C(89)-H(89C) | 109.5 |
| H(89A)-C(89)-H(89C) | 109.5 |
| H(89B)-C(89)-H(89C) | 109.5 |
| N(8)-C(90)-H(90A) | 109.5 |
| N(8)-C(90)-H(90B) | 109.5 |
| H(90A)-C(90)-H(90B) | 109.5 |
| N(8)-C(90)-H(90C) | 109.5 |
| H(90A)-C(90)-H(90C) | 109.5 |
| H(90B)-C(90)-H(90C) | 109.5 |
| C(96)-C(91)-C(92) | 119.5(4) |
| C(96)-C(91)-C(75) | 118.7(4) |
| C(92)-C(91)-C(75) | 121.8(4) |
| C(93)-C(92)-C(91) | 119.9(4) |
| C(93)-C(92)-H(92) | 120.1 |
| C(91)-C(92)-H(92) | 120.1 |
| C(92)-C(93)-C(94) | 120.5(5) |
| C(92)-C(93)-H(93) | 119.8 |
| C(94)-C(93)-H(93) | 119.8 |
| C(95)-C(94)-C(93) | 119.5(4) |
| C(95)-C(94)-H(94) | 120.3 |

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| C(93)-C(94)-H(94) | 120.3 |
| C(94)-C(95)-C(96) | 120.4(5) |
| C(94)-C(95)-H(95) | 119.8 |
| C(96)-C(95)-H(95) | 119.8 |
| C(91)-C(96)-C(95) | 120.2(4) |
| C(91)-C(96)-H(96) | 119.9 |
| C(95)-C(96)-H(96) | 119.9 |

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Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for DJL. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| C(1) | 51(3) | 30(2) | 38(3) | 3(2) | 0(2) | 5(2) |
| O(1) | 51(2) | 43(2) | 68(2) | -14(2) | 0(2) | 4(2) |
| C(2) | 40(3) | 33(2) | 46(3) | 6(2) | -4(2) | 2(2) |
| C(3) | 45(3) | 38(2) | 35(2) | 1(2) | -2(2) | -9(2) |
| C(4) | 36(3) | 35(2) | 44(3) | -1(2) | -1(2) | -4(2) |
| C(5) | 53(3) | 39(3) | 42(3) | 1(2) | -3(2) | -7(2) |
| C(6) | 58(3) | 61(3) | 54(3) | -11(2) | 16(3) | -17(3) |
| C(7) | 44(3) | 93(4) | 66(4) | -20(3) | 5(3) | -18(3) |
| C(8) | 48(3) | 98(4) | 52(3) | -18(3) | -8(3) | -18(3) |
| C(9) | 45(3) | 57(3) | 41(3) | -6(2) | -1(2) | -7(2) |
| N(1) | 38(2) | 43(2) | 50(2) | 13(2) | -5(2) | -2(2) |
| S(1) | 45(1) | 47(1) | 66(1) | 4(1) | 2(1) | -6(1) |
| O(2) | 74(2) | 42(2) | 81(2) | -6(2) | 11(2) | -17(2) |
| O(3) | 36(2) | 83(2) | 83(2) | 10(2) | -3(2) | 0(2) |
| C(10) | 37(3) | 47(3) | 63(3) | 11(2) | 7(2) | 3(2) |
| C(11) | 65(4) | 47(3) | 73(4) | 13(3) | 9(3) | 1(3) |
| C(12) | 69(4) | 61(4) | 68(4) | 23(3) | 12(3) | 2(3) |
| C(13) | 45(3) | 73(4) | 62(4) | 13(3) | 14(2) | 5(3) |
| C(14) | 51(3) | 56(3) | 64(3) | -5(3) | 13(2) | 1(2) |
| C(15) | 52(3) | 40(3) | 65(3) | 9(2) | 14(2) | 5(2) |
| C(16) | 78(4) | 107(5) | 61(4) | 7(3) | 16(3) | 4(3) |
| N(2) | 52(2) | 40(2) | 46(2) | -1(2) | -8(2) | 1(2) |
| C(17) | 67(4) | 51(3) | 63(3) | -11(2) | -5(3) | -11(3) |
| C(18) | 66(3) | 65(3) | 44(3) | 5(2) | -18(2) | 1(3) |
| C(19) | 45(3) | 27(2) | 42(3) | -2(2) | -4(2) | -1(2) |
| C(20) | 60(3) | 43(3) | 46(3) | -1(2) | 0(2) | -1(2) |
| C(21) | 48(3) | 48(3) | 90(4) | -2(3) | 6(3) | 9(3) |
| C(22) | 68(4) | 49(3) | 90(5) | -8(3) | -21(3) | 16(3) |
| C(23) | 92(5) | 47(3) | 58(4) | -2(3) | -27(3) | 16(3) |
| C(24) | 68(3) | 37(2) | 40(3) | 0(2) | -5(2) | 4(2) |
| C(25) | 41(3) | 27(2) | 36(3) | 4(2) | 2(2) | 1(2) |
| O(4) | 40(2) | 41(2) | 42(2) | -4(1) | 7(1) | -3(1) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C(26) | 35(3) | 31(2) | 39(2) | 5(2) | 2(2) | -2(2) |
| C(27) | 47(3) | 34(2) | 41(3) | 0(2) | 1(2) | -4(2) |
| C(28) | 36(3) | 30(2) | 36(2) | 1(2) | 7(2) | -2(2) |
| C(29) | 43(3) | 40(2) | 43(3) | 3(2) | 0(2) | 1(2) |
| C(30) | 47(3) | 54(3) | 56(3) | 9(2) | 16(2) | -11(2) |
| C(31) | 35(3) | 64(3) | 75(4) | -8(3) | 10(3) | -9(2) |
| C(32) | 45(3) | 90(4) | 51(3) | -8(3) | -1(2) | -16(3) |
| C(33) | 42(3) | 73(3) | 39(3) | -3(2) | 1(2) | -8(3) |
| N(3) | 42(2) | 35(2) | 43(2) | 5(2) | -3(2) | -4(2) |
| S(2) | 45(1) | 41(1) | 42(1) | 3(1) | -4(1) | -12(1) |
| O(5) | 81(2) | 51(2) | 43(2) | -12(2) | -2(2) | -24(2) |
| O(6) | 35(2) | 58(2) | 62(2) | 12(2) | -6(1) | -2(2) |
| C(34) | 30(2) | 38(2) | 42(3) | 1(2) | 3(2) | -8(2) |
| C(35) | 48(3) | 43(3) | 50(3) | -2(2) | 2(2) | -10(2) |
| C(36) | 46(3) | 69(3) | 45(3) | 14(3) | -3(2) | -18(3) |
| C(37) | 37(3) | 73(4) | 62(3) | 20(3) | -1(2) | -6(3) |
| C(38) | 56(3) | 40(3) | 95(4) | 23(3) | 5(3) | 9(2) |
| C(39) | 52(3) | 43(3) | 61(3) | -6(2) | 7(2) | 2(2) |
| C(40) | 68(4) | 119(5) | 86(4) | 62(4) | -8(3) | 4(3) |
| N(4) | 56(2) | 42(2) | 41(2) | -6(2) | 2(2) | 0(2) |
| C(41) | 115(5) | 66(4) | 58(3) | -25(3) | 0(3) | 5(3) |
| C(42) | 65(3) | 66(3) | 42(3) | 5(2) | 0(2) | 0(3) |
| C(43) | 47(3) | 31(2) | 47(3) | -5(2) | 2(2) | 6(2) |
| C(44) | 61(3) | 46(3) | 54(3) | -5(2) | 12(3) | 14(3) |
| C(45) | 54(3) | 62(3) | 79(4) | -5(3) | 13(3) | 18(3) |
| C(46) | 62(4) | 51(3) | 76(4) | -1(3) | -7(3) | 13(3) |
| C(47) | 67(4) | 42(3) | 61(3) | 5(2) | -6(3) | 11(3) |
| C(48) | 59(3) | 32(2) | 51(3) | 3(2) | 0(2) | 4(2) |
| C(49) | 38(3) | 31(2) | 35(3) | 7(2) | 2(2) | 3(2) |
| O(7) | 43(2) | 45(2) | 46(2) | 1(1) | 4(1) | -6(2) |
| C(50) | 39(3) | 34(2) | 36(3) | -4(2) | -2(2) | -1(2) |
| C(51) | 42(3) | 38(2) | 40(3) | -3(2) | 3(2) | -2(2) |
| C(52) | 44(3) | 28(2) | 38(3) | 5(2) | -4(2) | -1(2) |
| C(53) | 52(3) | 43(3) | 39(3) | -11(2) | 0(2) | -3(2) |
| C(54) | 58(3) | 61(3) | 53(3) | -10(2) | 5(3) | -5(3) |
| C(55) | 84(4) | 55(3) | 37(3) | -7(2) | 13(3) | -10(3) |
| C(56) | 68(4) | 55(3) | 46(3) | -4(2) | -16(3) | -9(3) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C(57) | 50(3) | 45(3) | 39(3) | -3(2) | -2(2) | -4(2) |
| N(5) | 53(2) | 35(2) | 35(2) | 1(2) | -8(2) | 4(2) |
| S(3) | 53(1) | 52(1) | 38(1) | -5(1) | 0(1) | -4(1) |
| O(8) | 60(2) | 60(2) | 59(2) | -20(2) | -3(2) | -21(2) |
| O(9) | 67(2) | 76(2) | 33(2) | 10(2) | 8(2) | 6(2) |
| C(58) | 49(3) | 43(3) | 36(2) | -4(2) | 3(2) | -8(2) |
| C(59) | 74(4) | 48(3) | 53(3) | -4(2) | 11(3) | 4(3) |
| C(60) | 95(4) | 43(3) | 58(3) | -4(2) | 19(3) | -2(3) |
| C(61) | 83(4) | 49(3) | 41(3) | 1(2) | 10(3) | 26(3) |
| C(62) | 63(3) | 58(3) | 41(3) | -5(2) | 10(2) | 6(3) |
| C(63) | 63(3) | 39(3) | 38(3) | 0(2) | 4(2) | 7(2) |
| C(64) | 108(5) | 78(4) | 67(4) | 15(3) | 9(3) | 38(4) |
| N(6) | 38(2) | 60(3) | 57(2) | -7(2) | -1(2) | -16(2) |
| C(65) | 67(4) | 80(4) | 77(4) | -5(3) | 8(3) | -37(3) |
| C(66) | 42(3) | 101(4) | 60(3) | -8(3) | -5(2) | 1(3) |
| C(67) | 41(3) | 34(2) | 46(3) | -2(2) | 9(2) | -3(2) |
| C(68) | 49(3) | 57(3) | 54(3) | 10(2) | 8(2) | -1(2) |
| C(69) | 74(4) | 62(3) | 57(3) | 5(3) | 27(3) | 1(3) |
| C(70) | 75(4) | 53(3) | 51(3) | 11(2) | 3(3) | 5(3) |
| C(71) | 56(3) | 41(3) | 58(3) | 7(2) | 3(3) | 5(2) |
| C(72) | 51(3) | 35(2) | 43(3) | 3(2) | 7(2) | -4(2) |
| C(73) | 38(3) | 28(2) | 50(3) | -6(2) | 0(2) | 0(2) |
| O(10) | 61(2) | 39(2) | 50(2) | -3(1) | -2(2) | 13(2) |
| C(74) | 37(3) | 33(2) | 42(3) | 3(2) | -3(2) | -1(2) |
| C(75) | 38(3) | 34(2) | 48(3) | 4(2) | 6(2) | -1(2) |
| C(76) | 45(3) | 25(2) | 44(3) | 3(2) | -4(2) | 1(2) |
| C(77) | 40(3) | 36(2) | 55(3) | 1(2) | -4(2) | -1(2) |
| C(78) | 50(3) | 51(3) | 63(3) | 1(2) | 15(3) | 1(2) |
| C(79) | 71(4) | 64(3) | 51(3) | 2(3) | 11(3) | 3(3) |
| C(80) | 66(4) | 79(4) | 47(3) | 1(3) | -7(3) | 8(3) |
| C(81) | 48(3) | 52(3) | 49(3) | 2(2) | 1(2) | 6(2) |
| N(7) | 36(2) | 44(2) | 39(2) | -1(2) | -3(2) | -10(2) |
| S(4) | 52(1) | 44(1) | 50(1) | 11(1) | 7(1) | -2(1) |
| O(11) | 76(2) | 39(2) | 81(2) | 18(2) | 19(2) | -2(2) |
| O(12) | 70(2) | 77(2) | 35(2) | 3(2) | 4(2) | 1(2) |
| C(82) | 46(3) | 42(3) | 48(3) | -1(2) | 9(2) | -10(2) |
| C(83) | 50(3) | 56(3) | 69(3) | 3(3) | 12(3) | -7(3) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C(84) | 57(4) | 68(4) | 63(3) | -5(3) | 2(3) | -22(3) |
| C(85) | 44(3) | 67(3) | 54(3) | 16(3) | 10(2) | -6(3) |
| C(86) | 55(3) | 46(3) | 74(3) | 6(2) | 18(3) | -9(3) |
| C(87) | 41(3) | 52(3) | 59(3) | -1(2) | 10(2) | -4(2) |
| C(88) | 55(4) | 97(4) | 79(4) | 28(3) | 6(3) | -6(3) |
| N(8) | 41(2) | 40(2) | 60(2) | 10(2) | -4(2) | 9(2) |
| C(89) | 60(4) | 48(3) | 109(4) | 30(3) | -10(3) | 5(3) |
| C(90) | 49(3) | 70(3) | 58(3) | 0(3) | -11(2) | 4(3) |
| C(91) | 36(3) | 23(2) | 58(3) | 5(2) | 1(2) | 0(2) |
| C(92) | 46(3) | 38(3) | 71(3) | -8(2) | 4(3) | 0(2) |
| C(93) | 68(4) | 44(3) | 79(4) | -13(3) | 18(3) | -2(3) |
| C(94) | 74(4) | 39(3) | 68(4) | -6(2) | -1(3) | 0(3) |
| C(95) | 50(3) | 36(3) | 77(4) | 4(2) | -14(3) | -2(2) |
| C(96) | 48(3) | 37(3) | 59(3) | 5(2) | 0(2) | 1(2) |

Table 5. Hydrogen coordinates ( x $10^4$) and isotropic displacement parameters ($Å^2$x $10^3$) for DJL.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(5) | 3523 | 7118 | -463 | 54 |
| H(6) | 4481 | 7229 | -455 | 69 |
| H(7) | 5020 | 7475 | 295 | 81 |
| H(8) | 4590 | 7686 | 1033 | 80 |
| H(9) | 3633 | 7618 | 1025 | 58 |
| H(1A) | 1832 | 7493 | -229 | 53 |
| H(11) | 1624 | 5131 | 1077 | 74 |
| H(12) | 1843 | 5386 | 1928 | 79 |
| H(14) | 1852 | 8289 | 1712 | 68 |
| H(15) | 1625 | 8058 | 861 | 62 |
| H(16A) | 2463 | 7001 | 2510 | 122 |
| H(16B) | 1902 | 6486 | 2654 | 122 |
| H(16C) | 1916 | 7642 | 2565 | 122 |
| H(17A) | 2563 | 4025 | -481 | 91 |
| H(17B) | 2383 | 4207 | -1063 | 91 |
| H(17C) | 1920 | 4163 | -670 | 91 |
| H(18A) | 1597 | 5971 | -860 | 90 |
| H(18B) | 1967 | 5758 | -1317 | 90 |
| H(18C) | 2097 | 6691 | -965 | 90 |
| H(20) | 3473 | 5085 | -711 | 60 |
| H(21) | 4314 | 4401 | -403 | 74 |
| H(22) | 4496 | 4152 | 451 | 84 |
| H(23) | 3828 | 4523 | 989 | 81 |
| H(24) | 2984 | 5215 | 691 | 58 |
| H(29) | 5647 | 4146 | 6978 | 50 |
| H(30) | 6514 | 4865 | 6937 | 62 |
| H(31) | 7127 | 4963 | 7655 | 70 |
| H(32) | 6851 | 4418 | 8418 | 74 |
| H(33) | 5970 | 3763 | 8467 | 62 |
| H(3A) | 4133 | 3515 | 7255 | 48 |
| H(35) | 4220 | 2491 | 8395 | 56 |

| | | | | |
|---|---|---|---|---|
| H(36) | 4453 | 1563 | 9112 | 65 |
| H(38) | 4387 | -890 | 8291 | 77 |
| H(39) | 4169 | 19 | 7565 | 63 |
| H(40A) | 4795 | 22 | 9490 | 138 |
| H(40B) | 4749 | -956 | 9161 | 138 |
| H(40C) | 4208 | -521 | 9389 | 138 |
| H(41A) | 5331 | 820 | 6528 | 120 |
| H(41B) | 5231 | 1328 | 5989 | 120 |
| H(41C) | 4716 | 873 | 6250 | 120 |
| H(42A) | 4202 | 2541 | 6305 | 87 |
| H(42B) | 4654 | 2826 | 5926 | 87 |
| H(42C) | 4606 | 3454 | 6425 | 87 |
| H(44) | 6136 | 2220 | 6610 | 64 |
| H(45) | 7000 | 1667 | 6947 | 77 |
| H(46) | 7096 | 975 | 7743 | 77 |
| H(47) | 6331 | 831 | 8210 | 69 |
| H(48) | 5467 | 1403 | 7888 | 57 |
| H(53) | 3126 | -919 | 9514 | 54 |
| H(54) | 3227 | -1519 | 8715 | 69 |
| H(55) | 2448 | -1698 | 8141 | 70 |
| H(56) | 1566 | -1315 | 8381 | 69 |
| H(57) | 1456 | -796 | 9198 | 54 |
| H(5A) | 2824 | -623 | 10847 | 50 |
| H(59) | 2454 | 2718 | 10830 | 69 |
| H(60) | 1718 | 3602 | 10428 | 77 |
| H(62) | 702 | 1279 | 10536 | 65 |
| H(63) | 1445 | 380 | 10919 | 57 |
| H(64A) | 718 | 3755 | 10159 | 126 |
| H(64B) | 312 | 2854 | 10238 | 126 |
| H(64C) | 672 | 2876 | 9762 | 126 |
| H(65A) | 3392 | 2496 | 9945 | 112 |
| H(65B) | 4026 | 2144 | 10037 | 112 |
| H(65C) | 3675 | 2377 | 10505 | 112 |
| H(66A) | 3768 | 584 | 10841 | 102 |
| H(66B) | 4216 | 566 | 10432 | 102 |
| H(66C) | 3726 | -227 | 10408 | 102 |
| H(68) | 3403 | 1209 | 9144 | 64 |

| | | | | |
|---|---|---|---|---|
| H(69) | 2988 | 1810 | 8388 | 75 |
| H(70) | 2058 | 2279 | 8317 | 71 |
| H(71) | 1539 | 2165 | 9005 | 62 |
| H(72) | 1943 | 1549 | 9762 | 52 |
| H(77) | -605 | 1094 | 8294 | 53 |
| H(78) | -769 | 1098 | 9136 | 65 |
| H(79) | -45 | 866 | 9748 | 74 |
| H(80) | 852 | 581 | 9522 | 77 |
| H(81) | 1022 | 529 | 8675 | 60 |
| H(7A) | -145 | 455 | 6867 | 48 |
| H(83) | 1520 | 2174 | 7037 | 69 |
| H(84) | 2385 | 1562 | 7324 | 75 |
| H(86) | 1894 | -1149 | 6891 | 69 |
| H(87) | 1024 | -533 | 6608 | 60 |
| H(88A) | 3089 | 49 | 7150 | 115 |
| H(88B) | 2808 | -965 | 7288 | 115 |
| H(88C) | 2875 | -105 | 7694 | 115 |
| H(89A) | -317 | 4040 | 7357 | 110 |
| H(89B) | -970 | 3911 | 7204 | 110 |
| H(89C) | -538 | 3864 | 6783 | 110 |
| H(90A) | -682 | 2032 | 6522 | 90 |
| H(90B) | -1238 | 2407 | 6749 | 90 |
| H(90C) | -941 | 1426 | 6958 | 90 |
| H(92) | -648 | 3114 | 8262 | 62 |
| H(93) | -257 | 3940 | 8968 | 76 |
| H(94) | 696 | 4276 | 9056 | 73 |
| H(95) | 1258 | 3743 | 8448 | 66 |
| H(96) | 882 | 2805 | 7774 | 58 |

Table 6. Torsion angles [°] for DJL.

| | |
|---|---|
| O(1)-C(1)-C(2)-C(3) | -163.9(4) |
| C(4)-C(1)-C(2)-C(3) | 20.8(6) |
| O(1)-C(1)-C(2)-N(1) | 16.3(5) |
| C(4)-C(1)-C(2)-N(1) | -159.0(3) |
| N(1)-C(2)-C(3)-N(2) | 24.5(6) |
| C(1)-C(2)-C(3)-N(2) | -155.3(4) |
| N(1)-C(2)-C(3)-C(19) | -156.1(4) |
| C(1)-C(2)-C(3)-C(19) | 24.1(6) |
| O(1)-C(1)-C(4)-C(9) | 38.0(5) |
| C(2)-C(1)-C(4)-C(9) | -146.6(4) |
| O(1)-C(1)-C(4)-C(5) | -137.5(4) |
| C(2)-C(1)-C(4)-C(5) | 37.9(6) |
| C(9)-C(4)-C(5)-C(6) | 2.3(6) |
| C(1)-C(4)-C(5)-C(6) | 177.8(4) |
| C(4)-C(5)-C(6)-C(7) | 0.1(7) |
| C(5)-C(6)-C(7)-C(8) | -1.8(7) |
| C(6)-C(7)-C(8)-C(9) | 0.9(8) |
| C(7)-C(8)-C(9)-C(4) | 1.7(7) |
| C(5)-C(4)-C(9)-C(8) | -3.2(6) |
| C(1)-C(4)-C(9)-C(8) | -179.0(4) |
| C(3)-C(2)-N(1)-S(1) | 71.6(4) |
| C(1)-C(2)-N(1)-S(1) | -108.5(3) |
| C(2)-N(1)-S(1)-O(3) | -178.6(3) |
| C(2)-N(1)-S(1)-O(2) | -48.6(3) |
| C(2)-N(1)-S(1)-C(10) | 66.1(3) |
| O(3)-S(1)-C(10)-C(11) | 121.9(4) |
| O(2)-S(1)-C(10)-C(11) | -9.1(4) |
| N(1)-S(1)-C(10)-C(11) | -124.6(4) |
| O(3)-S(1)-C(10)-C(15) | -57.9(4) |
| O(2)-S(1)-C(10)-C(15) | 171.1(3) |
| N(1)-S(1)-C(10)-C(15) | 55.6(4) |
| C(15)-C(10)-C(11)-C(12) | -0.6(7) |
| S(1)-C(10)-C(11)-C(12) | 179.6(4) |
| C(10)-C(11)-C(12)-C(13) | -0.6(7) |
| C(11)-C(12)-C(13)-C(14) | 1.4(7) |

| | |
|---|---|
| C(11)-C(12)-C(13)-C(16) | -176.5(4) |
| C(12)-C(13)-C(14)-C(15) | -1.0(7) |
| C(16)-C(13)-C(14)-C(15) | 176.9(4) |
| C(13)-C(14)-C(15)-C(10) | -0.1(7) |
| C(11)-C(10)-C(15)-C(14) | 0.9(7) |
| S(1)-C(10)-C(15)-C(14) | -179.3(3) |
| C(2)-C(3)-N(2)-C(17) | -144.9(4) |
| C(19)-C(3)-N(2)-C(17) | 35.7(6) |
| C(2)-C(3)-N(2)-C(18) | 20.7(6) |
| C(19)-C(3)-N(2)-C(18) | -158.8(4) |
| N(2)-C(3)-C(19)-C(24) | -134.5(4) |
| C(2)-C(3)-C(19)-C(24) | 46.0(6) |
| N(2)-C(3)-C(19)-C(20) | 51.0(5) |
| C(2)-C(3)-C(19)-C(20) | -128.5(4) |
| C(24)-C(19)-C(20)-C(21) | -2.4(6) |
| C(3)-C(19)-C(20)-C(21) | 172.3(4) |
| C(19)-C(20)-C(21)-C(22) | 0.5(7) |
| C(20)-C(21)-C(22)-C(23) | 1.5(7) |
| C(21)-C(22)-C(23)-C(24) | -1.7(8) |
| C(22)-C(23)-C(24)-C(19) | -0.2(7) |
| C(20)-C(19)-C(24)-C(23) | 2.2(6) |
| C(3)-C(19)-C(24)-C(23) | -172.5(4) |
| O(4)-C(25)-C(26)-C(27) | -162.4(4) |
| C(28)-C(25)-C(26)-C(27) | 25.8(5) |
| O(4)-C(25)-C(26)-N(3) | 20.9(5) |
| C(28)-C(25)-C(26)-N(3) | -150.9(3) |
| N(3)-C(26)-C(27)-N(4) | 28.0(6) |
| C(25)-C(26)-C(27)-N(4) | -148.5(4) |
| N(3)-C(26)-C(27)-C(43) | -150.1(3) |
| C(25)-C(26)-C(27)-C(43) | 33.4(6) |
| O(4)-C(25)-C(28)-C(33) | 41.7(5) |
| C(26)-C(25)-C(28)-C(33) | -146.3(4) |
| O(4)-C(25)-C(28)-C(29) | -134.0(4) |
| C(26)-C(25)-C(28)-C(29) | 38.1(5) |
| C(33)-C(28)-C(29)-C(30) | 0.3(6) |
| C(25)-C(28)-C(29)-C(30) | 176.0(4) |
| C(28)-C(29)-C(30)-C(31) | 1.5(6) |

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| C(29)-C(30)-C(31)-C(32) | -1.8(7) |
| C(30)-C(31)-C(32)-C(33) | 0.3(7) |
| C(31)-C(32)-C(33)-C(28) | 1.5(7) |
| C(29)-C(28)-C(33)-C(32) | -1.8(6) |
| C(25)-C(28)-C(33)-C(32) | -177.6(4) |
| C(27)-C(26)-N(3)-S(2) | 63.4(4) |
| C(25)-C(26)-N(3)-S(2) | -119.8(3) |
| C(26)-N(3)-S(2)-O(5) | -69.4(3) |
| C(26)-N(3)-S(2)-O(6) | 161.5(3) |
| C(26)-N(3)-S(2)-C(34) | 46.0(3) |
| O(5)-S(2)-C(34)-C(35) | 170.9(3) |
| O(6)-S(2)-C(34)-C(35) | -60.2(4) |
| N(3)-S(2)-C(34)-C(35) | 53.2(4) |
| O(5)-S(2)-C(34)-C(39) | -15.5(4) |
| O(6)-S(2)-C(34)-C(39) | 113.4(4) |
| N(3)-S(2)-C(34)-C(39) | -133.2(3) |
| C(39)-C(34)-C(35)-C(36) | -1.9(6) |
| S(2)-C(34)-C(35)-C(36) | 171.7(3) |
| C(34)-C(35)-C(36)-C(37) | -0.4(7) |
| C(35)-C(36)-C(37)-C(38) | 1.9(7) |
| C(35)-C(36)-C(37)-C(40) | -177.4(4) |
| C(36)-C(37)-C(38)-C(39) | -1.3(7) |
| C(40)-C(37)-C(38)-C(39) | 178.0(4) |
| C(35)-C(34)-C(39)-C(38) | 2.5(6) |
| S(2)-C(34)-C(39)-C(38) | -171.2(3) |
| C(37)-C(38)-C(39)-C(34) | -0.9(7) |
| C(26)-C(27)-N(4)-C(42) | 23.8(6) |
| C(43)-C(27)-N(4)-C(42) | -158.1(4) |
| C(26)-C(27)-N(4)-C(41) | -142.7(4) |
| C(43)-C(27)-N(4)-C(41) | 35.4(6) |
| N(4)-C(27)-C(43)-C(44) | 46.8(5) |
| C(26)-C(27)-C(43)-C(44) | -135.0(4) |
| N(4)-C(27)-C(43)-C(48) | -136.9(4) |
| C(26)-C(27)-C(43)-C(48) | 41.3(5) |
| C(48)-C(43)-C(44)-C(45) | -2.2(6) |
| C(27)-C(43)-C(44)-C(45) | 174.1(4) |
| C(43)-C(44)-C(45)-C(46) | 1.4(7) |

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| C(44)-C(45)-C(46)-C(47) | 0.1(7) |
| C(45)-C(46)-C(47)-C(48) | -0.7(7) |
| C(46)-C(47)-C(48)-C(43) | -0.2(6) |
| C(44)-C(43)-C(48)-C(47) | 1.6(6) |
| C(27)-C(43)-C(48)-C(47) | -174.7(4) |
| O(7)-C(49)-C(50)-C(51) | -152.3(4) |
| C(52)-C(49)-C(50)-C(51) | 34.2(6) |
| O(7)-C(49)-C(50)-N(5) | 27.9(5) |
| C(52)-C(49)-C(50)-N(5) | -145.6(3) |
| N(5)-C(50)-C(51)-N(6) | 26.9(6) |
| C(49)-C(50)-C(51)-N(6) | -152.9(4) |
| N(5)-C(50)-C(51)-C(67) | -153.2(3) |
| C(49)-C(50)-C(51)-C(67) | 27.0(6) |
| O(7)-C(49)-C(52)-C(53) | -138.7(4) |
| C(50)-C(49)-C(52)-C(53) | 35.1(5) |
| O(7)-C(49)-C(52)-C(57) | 35.9(5) |
| C(50)-C(49)-C(52)-C(57) | -150.3(4) |
| C(57)-C(52)-C(53)-C(54) | 1.6(6) |
| C(49)-C(52)-C(53)-C(54) | 176.1(4) |
| C(52)-C(53)-C(54)-C(55) | 0.8(6) |
| C(53)-C(54)-C(55)-C(56) | -1.2(7) |
| C(54)-C(55)-C(56)-C(57) | -0.7(7) |
| C(55)-C(56)-C(57)-C(52) | 3.0(6) |
| C(53)-C(52)-C(57)-C(56) | -3.5(6) |
| C(49)-C(52)-C(57)-C(56) | -178.1(4) |
| C(51)-C(50)-N(5)-S(3) | 64.5(5) |
| C(49)-C(50)-N(5)-S(3) | -115.7(3) |
| C(50)-N(5)-S(3)-O(8) | -79.8(3) |
| C(50)-N(5)-S(3)-O(9) | 152.2(3) |
| C(50)-N(5)-S(3)-C(58) | 34.3(4) |
| O(8)-S(3)-C(58)-C(59) | 6.6(4) |
| O(9)-S(3)-C(58)-C(59) | 136.2(3) |
| N(5)-S(3)-C(58)-C(59) | -110.5(4) |
| O(8)-S(3)-C(58)-C(63) | -175.4(3) |
| O(9)-S(3)-C(58)-C(63) | -45.8(4) |
| N(5)-S(3)-C(58)-C(63) | 67.5(4) |
| C(63)-C(58)-C(59)-C(60) | -2.2(6) |

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| S(3)-C(58)-C(59)-C(60) | 175.7(3) |
| C(58)-C(59)-C(60)-C(61) | -0.1(7) |
| C(59)-C(60)-C(61)-C(62) | 3.2(7) |
| C(59)-C(60)-C(61)-C(64) | -174.5(4) |
| C(60)-C(61)-C(62)-C(63) | -4.0(6) |
| C(64)-C(61)-C(62)-C(63) | 173.7(4) |
| C(59)-C(58)-C(63)-C(62) | 1.4(6) |
| S(3)-C(58)-C(63)-C(62) | -176.6(3) |
| C(61)-C(62)-C(63)-C(58) | 1.9(6) |
| C(50)-C(51)-N(6)-C(65) | -139.2(4) |
| C(67)-C(51)-N(6)-C(65) | 40.9(6) |
| C(50)-C(51)-N(6)-C(66) | 24.4(6) |
| C(67)-C(51)-N(6)-C(66) | -155.5(4) |
| N(6)-C(51)-C(67)-C(72) | -137.4(4) |
| C(50)-C(51)-C(67)-C(72) | 42.7(5) |
| N(6)-C(51)-C(67)-C(68) | 45.3(5) |
| C(50)-C(51)-C(67)-C(68) | -134.7(4) |
| C(72)-C(67)-C(68)-C(69) | -2.5(6) |
| C(51)-C(67)-C(68)-C(69) | 174.9(4) |
| C(67)-C(68)-C(69)-C(70) | 1.2(7) |
| C(68)-C(69)-C(70)-C(71) | 0.5(7) |
| C(69)-C(70)-C(71)-C(72) | -0.9(7) |
| C(68)-C(67)-C(72)-C(71) | 2.1(6) |
| C(51)-C(67)-C(72)-C(71) | -175.3(4) |
| C(70)-C(71)-C(72)-C(67) | -0.4(6) |
| O(10)-C(73)-C(74)-C(75) | -163.2(4) |
| C(76)-C(73)-C(74)-C(75) | 25.3(6) |
| O(10)-C(73)-C(74)-N(7) | 13.0(5) |
| C(76)-C(73)-C(74)-N(7) | -158.5(3) |
| N(7)-C(74)-C(75)-N(8) | 27.1(6) |
| C(73)-C(74)-C(75)-N(8) | -156.9(4) |
| N(7)-C(74)-C(75)-C(91) | -149.8(4) |
| C(73)-C(74)-C(75)-C(91) | 26.2(6) |
| O(10)-C(73)-C(76)-C(77) | -132.9(4) |
| C(74)-C(73)-C(76)-C(77) | 38.9(6) |
| O(10)-C(73)-C(76)-C(81) | 41.6(5) |
| C(74)-C(73)-C(76)-C(81) | -146.6(4) |

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| C(81)-C(76)-C(77)-C(78) | 0.5(6) |
| C(73)-C(76)-C(77)-C(78) | 175.0(4) |
| C(76)-C(77)-C(78)-C(79) | 0.7(6) |
| C(77)-C(78)-C(79)-C(80) | -1.1(7) |
| C(78)-C(79)-C(80)-C(81) | 0.1(7) |
| C(79)-C(80)-C(81)-C(76) | 1.2(7) |
| C(77)-C(76)-C(81)-C(80) | -1.5(6) |
| C(73)-C(76)-C(81)-C(80) | -176.3(4) |
| C(75)-C(74)-N(7)-S(4) | 74.8(4) |
| C(73)-C(74)-N(7)-S(4) | -101.5(4) |
| C(74)-N(7)-S(4)-O(11) | -43.9(3) |
| C(74)-N(7)-S(4)-O(12) | -172.2(3) |
| C(74)-N(7)-S(4)-C(82) | 73.0(3) |
| O(11)-S(4)-C(82)-C(87) | -173.4(3) |
| O(12)-S(4)-C(82)-C(87) | -43.2(4) |
| N(7)-S(4)-C(82)-C(87) | 70.2(4) |
| O(11)-S(4)-C(82)-C(83) | 7.6(4) |
| O(12)-S(4)-C(82)-C(83) | 137.9(4) |
| N(7)-S(4)-C(82)-C(83) | -108.7(4) |
| C(87)-C(82)-C(83)-C(84) | 0.0(7) |
| S(4)-C(82)-C(83)-C(84) | 178.9(3) |
| C(82)-C(83)-C(84)-C(85) | -0.4(7) |
| C(83)-C(84)-C(85)-C(86) | 0.9(7) |
| C(83)-C(84)-C(85)-C(88) | 180.0(4) |
| C(84)-C(85)-C(86)-C(87) | -1.1(7) |
| C(88)-C(85)-C(86)-C(87) | 179.8(4) |
| C(83)-C(82)-C(87)-C(86) | -0.2(7) |
| S(4)-C(82)-C(87)-C(86) | -179.1(3) |
| C(85)-C(86)-C(87)-C(82) | 0.8(7) |
| C(74)-C(75)-N(8)-C(89) | -150.5(4) |
| C(91)-C(75)-N(8)-C(89) | 26.4(6) |
| C(74)-C(75)-N(8)-C(90) | 15.8(6) |
| C(91)-C(75)-N(8)-C(90) | -167.3(4) |
| N(8)-C(75)-C(91)-C(96) | -122.0(4) |
| C(74)-C(75)-C(91)-C(96) | 55.1(5) |
| N(8)-C(75)-C(91)-C(92) | 59.1(5) |
| C(74)-C(75)-C(91)-C(92) | -123.7(4) |

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| C(96)-C(91)-C(92)-C(93) | -3.1(6) |
| C(75)-C(91)-C(92)-C(93) | 175.7(4) |
| C(91)-C(92)-C(93)-C(94) | 3.4(7) |
| C(92)-C(93)-C(94)-C(95) | -0.8(7) |
| C(93)-C(94)-C(95)-C(96) | -1.9(7) |
| C(92)-C(91)-C(96)-C(95) | 0.4(6) |
| C(75)-C(91)-C(96)-C(95) | -178.5(4) |
| C(94)-C(95)-C(96)-C(91) | 2.2(6) |

Symmetry transformations used to generate equivalent atoms: