Supporting Information

Regio- and stereoselective synthesis of 2-cyclopentenones *via* a hydrogenolysis-terminated Heck cyclization of *β*-alkylthio dienones

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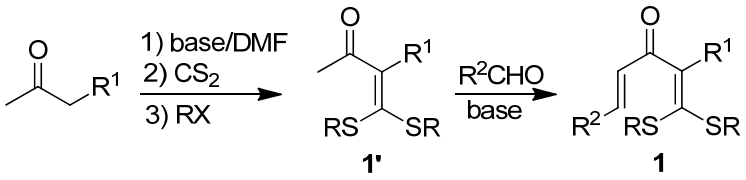
I. General

All reagents were purchased from commercial sources and used without treatment, unless otherwise indicated. The products were purified by column chromatography over silica gel. ^{1}H NMR and ^{13}C NMR spectra were recorded at 25ºC on a Varian 500 MHz and 125 MHz, and using TMS as internal standard. High-resolution mass spectra (HRMS) were obtained using a Bruker microTOF II focus spectrometer (ESI). Melting points were uncorrected. The compound **2a** with dimension 0.40 × 0.35 × 0.30 mm, was glued on a glass fiber. Data were collected at 293K using graphite-monochromated Mo Kα radiation (λ = 0.71073Å) and Bruker APEX CCD area-detector in the range 3.09° < θ < 25.00°. Substrates **1** were prepared following the known procedure.[1] **1′a**,[2] **1′e**,[3] **1′f**,[4] **1′g**,[5] **1′h**,[1] **1′i**,[6] **1′j**,[7] **1′k**,[8] **1a**,[2] **1b**,[2] **1e**,[2] **1g**,[2] **1v**,[9] **1w**,[9] **1x**,[4] and **1y**[10] are known compounds.

II. Synthetic procedures/analytical data of compounds 1



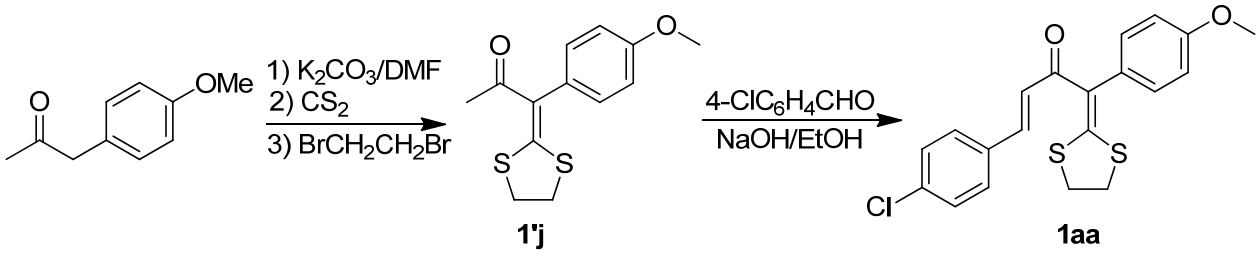
1′/R, R^1	**1**/R, R^1, R^2
1′a/Et, 4-$MeOC_6H_4$	**1a**/Et, 4-$MeOC_6H_4$, Ph
	1b/Et, 4-$MeOC_6H_4$, 4-$MeOC_6H_4$
	1c/Et, 4-$MeOC_6H_4$, 4-MeC_6H_4
	1d/Et, 4-$MeOC_6H_4$, 2,3-$CH_2O_2C_6H_3$
	1e/Et, 4-$MeOC_6H_4$, 4-ClC_6H_4
	1f/Et, 4-$MeOC_6H_4$, 2-ClC_6H_4
	1g/Et, 4-$MeOC_6H_4$, 2-furyl
	1h/Et, 4-$MeOC_6H_4$, *t*Bu
1′b/Et, 2-$MeOC_6H_4$	**1i**/Et, 2-$MeOC_6H_4$, Ph
	1j/Et, 2-$MeOC_6H_4$, 2,3-$CH_2O_2C_6H_3$
	1k/Et, 2-$MeOC_6H_4$, 4-ClC_6H_4
1′c/Et, 4-ClC_6H_4	**1*l***/Et, 4-ClC_6H_4, Ph
	1m/Et, 4-ClC_6H_4, 2,3-$CH_2O_2C_6H_3$
	1n/Et, 4-ClC_6H_4, 4-ClC_6H_4
	1o/Et, 4-ClC_6H_4, 2-furyl
1′d/Et, 4-FC_6H_4	**1p**/Et, 4-FC_6H_4, Ph
	1q/Et, 4-FC_6H_4, 2,3-$CH_2O_2C_6H_3$
	1r/Et, 4-FC_6H_4, 4-ClC_6H_4
	1s/Et, 4-FC_6H_4, 2-furyl
1′e/Me, 4-ClC_6H_4	**1t**/Me, 4-ClC_6H_4, Ph
	1u/Me, 4-ClC_6H_4, 4-ClC_6H_4
1′f/Me, Me	**1v**/Me, Me, Ph
	1w/Me, Me, 2,3-$CH_2O_2C_6H_3$
1′g/Me, *n*Bu	**1x**/Me, *n*Bu, Ph
1′h/Et, COPh	**1y**/Et, COPh, 4-ClC_6H_4
1′i/Et, H	**1z**/Et, H, 4-ClC_6H_4

General procedure for the synthesis of ketene dithioacetals of 1a-u and **1y** (taking **1a** as an example)**:** To a well-stirred suspension of 1-(4-methoxyphenyl)propan-2-one (15.4 mL, 100 mmol), K_2CO_3 (34.5 g, 250 mmol) and DMF (50 mL) at room temperature was added CS_2 (6.6 mL, 110 mmol) at 0 °C. After the reaction mixture was stirred at 0 °C for 0.5 h, EtBr (16.4 mL, 220 mmol) was added dropwise within 15 min. The mixture was allowed to warm to room temperature and stirred for 24 h, and then poured into ice-water (100 mL) under stirring and extracted with CH_2Cl_2 (3 × 30 mL). The combined organic phase was washed with water (3 × 25 mL), dried over $MgSO_4$ and concentrated in vacuo. The crude product was purified by flash chromatography (silica gel, petroleum ether/ ethyl acetate 60/1, v/v) to give 4,4-bis(ethylthio)-3-(4-methoxyphenyl) but-3-en-2-one **1a'** (23.7 g, 80%) as a yellow liquid. Then, to a stirred solution of **1a'** (296 mg, 1.0 mmol) and benzaldehyde (0.12 mL, 1.2 mmol) in EtOH (3 mL) was added NaOH (80 mg, 2.0 mmol) in one portion at room temperature. After **1a'** was consumed as indicated by TLC, the resulting mixture was quenched by ice-water (20 mL). The precipitate was collected by filtration, washed with water (3 × 15 mL) and dried at ambience to give **1a** (353 mg, 92%) as a yellow crystal.

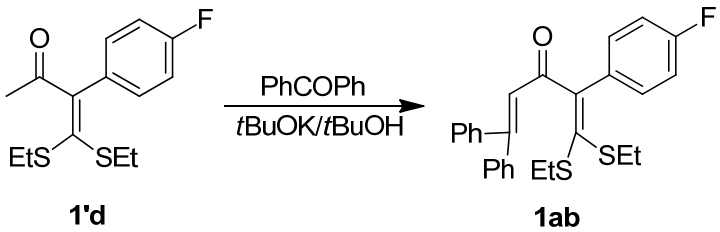
General procedure for the synthesis of ketene dithioacetals 1v-x (taking **1v** as an example): To a well-stirred suspension of anhydrous t-BuOK (4.94 g, 44 mmol) and butan-2-one (1.79 mL, 20 mmol) in 40 mL of anhydrous DMF were added CS_2 (1.32 mL, 20 mmol) at 0 ºC. After the reaction mixture was stirred at 0 °C for 1.5 h, MeI (2.49 mL, 40 mmol) was added dropwise within 30 min. The mixture was allowed to warm to room temperature and stirred for 5 h, and then poured into saturated aqueous NH_4Cl (100 mL) under stirring. The resulting mixture was extracted with CH_2Cl_2 (3 × 30 mL). The combined organic phase was washed with water (3 × 15 mL), dried over anhydrous $MgSO_4$, filtered and concentrated in vacuo. The crude product was purified by flash chromatography (silica gel, petroleum ether/ ethyl acetate: 80/1, v/v) to give 3-methyl-4,4-bis(methylthio)but-3-en-2-one **1'f** (705 mg, 20%) as a lightyellow liquid. Then, to a stirred solution of **1'f** (176 mg, 1.0 mmol) and benzaldehyde (0.12 mL, 1.2 mmol) in EtOH (3 mL) was added NaOH (80 mg, 2.0 mmol) in one portion at room temperature. After **1'f** was consumed as indicated by TLC, the resulting mixture was quenched by ice-water (20 mL) under stirring. The precipitate was collected by filtration, washed with water (15 mL × 3) and dried at ambience to give **1v** (198 mg, 75%) as a light yellow crystal.

Procedure for the synthesis of ketene dithioacetal 1z: To a well-stirred suspension of pentane-2,4-dione (10.2 mL, 100 mmol), K_2CO_3 (34.5 g, 250 mmol) and DMF (50 mL) at room temperature was added CS_2 (6.6 mL, 110 mmol) at 0 °C. After the reaction mixture was stirred at 0 °C for 0.5 h, EtBr (16.4mL, 220 mmol) was added dropwise within 15 min. The mixture was

allowed to warm to room temperature and stirred for 16.0 h, and then poured into ice-water (200 mL) under stirring and extracted with CH_2Cl_2 (3 × 30 mL). The combined organic phase was washed with water (3 × 25 mL), dried over $MgSO_4$ and concentrated in vacuo. The crude product was purified by flash chromatography (silica gel, petroleum ether/ ethyl acetate 20/1, v/v) to give 3-(bis(ethylthio)methylene)pentane-2,4-dione (20.8g, 90%) as a yellow liquid. Then to a solution of 3-(bis(ethylthio)methylene)pentane-2,4-dione (1.16 g, 5.0 mmol) in 20 mL of CH_2Cl_2 was added concentrated H_2SO_4 (1.1 mL, 20 mmol) at 0 ^oC. The mixture was allowed to warm to room temperature and stirred for 10 h, and then poured onto saturated NaCl ice-water (50 mL) under stirring. The mixture was neutralized with aqueous Na_2CO_3, and extracted with CH_2Cl_2 (3 × 15 mL). The combined organic phase was washed with water (3 × 10 mL), dried over $MgSO_4$ and concentrated in vacuo. The crude product was purified by flash chromatography (silica gel, petroleum ether/ ethyl acetate 30/1, V/V) to give 4,4-bis(ethylthio)but-3-en-2-one **1′i** (855 mg, 90%) as a white solid. Then, to a stirred solution of **1′i** (190 mg, 1.0 mmol) and 4-chlorobenzaldehyde (154 mg, 1.1 mmol) in EtOH (3 mL) was added NaOH (80 mg, 2.0 mmol) in one portion at room temperature. After **1′i** was consumed as indicated by TLC, the resulting mixture was quenched by ice-water (20 mL) under stirring. The precipitate was collected by filtration, washed with water (3 × 15 mL) and dried at ambience to give **1z** (281 mg, 90%) as a yellow crystal.

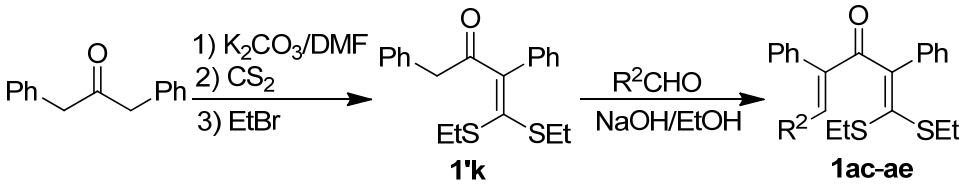


Procedure for the synthesis of ketene dithioacetal 1aa: The procedure for the synthesis of **1aa** is the same as that of **1a**.



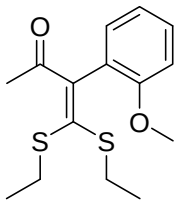
Procedure for the synthesis of ketene dithioacetal 1ab : To a stirred solution of **1'd** (284 mg, 1.0 mmol) and benzophenone (182 mg, 1.0 mmol) in *t*BuOH (5.0 mL) was added *t*BuOK (448 mg, 4.0 mmol) in one portion at room temperature. The reaction mixture was stirred for 15 min at room temperature and then heated to 50°C to stir for additional 7 h. After **1'd** was consumed (monitored

by TLC), the reaction mixture was poured into ice water (30 mL), neutralized with diluted hydrochloric acid, extracted with CH_2Cl_2 (3 × 15 mL). The combined organic extracts were washed with water (3 × 15 mL), dried over anhydrous $MgSO_4$, filtered and concentrated under reduced pressure to yield the crude product, which was purified by silica gel chromatography (eluent, petroleum ether/ ethyl acetate: 20/1, v/v) to give **1ab** (166 mg, 37%) as a yellow crystal.



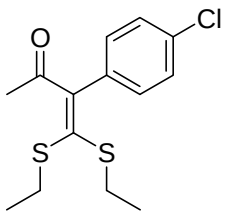
General procedure for the synthesis of ketene dithioacetals 1ac–ae: General procedure for the synthesis of **1ac–ae** is the same as that of **1a**.

4,4-Bis(ethylthio)-3-(2-methoxyphenyl)but-3-en-2-one(1'b)



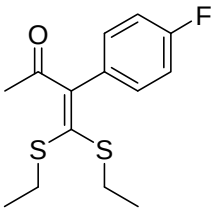
Yellow liquid. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.13 (t, *J* = 7.5 Hz, 3H), 1.29 (t, *J* = 7.5 Hz, 3H), 2.28 (s, 3H), 2.60 (q, *J* = 7.5 Hz, 2H), 2.91 (q, *J* = 7.5 Hz, 2H), 3.79 (s, 3H), 6.88-6.90 (m, 1H), 6.94-6.98 (m, 1H), 7.22-7.24 (m, 1H), 7.30-7.33 (m, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 200.7, 156.7, 143.9, 140.7, 131.1, 129.6, 127.6, 120.5, 110.7, 55.3, 30.0, 28.5 (2C), 14.6, 14.5. **HRMS** (ESI-TOF) calcd for $C_{15}H_{21}O_2S_2^+$ ($[M+H]^+$) 297.0977, found 297.0983.

3-(4-Chlorophenyl)-4,4-bis(ethylthio)but-3-en-2-one(1'c)



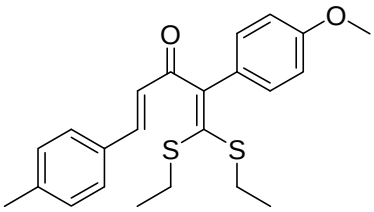
White solid. mp 62-63 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.15 (t, *J* = 7.0 Hz, 3H), 1.32 (t, *J* = 7.0 Hz, 3H), 2.29 (s, 3H), 2.68 (q, *J* = 7.5 Hz, 2H), 2.89 (q, *J* = 7.5 Hz, 2H), 7.23 (dd, *J* = 2.0, 6.5 Hz, 2H), 7.34 (dd, *J* = 2.0, 6.5 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 200.9, 147.9, 136.7, 134.8, 134.0, 130.4 (2C), 128.5 (2C), 30.4, 28.4, 28.2, 14.6, 14.5. **HRMS** (ESI-TOF) calcd for $C_{14}H_{18}ClOS_2^+$ ($[M+H]^+$) 301.0482, found 301.0484.

4,4-Bis(ethylthio)-3-(4-fluorophenyl)but-3-en-2-one(1'd)



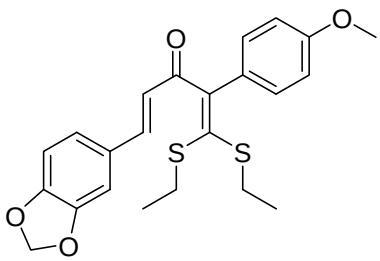
Yellow solid. mp 40-41 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.15 (t, *J* = 7.5 Hz, 3H), 1.32 (t, *J* = 7.5 Hz, 3H), 2.29 (s, 3H), 2.67 (q, *J* = 7.5 Hz, 2H), 2.88 (q, *J* = 7.5 Hz, 2H), 7.05 (t, *J* = 8.5 Hz, 2H), 7.26-7.29 (m, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 201.2, 162.3 (d, *J* = 247 Hz, 1C), 148.2, 135.9, 132.2 (d, *J* = 3.4 Hz, 1C), 130.8 (d, *J* = 8.1 Hz, 2C), 115.3 (d, *J* = 21.4 Hz, 2C), 30.3, 28.3, 28.0, 14.6, 14.5. **HRMS** (ESI-TOF) calcd for $C_{14}H_{18}FOS_2^+$ ($[M+H]^+$) 285.0778, found 285.0778.

(E)-1,1-Bis(ethylthio)-2-(4-methoxyphenyl)-5-p-tolylpenta-1,4-dien-3-one (1c)



Yellow solid. mp 82-83 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.22 (t, *J* = 7.5 Hz, 3H), 1.26 (t, *J* = 7.5 Hz, 3H), 2.36 (s, 3H), 2.73 (q, *J* = 7.5 Hz, 2H), 2.84 (q, *J* = 7.5 Hz, 2H), 3.80 (s, 3H), 6.77 (d, *J* = 16.5 Hz, 1H), 6.88 (d, *J* = 8.5 Hz, 2H), 7.17 (d, *J* = 8.0 Hz, 2H), 7.35 (d, *J* = 8.5 Hz, 2H), 7.39 (d, *J* = 8.0 Hz, 2H), 7.51 (d, *J* = 16.5 Hz, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 194.7, 159.3, 147.8, 144.6, 140.9, 134.1, 131.9, 130.5 (2C), 129.6 (2C), 128.9, 128.3 (2C), 126.1, 113.7 (2C), 55.2, 28.6, 27.9, 21.5, 14.8, 14.6. **HRMS** (ESI-TOF) calcd for $C_{23}H_{27}O_2S_2^+$ ($[M+H]^+$) 399.1447, found 399.1454.

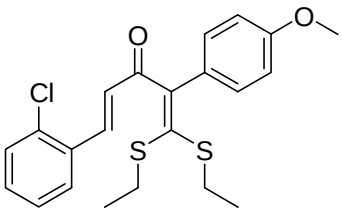
(E)-5-(Benzo[d][1,3]dioxol-5-yl)-1,1-bis(ethylthio)-2-(4-methoxyphenyl)penta-1,4-dien-3-one(1d)



Yellow solid. mp 60-61 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.21 (t, *J* = 7.5 Hz, 3H), 1.27 (t, *J* = 7.5 Hz, 3H), 2.72 (q, *J* = 7.5 Hz, 2H), 2.84 (q, *J* = 7.5 Hz, 2H), 3.81 (s, 3H), 5.99 (s, 2H), 6.63 (d, *J* = 16.0 Hz, 1H), 6.79 (d, *J* = 8.0 Hz, 1H), 6.87-6.89 (m, 2H), 6.97-6.99 (m, 2H), 7.33-7.35 (m, 2H),

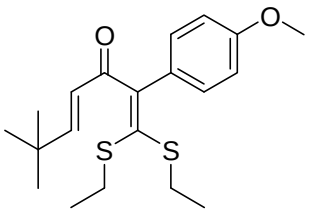
7.44 (d, *J* = 16.0 Hz, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 194.4, 159.3, 149.8, 148.3, 147.8, 144.3, 134.2, 130.5 (2C), 129.1, 128.9, 125.1, 124.9, 113.7 (2C), 108.6, 106.6, 101.6, 55.2, 28.6, 27.9, 14.8, 14.6. **HRMS** (ESI-TOF) calcd for $C_{23}H_{25}O_4S_2^+$ ($[M+H]^+$) 429.1189, found 429.1187.

(E)-5-(2-Chlorophenyl)-1,1-bis(ethylthio)-2-(4-methoxyphenyl)penta-1,4-dien-3-one(1f)



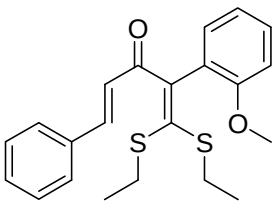
Yellow solid. mp 65-66 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.23 (t, *J* = 7.5 Hz, 3H), 1.26 (t, *J* = 7.5 Hz, 3H), 2.73 (q, *J* = 7.5 Hz, 2H), 2.85 (q, *J* = 7.5 Hz, 2H), 3.80 (s, 3H), 6.77 (d, *J* = 16.5 Hz, 1H), 6.89 (d, *J* = 9.0 Hz, 2H), 7.27-7.29 (m, 2H), 7.36-7.40 (m, 3H), 7.60-7.62 (m, 1H), 7.97 (d, *J* = 16.5 Hz, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 194.8, 159.4, 147.3, 140.3, 135.2, 134.7, 132.8, 131.2, 130.5 (2C), 130.2, 129.3, 128.8, 127.5, 127.1, 113.7 (2C), 55.2, 28.7, 27.9, 14.8, 14.5. **HRMS** (ESI-TOF) calcd for $C_{22}H_{24}ClO_2S_2^+$ ($[M+H]^+$) 419.0901, found 419.0902.

(E)-1,1-Bis(ethylthio)-2-(4-methoxyphenyl)-6,6-dimethylhepta-1,4-dien-3-one(1h)



Yellow solid. mp 57-58 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.05 (s, 9H), 1.19 (t, *J* = 7.0 Hz, 3H), 1.27 (t, *J* = 7.5 Hz, 3H), 2.70 (q, *J* = 7.0 Hz, 2H), 2.81 (q, *J* = 7.5 Hz, 2H), 3.80 (s, 3H), 6.10 (d, *J* = 16.0 Hz, 1H), 6.80 (d, *J* = 16.0 Hz, 1H), 6.86 (d, *J* = 8.5 Hz, 2H), 7.28 (d, *J* = 8.5 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 195.8, 159.8, 159.2, 148.0, 132.6, 130.2 (2C), 128.8, 126.0, 113.5 (2C), 55.1, 33.9, 28.5 (3C), 28.4, 27.6, 14.7, 14.5. **HRMS** (ESI-TOF) calcd for $C_{20}H_{29}O_2S_2^+$ ($[M+H]^+$) 365.1603, found 365.1605.

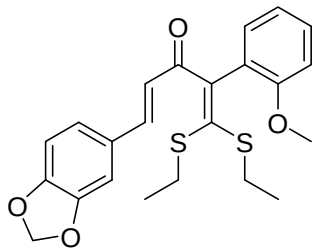
(E)-1,1-Bis(ethylthio)-2-(2-methoxyphenyl)-5-phenylpenta-1,4-dien-3-one(1i)



Yellow solid. mp 76-77 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.18 (t, *J* = 7.5 Hz, 3H), 1.30 (t, *J* = 7.5

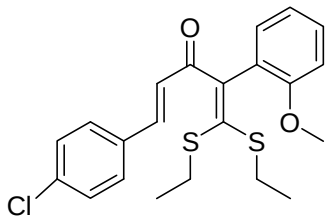
Hz, 3H), 2.65 (q, *J* = 7.5 Hz, 2H), 2.87 (q, *J* = 7.5 Hz, 2H), 3.79 (s, 3H), 6.88-6.92 (m, 2H), 6.96-6.98 (m, 1H), 7.29-7.36 (m, 5H), 7.48-7.50 (m, 2H), 7.71 (d, *J* = 16.0 Hz, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 193.5, 156.6, 143.8, 142.6, 139.6, 135.2, 130.8, 129.9, 129.6, 128.8 (2C), 128.1 (2C), 127.0, 126.9, 120.5, 110.9, 55.3, 28.7, 28.2, 14.8, 14.7. **HRMS** (ESI-TOF) calcd for $C_{22}H_{25}O_2S_2^+$ ($[M+H]^+$) 385.1290, found 385.1289.

(E)-5-(Benzo[d][1,3]dioxol-5-yl)-1,1-bis(ethylthio)-2-(2-methoxyphenyl)penta-1,4-dien-3-one(1j)



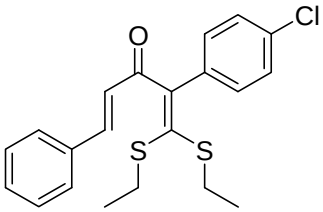
Yellow solid. mp 128-129 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.17 (t, *J* = 7.5 Hz, 3H), 1.29 (t, *J* = 7.5 Hz, 3H), 2.64 (q, *J* = 7.5 Hz, 2H), 2.86 (q, *J* = 7.5 Hz, 2H), 3.79 (s, 3H), 5.97 (s, 2H), 6.71 (d, *J* = 16.0 Hz, 1H), 6.79 (d, *J* = 8.0 Hz, 1H), 6.88 (d, *J* = 8.5 Hz, 1H), 6.95-6.98 (m, 3H), 7.30-7.32 (m, 2H), 7.62 (d, *J* = 16.0 Hz, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 193.4, 156.5, 149.4, 148.2, 144.0, 142.8, 139.1, 130.7, 129.6, 129.5, 126.9, 125.1, 124.5, 120.5, 110.8, 108.5, 106.5, 101.4, 55.3, 28.6, 28.1, 14.8, 14.7. **HRMS** (ESI-TOF) calcd for $C_{23}H_{25}O_4S_2^+$ ($[M+H]^+$) 429.1189, found 429.1188.

(E)-5-(4-Chlorophenyl)-1,1-bis(ethylthio)-2-(2-methoxyphenyl)penta-1,4-dien-3-one(1k)



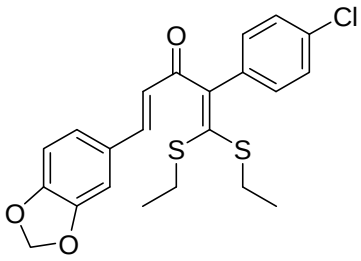
Yellow solid. mp 118-119 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.17 (t, *J* = 7.5 Hz, 3H), 1.30 (t, *J* = 7.5 Hz, 3H), 2.64 (q, *J* = 7.5 Hz, 2H), 2.88 (q, *J* = 7.5 Hz, 2H), 3.77 (s, 3H), 6.86-6.90 (m, 2H), 6.97 (t, *J* = 7.5 Hz, 1H), 7.29-7.34 (m, 4H), 7.42 (d, *J* = 8.5 Hz, 2H), 7.64 (d, *J* = 16.0 Hz, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 193.1, 156.6, 143.5, 140.7, 140.3, 135.7, 133.7, 130.9, 129.7, 129.2 (2C), 129.1 (2C), 127.4, 127.0, 120.6, 110.9, 55.3, 28.8, 28.3, 14.8, 14.6. **HRMS** (ESI-TOF) calcd for $C_{22}H_{24}ClO_2S_2^+$ ($[M+H]^+$) 419.1158, found 419.1152.

(E)-2-(4-Chlorophenyl)-1,1-bis(ethylthio)-5-phenylpenta-1,4-dien-3-one(1l)



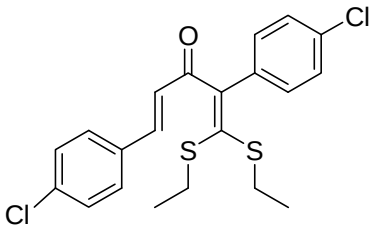
Yellow solid. mp 138-139 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.22 (t, *J* = 7.5 Hz, 3H), 1.28 (t, *J* = 7.5 Hz, 3H), 2.73 (q, *J* = 7.5 Hz, 2H), 2.87 (q, *J* = 7.5 Hz, 2H), 6.84 (d, *J* = 16.0 Hz, 1H), 7.32-7.38 (m, 7H), 7.49-7.51 (m, 2H), 7.54 (d, *J* = 16.0 Hz, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 193.7, 146.2, 144.4, 137.2, 135.1, 134.4, 133.9, 130.5, 130.4 (2C), 128.9 (2C), 128.5 (2C), 128.3 (2C), 126.7, 28.6, 28.1, 14.7, 14.6. **HRMS** (ESI-TOF) calcd for $C_{21}H_{22}ClOS_2^+$ ($[M+H]^+$) 389.0795, found 389.0802.

(E)-5-(Benzo[d][1,3]dioxol-5-yl)-2-(4-chlorophenyl)-1,1-bis(ethylthio)penta-1,4-dien-3-one(1m)



Yellow solid. mp 149-150 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.21 (t, *J* = 7.5 Hz, 3H), 1.28 (t, *J* = 7.5 Hz, 3H), 2.72 (q, *J* = 7.5 Hz, 2H), 2.86 (q, *J* = 7.5 Hz, 2H), 5.99 (s, 2H), 6.65 (d, *J* = 16.0 Hz, 1H), 6.80 (d, *J* = 8.0 Hz, 1H), 6.99 (d, *J* = 8.5 Hz, 2H), 7.31-7.35 (m, 4H), 7.45 (d, *J* = 16.0 Hz, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 193.7, 149.9, 148.4, 146.5, 144.4, 136.8, 135.2, 133.9, 130.5 (2C), 128.9, 128.5 (2C), 125.0, 124.8, 108.6, 106.6, 101.6, 28.6, 28.2, 14.8, 14.7. **HRMS** (ESI-TOF) calcd for $C_{22}H_{22}ClO_3S_2^+$ ($[M+H]^+$) 433.0693, found 433.0701.

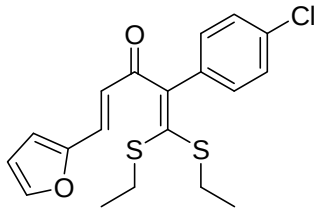
(E)-2,5-Bis(4-chlorophenyl)-1,1-bis(ethylthio)penta-1,4-dien-3-one(1n)



Yellow solid. mp 120-121 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.21 (t, *J* = 7.5 Hz, 3H), 1.28 (t, *J* = 7.0 Hz, 3H), 2.72 (q, *J* = 7.5 Hz, 2H), 2.87 (q, *J* = 7.0 Hz, 2H), 6.80 (d, *J* = 16.0 Hz, 1H), 7.33-7.35 (m, 6H), 7.42 (d, *J* = 8.5 Hz, 2H), 7.49 (d, *J* = 16.0 Hz, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 193.2, 146.0, 142.6, 138.0, 136.4, 135.1, 134.0, 133.0, 130.6 (2C), 129.4 (2C), 129.2 (2C), 128.5 (2C), 127.1, 28.7, 28.3, 14.8, 14.7. **HRMS** (ESI-TOF) calcd for $C_{21}H_{21}Cl_2OS_2^+$ ($[M+H]^+$) 423.0405,

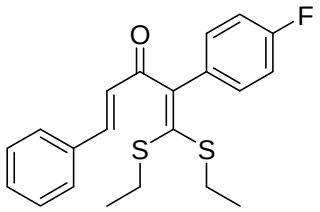
found 423.0409.

(E)-2-(4-Chlorophenyl)-1,1-bis(ethylthio)-5-(furan-2-yl)penta-1,4-dien-3-one(1o)



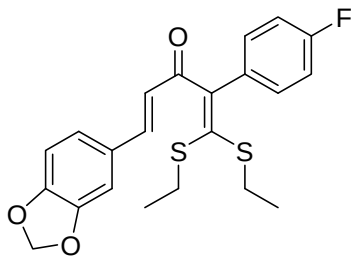
Yellow solid. mp 87-88 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.20 (t, *J* = 7.5 Hz, 3H), 1.30 (t, *J* = 7.5 Hz, 3H), 2.71 (q, *J* = 7.5 Hz, 2H), 2.88 (q, *J* = 7.5 Hz, 2H), 6.47 (dd, *J* = 2.0, 3.5 Hz, 1H), 6.64 (d, *J* = 3.0 Hz, 1H), 6.73 (d, *J* = 15.5 Hz, 1H), 7.27-7.32 (m, 5H), 7.47 (d, *J* = 1.5 Hz, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 193.0, 151.2, 146.3, 145.1, 137.8, 135.3, 133.9, 130.6 (2C), 130.0, 128.5 (2C), 124.1, 115.9, 112.6, 28.7, 28.3, 14.7, 14.6. **HRMS** (ESI-TOF) calcd for $C_{19}H_{20}ClO_2S_2^+$ ($[M+H]^+$) 379.0588, found 379.0587.

(E)-1,1-Bis(ethylthio)-2-(4-fluorophenyl)-5-phenylpenta-1,4-dien-3-one(1p)



Yellow solid. mp 125-126 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.22 (t, *J* = 7.5 Hz, 3H), 1.28 (t, *J* = 7.5 Hz, 3H), 2.72 (q, *J* = 7.5 Hz, 2H), 2.86 (q, *J* = 7.5 Hz, 2H), 6.84 (d, *J* = 16.0 Hz, 1H), 7.03-7.06 (m, 2H), 7.37-7.40 (m, 5H), 7.49-7.51 (m, 2H), 7.55 (d, *J* = 16.0 Hz, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 193.9, 162.3 (d, *J* = 247.0 Hz, 1C), 146.5, 144.4, 136.7, 134.5, 132.7, 131.0 (d, *J* = 8.1 Hz, 2C), 130.5, 128.9 (2C), 128.3 (2C), 126.8, 115.3 (d, *J* = 21.5 Hz, 2C), 28.7, 28.1, 14.8, 14.7. **HRMS** (ESI-TOF) calcd for $C_{21}H_{22}FOS_2^+$ ($[M+H]^+$) 373.1091, found 373.1086.

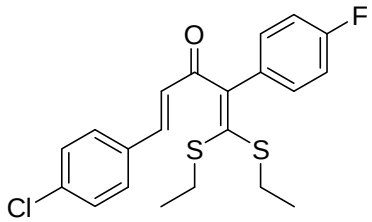
(E)-5-(Benzo[d][1,3]dioxol-5-yl)-1,1-bis(ethylthio)-2-(4-fluorophenyl)penta-1,4-dien-3-one(1q)



Yellow solid. mp 134-136 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.21 (t, *J* = 7.5 Hz, 3H), 1.28 (t, *J* = 7.5 Hz, 3H), 2.72 (q, *J* = 7.5 Hz, 2H), 2.86 (q, *J* = 7.5 Hz, 2H), 6.00 (s, 2H), 6.65 (d, *J* = 16.0 Hz,

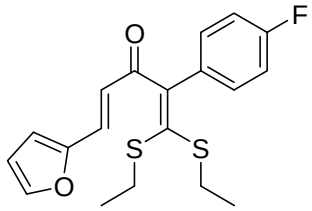
1H), 6.80 (d, *J* = 8.0 Hz, 1H), 6.98-7.06 (m, 4H), 7.36-7.39 (m, 2H), 7.46 (d, *J* = 16.0 Hz, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 193.9, 162.3 (d, *J* = 247.0 Hz, 1C), 149.9, 148.4, 146.8, 144.4, 136.3, 132.7, 131.0 (d, *J* = 8.1 Hz, 2C), 129.0, 125.0 (d, *J* = 3.5 Hz, 2C), 115.3 (d, *J* = 21.4 Hz, 2C), 108.6, 106.6, 101.6, 28.6, 28.1, 14.8, 14.7. **HRMS** (ESI-TOF) calcd for $C_{22}H_{22}FO_3S_2^+$ ($[M+H]^+$) 417.0989, found 417.0983.

(E)-5-(4-Chlorophenyl)-1,1-bis(ethylthio)-2-(4-fluorophenyl)penta-1,4-dien-3-one(1r)



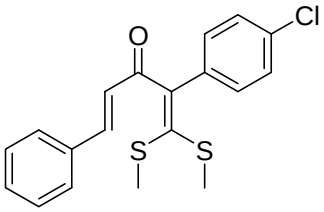
Yellow solid. mp 123-125 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.21 (t, *J* = 7.5 Hz, 3H), 1.28 (t, *J* = 7.5 Hz, 3H), 2.72 (q, *J* = 7.5 Hz, 2H), 2.84 (q, *J* = 7.5 Hz, 2H), 6.80 (d, *J* = 16.0 Hz, 1H), 7.03-7.07 (m, 2H), 7.33-7.39 (m, 4H), 7.42 (d, *J* = 8.5 Hz, 2H), 7.49 (d, *J* = 16.0 Hz, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 193.5, 162.4 (d, *J* = 247.1 Hz, 1C), 146.3, 142.5, 137.5, 136.4, 133.1, 132.7, 131.0 (d, *J* = 8.1 Hz, 2C), 129.4 (2C), 129.2 (2C), 127.1, 115.3 (d, *J* = 21.4 Hz, 2C), 28.7, 28.2, 14.8, 14.7. **HRMS** (ESI-TOF) calcd for $C_{21}H_{21}ClFOS_2^+$ ($[M+H]^+$) 407.0701, found 407.0698.

(E)-1,1-bis(ethylthio)-2-(4-fluorophenyl)-5-(furan-2-yl)penta-1,4-dien-3-one(1s)



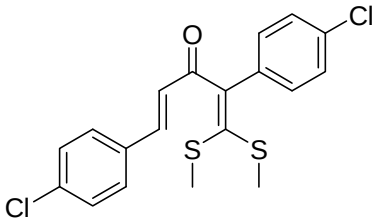
Yellow solid. mp 59-60 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.20 (t, *J* = 7.5 Hz, 3H), 1.30 (t, *J* = 7.5 Hz, 3H), 2.71 (q, *J* = 7.5 Hz, 2H), 2.88 (q, *J* = 7.5 Hz, 2H), 6.46 (dd, *J* = 2.0 Hz, 1H), 6.64 (d, *J* = 3.5 Hz, 1H), 6.74 (d, *J* = 15.5 Hz, 1H), 7.02-7.06 (m, 2H), 7.31 (d, *J* = 15.5 Hz, 1H), 7.35-7.37 (m, 2H), 7.47 (d, *J* = 1.0 Hz, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 193.2, 162.3 (d, *J* = 247.1 Hz, 1C), 151.2, 146.6, 145.0, 137.2, 132.8 (d, *J* = 3.4 Hz, 1C), 131.0 (d, *J* = 8.1 Hz, 2C), 129.9, 124.1, 115.8, 115.3 (d, *J* = 21.4 Hz, 2C), 112.6, 28.7, 28.2, 14.7, 14.6. **HRMS** (ESI-TOF) calcd for $C_{19}H_{20}FO_2S_2^+$ ($[M+H]^+$) 363.0883, found 363.0883.

(E)-2-(4-Chlorophenyl)-1,1-bis(methylthio)-5-phenylpenta-1,4-dien-3-one(1t)



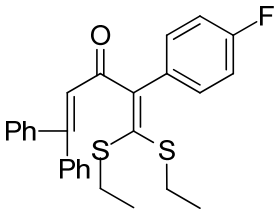
Yellow solid. mp 134-135 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 2.26 (s, 3H), 2.37 (s, 3H), 6.82 (d, *J* = 16.5 Hz, 1H), 7.34-7.38 (m, 7H), 7.50-7.51 (m, 2H), 7.54 (d, *J* = 16.5 Hz, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 193.1, 144.2, 143.7, 141.7, 135.2, 134.5, 134.1, 130.6 (3C), 128.9 (2C), 128.6 (2C), 128.4 (2C), 126.6, 18.1, 17.4. **HRMS** (ESI-TOF) calcd for $C_{19}H_{18}ClOS_2^+$ ($[M+H]^+$) 361.0482, found 361.0478.

(E)-2,5-Bis(4-chlorophenyl)-1,1-bis(methylthio)penta-1,4-dien-3-one(1u)



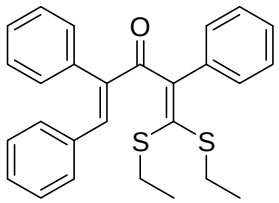
Yellow solid. mp 114-115 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 2.26 (s, 3H), 2.38 (s, 3H), 6.77 (d, *J* = 16.0 Hz, 1H), 7.32-7.36 (m, 6H), 7.42 (d, *J* = 8.5 Hz, 2H), 7.49 (d, *J* = 16.0 Hz, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 192.6, 143.4, 142.6, 142.3, 136.4, 135.1, 134.2, 133.0, 130.6 (2C), 129.5 (2C), 129.2 (2C), 128.7 (2C), 126.9, 18.2, 17.5. **HRMS** (ESI-TOF) calcd for $C_{19}H_{17}Cl_2OS_2^+$ ($[M+H]^+$) 395.0092, found 395.0085.

1,1-Bis(ethylthio)-2-(4-fluorophenyl)-5,5-diphenylpenta-1,4-dien-3-one (1ab)



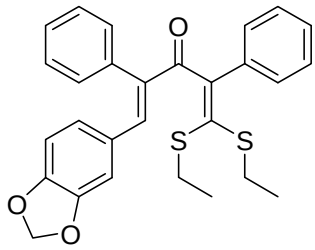
Yellow solid. mp 99-100 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.11 (t, *J* = 7.5 Hz, 3H), 1.31 (t, *J* = 7.5 Hz, 3H), 2.61 (q, *J* = 7.5 Hz, 2H), 2.91 (q, *J* = 7.5 Hz, 2H), 6.72 (s, 1H), 6.97 (t, *J* = 8.0 Hz, 2H), 7.07-7.10 (m, 2H), 7.15 (d, *J* = 8.0 Hz, 2H), 7.21 (d, *J* = 8.0 Hz, 2H), 7.28-7,36 (m, 6H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 192.9, 162.2 (d, *J* = 246.5 Hz, 1C), 153.0, 147.8, 141.4, 138.8, 132.9 (d, *J* = 3.4 Hz, 1C), 131.3 (d, *J* = 8.1 Hz, 2C), 129.9 (2C), 129.2, 128.4 (2C), 128.3, 128.2 (3C) 127.9 (2C), 126.2, 114.8 (d, *J* = 21.5 Hz, 2C), 28.8, 28.3, 14.8, 14.7. **HRMS** (ESI-TOF) calcd for $C_{27}H_{26}FOS_2^+$ ($[M+H]^+$) 449.1404, found 449.1400.

(E)-1,1-Bis(ethylthio)-2,4,5-triphenylpenta-1,4-dien-3-one(1ac)



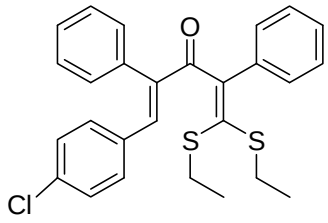
Yellow solid. mp 114-115 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.21 (t, *J* = 7.0 Hz, 3H), 1.26 (t, *J* = 7.0 Hz, 3H), 2.73 (q, *J* = 7.0 Hz, 2H), 2.85 (q, *J* = 7.0 Hz, 2H), 7.01 (d, *J* = 7.0 Hz, 2H), 7.12-7.20 (m, 5H), 7.25-7.35 (m, 6H), 7.43 (d, *J* = 7.5 Hz, 2H), 7.67 (s, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 196.0, 148.8, 142.2, 141.0, 136.2, 135.6, 134.6, 133.2, 130.7 (2C), 129.8 (2C), 129.3, 128.9 (2C), 128.5 (2C), 128.2 (2C), 128.1 (2C), 128.0, 127.8, 28.5, 27.7, 14.9, 14.6. **HRMS** (ESI-TOF) calcd for $C_{27}H_{27}OS_2^+$ ($[M+H]^+$) 431.1498, found 431.1499.

(E)-5-(Benzo[d][1,3]dioxol-5-yl)-1,1-bis(ethylthio)-2,4-diphenylpenta-1,4-dien-3-one(1ad)



Yellow solid. mp 86-87 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.20 (t, *J* = 7.0 Hz, 3H), 1.26 (t, *J* = 7.5 Hz, 3H), 2.72 (q, *J* = 7.0 Hz, 2H), 2.84 (q, *J* = 7.5 Hz, 2H), 5.88 (s, 2H), 6.31 (d, *J* = 1.5 Hz, 1H), 6.64-6.70 (m, 2H), 7.14-7.16 (m, 2H), 7.29-7.37 (m, 6H), 7.41 (t, *J* = 7.0 Hz, 2H), 7.59 (s, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 195.9, 149.0, 148.8, 147.5, 142.2, 139.1, 136.3, 135.7, 132.8, 129.7 (2C), 128.9 (2C), 128.8, 128.7 (2C), 128.1 (2C), 128.0, 127.9, 127.1, 109.6, 108.2, 101.3, 28.4, 27.6, 14.9, 14.7. **HRMS** (ESI-TOF) calcd for $C_{28}H_{27}O_3S_2^+$ ($[M+H]^+$) 475.1396, found 475.1400.

(E)-5-(4-Chlorophenyl)-1,1-bis(ethylthio)-2,4-diphenylpenta-1,4-dien-3-one(1ae)



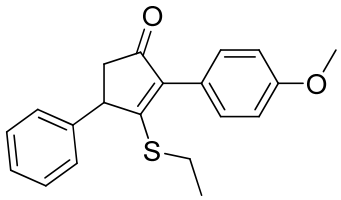
Yellow solid. mp 94-95 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.19 (t, *J* = 7.0 Hz, 3H), 1.25 (t, *J* = 7.0 Hz, 3H), 2.72 (q, *J* = 7.0 Hz, 2H), 2.84 (q, *J* = 7.0 Hz, 2H), 6.95 (d, *J* = 8.5 Hz, 2H), 7.10-7.14 (m, 4H), 7.30-7.36 (m, 6H), 7.40 (d, *J* = 7.5 Hz, 2H), 7.60 (s, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 195.8, 148.5, 141.4, 140.4, 136.1, 135.3, 135.2, 133.5, 133.1, 131.8 (2C), 129.7 (2C), 128.9 (2C), 128.6 (2C), 128.5 (2C), 128.2 (2C), 128.1, 128.0, 28.5, 27.7, 14.9, 14.6. **HRMS** (ESI-TOF) calcd

for $C_{27}H_{26}ClOS_2^+$ ($[M+H]^+$) 465.1114, found 465.1117.

III. Synthetic procedures/analytical data of compounds 2

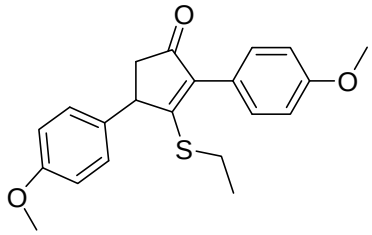
General procedure for the synthesis of cyclopentenones 2 (taking **2a** as an example): To a starting **1a** (192 mg, 0.5 mmol) in a dried flask under N_2 were added triphenylsilane (262 mg, 1.0 mmol), $Pd(PPh_3)_2Cl_2$ (35 mg, 0.05 mmol) and anhydrous DMF (5.0 mL) at room temperature. After the reaction mixture was stirred for 0.5 h at room temperature, it was heated to 90°C and stirred for 10 h. After **1a** was consumed (monitored by TLC), the reaction mixture was poured into ice water (30 mL), extracted with CH_2Cl_2 (3 × 15 mL). The combined organic extracts were washed with water (3 × 15 mL), dried over anhydrous $MgSO_4$, filtered and concentrated under reduced pressure to yield the crude product, which was purified by silica gel chromatography (eluent, petroleum ether/ ethyl acetate: 15/1, v/v) to give **2a** (148 mg, 92%) as a light yellow crystal.

3-(Ethylthio)-2-(4-methoxyphenyl)-4-phenylcyclopent-2-enone (2a)



Light yellow solid. mp 159-160 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.08 (t, *J* = 7.5 Hz, 3H), 2.41 (dd, *J* = 2.0, 18.5 Hz, 1H), 2.47-2.51 (m, 1H), 2.78-2.81 (m, 1H), 3.12 (dd, *J* = 7.5, 18.5 Hz, 1H), 3.84 (s, 3H), 4.35 (t, *J* = 6.0 Hz, 1H), 6.98 (d, *J* = 8.5 Hz, 2H), 7.25 (d, *J* = 7.5 Hz, 2H), 7.30 (d, *J* = 7.5 Hz, 1H), 7.37 (t, *J* = 7.5 Hz, 2H), 7.50 (d, *J* = 8.5 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 201.8, 172.7, 158.9, 142.0, 137.2, 130.1 (2C), 128.9 (2C), 127.0, 126.5 (2C), 123.2, 113.3 (2C), 54.9, 46.5, 45.8, 24.6, 13.8. **HRMS** (ESI-TOF) calcd for $C_{20}H_{21}O_2S^+$ ($[M+H]^+$) 325.1257, found 325.1255.

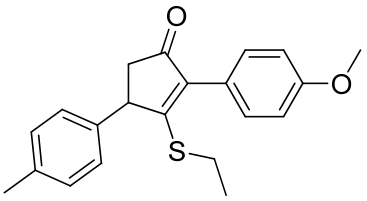
3-(Ethylthio)-2,4-bis(4-methoxyphenyl)cyclopent-2-enone (2b)



Yellow oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.08 (t, *J* = 8.0 Hz, 3H), 2.37 (d, *J* = 18.0 Hz, 1H), 2.48-2.53 (m, 1H), 2.75-2.80 (m, 1H), 3.09 (dd, *J* = 7.5, 18.0 Hz, 1H), 3.78 (s, 3H), 3.81 (s, 3H),

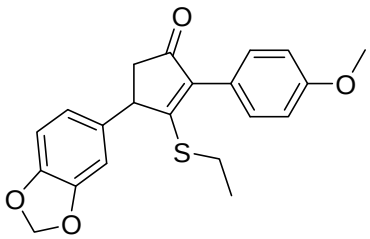
4.30 (t, *J* = 7.0 Hz, 1H), 6.90 (d, *J* = 8.5 Hz, 2H), 6.97 (d, *J* = 8.5 Hz, 2H), 7.17 (d, *J* = 8.5 Hz, 2H), 7.50 (d, *J* = 8.5 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 202.3, 173.0, 159.2, 158.7, 137.4, 134.2, 130.3 (2C), 127.8 (2C), 123.5, 114.5 (2C), 113.6 (2C), 55.2, 55.1, 46.2, 46.1, 24.8, 14.1. **HRMS** (ESI-TOF) calcd for $C_{21}H_{23}O_3S^+$ ($[M+H]^+$) 355.1362, found 355.1366.

3-(Ethylthio)-2-(4-methoxyphenyl)-4-p-tolylcyclopent-2-enone (2c)



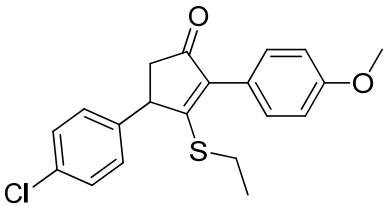
Yellow solid. mp 91-92 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.06 (t, *J* = 7.0 Hz, 3H), 2.33 (s, 3H), 2.37 (dd, *J* = 2.0, 18.5 Hz, 1H), 2.47-2.51 (m, 1H), 2.76-2.82 (m, 1H), 3.08 (dd, *J* = 7.5, 18.5 Hz, 1H), 3.81 (s, 3H), 4.29 (dd, *J* = 2.0, 7.5 Hz, 1H), 6.96-6.98 (m, 2H), 7.12-7.17 (m, 4H), 7.51 (dd, *J* = 2.0, 7.5 Hz, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 202.1, 172.9, 159.1, 139.2, 137.4, 136.9, 130.3 (2C), 129.8 (2C), 126.6 (2C), 123.5, 113.5 (2C), 55.1, 46.5, 46.1, 24.8, 20.9, 14.0. **HRMS** (ESI-TOF) calcd for $C_{21}H_{23}O_2S^+$ ($[M+H]^+$) 339.1413, found 339.1417.

4-(Benzo[d][1,3]dioxol-5-yl)-3-(ethylthio)-2-(4-methoxyphenyl)cyclopent-2-enone (2d)



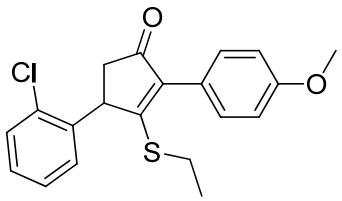
White solid. mp 55-56 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.20 (t, *J* = 7.0 Hz, 3H), 2.41 (dd, *J* = 1.5, 18.0 Hz, 1H), 2.55-2.58 (m, 1H), 2.81-2.85 (m, 1H), 3.09 (dd, *J* = 7.5, 18.0 Hz, 1H), 3.84 (s, 3H), 4.26 (t, *J* = 7.0 Hz, 1H), 5.98 (d, *J* = 2.5 Hz, 2H), 6.71-6.75 (m, 2H), 6.80 (d, *J* = 8.5 Hz, 1H), 6.98 (d, *J* = 8.5 Hz, 2H), 7.48 (d, *J* = 8.5 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 202.0, 172.7, 159.2, 148.3, 146.7, 137.6, 135.9, 130.3 (2C), 123.3, 120.1, 113.6 (2C), 108.7, 106.8, 101.1, 55.2, 46.6, 46.1, 24.9, 14.1. **HRMS** (ESI-TOF) calcd for $C_{21}H_{21}O_4S^+$ ($[M+H]^+$) 369.1155, found 369.1157.

4-(4-Chlorophenyl)-3-(ethylthio)-2-(4-methoxyphenyl)cyclopent-2-enone (2e)



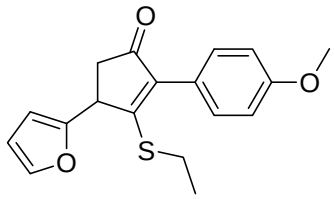
Yellow oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.76 (t, *J* = 7.0 Hz, 3H), 2.37 (dd, *J* = 0.5, 18.5 Hz, 1H), 2.45-2.49 (m, 1H), 2.74-2.78 (m, 1H), 3.10 (dd, *J* = 7.5, 18.5 Hz, 1H), 3.81 (s, 3H), 4.30 (d, *J* = 7.0 Hz, 1H), 6.97 (d, *J* = 8.5 Hz, 2H), 7.19 (d, *J* = 8.0 Hz, 2H), 7.33 (d, *J* = 8.5 Hz, 2H), 7.50 (d, *J* = 8.0 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 201.7, 172.0, 159.3, 140.9, 137.9, 133.1, 130.4 (2C), 129.4 (2C), 128.3 (2C), 123.3, 113.7 (2C), 55.2, 46.3, 45.9, 25.0, 14.1. **HRMS** (ESI-TOF) calcd for $C_{20}H_{20}ClO_2S^+$ ($[M+H]^+$) 359.0867, found 359.0863.

4-(2-Chlorophenyl)-3-(ethylthio)-2-(4-methoxyphenyl)cyclopent-2-enone (2f)



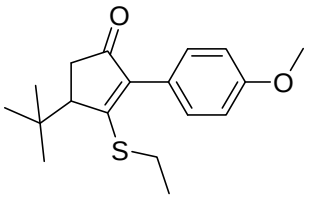
White solid. mp 99-100 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.11 (t, *J* = 7.5 Hz, 3H), 2.30 (d, *J* = 18.5 Hz, 1H), 2.37-2.41 (m, 1H), 2.73-2.77 (m, 1H), 3.18 (dd, *J* = 7.5, 18.5 Hz, 1H), 3.84 (s, 3H), 4.85 (d, *J* = 7.5 Hz, 1H), 6.98 (d, *J* = 8.5 Hz, 2H), 7.24 (d, *J* = 8.0 Hz, 2H), 7.29 (d, *J* = 8.0 Hz, 1H), 7.42 (d, *J* = 8.0 Hz, 1H), 7.52 (d, *J* = 8.5 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 201.5, 171.9, 159.3, 139.9, 137.9, 133.3, 130.3 (2C), 129.6, 128.6, 127.9, 127.7, 127.0, 123.4, 113.7 (2C), 55.2, 44.6, 42.9, 24.8, 14.1. **HRMS** (ESI-TOF) calcd for $C_{20}H_{20}ClO_2S^+$ ($[M+H]^+$) 359.0867, found 359.0869.

3-(Ethylthio)-4-(furan-2-yl)-2-(4-methoxyphenyl)cyclopent-2-enone (2g)



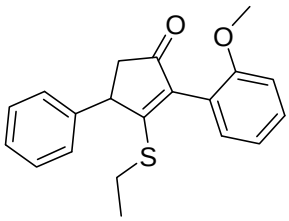
Yellow solid. mp 69-70 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.16 (t, *J* = 7.5 Hz, 3H), 2.61 (dd, *J* = 2.0, 18.0 Hz, 1H), 2.66-2.70 (m, 1H), 2.84-2.88 (m, 1H), 3.01 (dd, *J* = 2.0, 18.0 Hz, 1H), 3.83 (s, 3H), 4.43 (dd, *J* = 2.0, 7.5 Hz, 1H), 6.24 (d, *J* = 3.5 Hz, 1H), 6.36 (dd, *J* = 1.5, 3.0 Hz, 1H), 6.95-6.98 (m, 2H), 7.38 (d, *J* = 1.0 Hz, 1H), 7.44-7.46 (m, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 201.7, 169.4, 159.3, 154.2, 142.0, 137.6, 130.4 (2C), 123.3, 113.6 (2C), 110.6, 106.2, 55.2, 42.8, 40.3, 24.9, 14.3. **HRMS** (ESI-TOF) calcd for $C_{18}H_{19}O_3S^+$ ($[M+H]^+$) 315.1049, found 315.1043.

4-Tert-butyl-3-(ethylthio)-2-(4-methoxyphenyl)cyclopent-2-enone (2h)



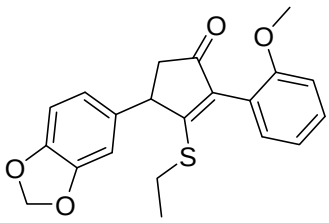
Yellow oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.05 (d, *J* = 10.5 Hz, 12H), 2.45-2.65 (m, 4H), 2.92 (d, *J* = 12.0 Hz, 1H), 3.82 (s, 3H), 6.92 (d, *J* = 7.5 Hz, 2H), 7.34 (d, *J* = 7.5 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 204.0, 172.0, 159.3, 139.4, 130.7 (2C), 124.1, 113.6 (2C), 55.2, 54.0, 40.8, 35.4, 27.9 (3C), 27.8, 14.0. **HRMS** (ESI-TOF) calcd for $C_{18}H_{25}O_2S^+$ ($[M+H]^+$) 305.1570, found 305.1578.

3-(Ethylthio)-2-(2-methoxyphenyl)-4-phenylcyclopent-2-enone (2i)



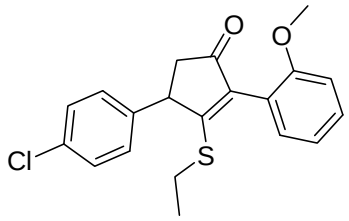
Yellow oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.01 (t, *J* = 7.5 Hz, 3H), 2.40-2.45 (m, 2H), 2.65-2.69 (m, 1H), 3.12 (dd, *J* = 7.5, 18.0 Hz, 1H), 3.84 (s, 3H), 4.33 (t, *J* = 6.0 Hz, 1H), 6.96 (d, *J* = 8.0 Hz, 1H), 7.01 (q, *J* = 8.0 Hz, 1H), 7.21-7.24 (m, 1H), 7.28-7.38 (m, 6H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 201.8, 174.9, 157.1, 142.3, 136.7, 130.7, 129.8, 129.0, 127.2 (2C), 126.9, 120.6, 120.4 (2C), 111.9, 55.5, 47.7, 45.9, 24.6, 14.1. **HRMS** (ESI-TOF) calcd for $C_{20}H_{21}O_2S^+$ ($[M+H]^+$) 325.1257, found 325.1251.

4-(Benzo[d][1,3]dioxol-5-yl)-3-(ethylthio)-2-(2-methoxyphenyl)cyclopent-2-enone (2j)



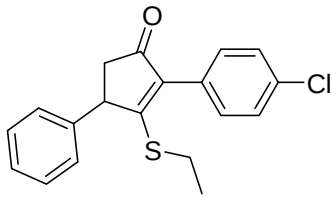
White solid. mp 127-128 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.05 (t, *J* = 7.5 Hz, 3H), 2.38 (dd, *J* = 1.5, 18.0 Hz, 1H), 2.45-2.52 (m, 1H), 2.67-2.73 (m, 1H), 3.09 (dd, *J* = 7.5, 18.5 Hz, 1H), 3.84 (s, 3H), 4.27 (t, *J* = 6.0 Hz, 1H), 5.96 (d, *J* = 4.5 Hz, 2H), 6.79 (s, 2H), 6.82 (s, 1H), 6.96 (d, *J* = 8.5 Hz, 1H), 7.01 (t, *J* = 7.5 Hz, 1H), 7.20 (q, *J* = 7.5 Hz, 1H), 7.34 (m, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 201.8, 175.0, 157.1, 148.4, 146.7, 136.6, 136.1, 130.7, 129.8, 120.6, 120.5, 120.4, 111.0, 108.5, 107.0, 101.1, 55.5, 47.4, 46.0, 24.6, 14.1. **HRMS** (ESI-TOF) calcd for $C_{21}H_{21}O_4S^+$ ($[M+H]^+$) 369.1155, found 369.1159.

4-(4-Chlorophenyl)-3-(ethylthio)-2-(2-methoxyphenyl)cyclopent-2-enone (2k)



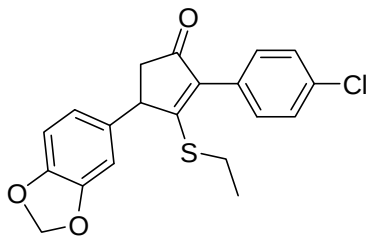
Yellow oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.02 (t, *J* = 7.5 Hz, 3H), 2.35-2.44 (m, 2H), 2.62-2.69 (m, 1H), 3.11 (dd, *J* = 7.5, 18.0 Hz, 1H), 3.84 (s, 3H), 4.31 (d, *J* = 7.5 Hz, 1H), 6.96 (d, *J* = 8.0 Hz, 1H), 7.01 (t, *J* = 7.5 Hz, 1H), 7.20-7.22 (m, 1H), 7.26 (d, *J* = 8.5 Hz, 2H), 7.34-7.37 (m, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 201.4, 174.3, 157.0, 140.9, 132.9, 130.6, 129.8, 129.5, 129.2 (2C), 128.3 (2C), 120.4, 120.3, 110.1, 55.5, 47.0, 45.7, 24.6, 14.0. **HRMS** (ESI-TOF) calcd for $C_{20}H_{20}ClO_2S^+$ ($[M+H]^+$) 359.0867, found 359.0861.

2-(4-Chlorophenyl)-3-(ethylthio)-4-phenylcyclopent-2-enone (2*l*)



Yellow solid. mp 151-152 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.08 (t, *J* = 7.5 Hz, 3H), 2.42 (dd, *J* = 2.0, 18.5 Hz, 1H), 2.47-2.53 (m, 1H), 2.77-2.82 (m, 1H), 3.13 (dd, *J* = 2.0, 18.5 Hz, 1H), 4.36 (dd, *J* = 2.0, 7.5 Hz, 1H), 7.24 (d, *J* = 8.0 Hz, 2H), 7.31 (t, *J* = 7.5 Hz, 1H), 7.37-7.43 (m, 4H), 7.50 (dd, *J* = 2.0, 7.5 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 201.5, 174.4, 142.0, 136.8, 133.9, 130.5 (2C), 129.6, 129.3 (2C), 128.5 (2C), 127.5, 126.8 (2C), 47.2, 46.1, 25.1, 14.1. **HRMS** (ESI-TOF) calcd for $C_{19}H_{18}ClOS^+$ ($[M+H]^+$) 329.0761, found 329.0765.

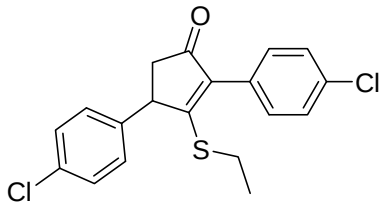
4-(Benzo[d][1,3]dioxol-5-yl)-2-(4-chlorophenyl)-3-(ethylthio)cyclopent-2-enone (2m)



White solid. mp 142-143 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.12 (t, *J* = 7.5 Hz, 3H), 2.40 (d, *J* = 18.5 Hz, 1H), 2.55-2.59 (m, 1H), 2.81-2.85 (m, 1H), 3.09 (dd, *J* = 2.5, 18.5 Hz, 1H), 4.28 (d, *J* = 7.5 Hz, 1H), 5.98 (s, 2H), 6.69 (s, 1H), 6.72 (d, *J* = 8.0 Hz, 1H), 6.90 (d, *J* = 8.0 Hz, 1H), 7.40 (d, *J* = 8.0 Hz, 2H), 7.49 (d, *J* = 8.0 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 201.4, 174.3, 148.4, 146.9, 136.7, 135.6, 133.8, 130.4 (2C), 129.6, 128.4 (2C), 120.2, 108.8, 106.8, 101.2, 46.8, 46.1, 25.0,

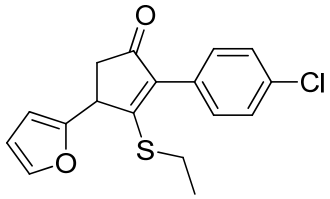
14.1. **HRMS** (ESI-TOF) calcd for $C_{20}H_{18}ClO_3S^+$ ($[M+H]^+$) 373.0660, found 373.0664

2,4-Bis(4-chlorophenyl)-3-(ethylthio)cyclopent-2-enone (2n)



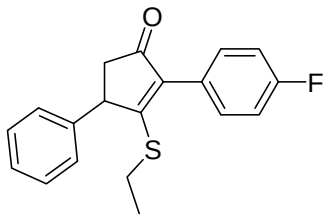
Yellow solid. mp 97-98 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.09 (t, *J* = 7.5 Hz, 3H), 2.42 (d, *J* = 18.5 Hz, 1H), 2.46-2.50 (m, 1H), 2.75-2.80 (m, 1H), 3.11 (dd, *J* = 7.5, 18.5 Hz, 1H), 4.33 (d, *J* = 7.0 Hz, 1H), 7.19 (d, *J* = 8.5 Hz, 2H), 7.35 (d, *J* = 8.5 Hz, 2H), 7.41 (d, *J* = 8.5 Hz, 2H), 7.50 (d, *J* = 8.5 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 201.1, 173.7, 140.4, 137.0, 133.9, 133.2, 130.4 (2C), 129.5, 129.4 (2C), 128.4 (2C), 128.1 (2C), 46.4, 45.8, 25.1, 14.0. **HRMS** (ESI-TOF) calcd for $C_{19}H_{17}Cl_2OS^+$ ($[M+H]^+$) 363.0372, found 363.0378.

2-(4-Chlorophenyl)-3-(ethylthio)-4-(furan-2-yl)cyclopent-2-enone (2o)



Yellow solid. mp 70-71°C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.17 (t, *J* = 7.5 Hz, 3H), 2.62 (dd, *J* = 2.0, 18.5 Hz, 1H), 2.67-2.71 (m, 1H), 2.85-2.89 (m, 1H), 3.01 (dd, *J* = 7.5, 18.5 Hz, 1H), 4.45 (dd, *J* = 2.0, 7.5 Hz, 1H), 6.24 (d, *J* = 3.0 Hz, 1H), 6.36-6.37 (m, 1H), 7.39 (q, *J* = 8.0 Hz, 3H), 7.46 (t, *J* = 8.0 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 201.1, 171.1, 153.8, 142.1, 136.8, 133.9, 130.5 (2C), 129.5, 128.4 (2C), 110.7, 106.4, 42.8, 40.6, 25.1, 14.2. **HRMS** (ESI-TOF) calcd for $C_{17}H_{16}ClO_2S^+$ ($[M+H]^+$) 319.0554, found 319.0556.

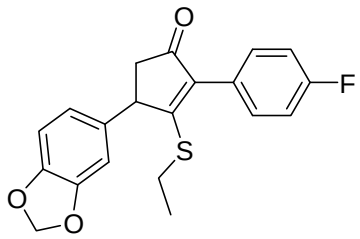
3-(Ethylthio)-2-(4-fluorophenyl)-4-phenylcyclopent-2-enone (2p)



White solid. mp 145-146 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.08 (t, *J* = 7.5 Hz, 3H), 2.42 (dd, *J* = 2.0, 18.5 Hz, 1H), 2.47-2.51 (m, 1H), 2.78-2.82 (m, 1H), 3.13 (dd, *J* = 7.5, 18.5 Hz, 1H), 4.36 (dd, *J* = 2.0, 7.5 Hz, 1H), 7.12-7.16 (m, 2H), 7.25-7.29 (m, 2H), 7.29-7.32 (m, 1H), 7.37-7.39 (m, 2H), 7.39-7.56 (m, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 201.7, 174.0, 162.2 (d, *J* = 246.6 Hz, 1C), 142.0,

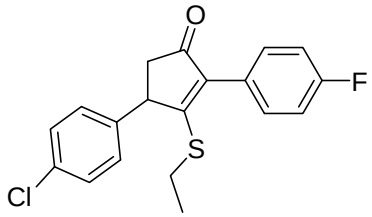
137.0, 130.9 (d, J = 8.1 Hz, 2C), 129.3 (2C), 127.4, 127.1 (d, J = 3.4 Hz, 1C), 126.8 (2C), 115.2 (d, J = 21.5 Hz, 2C), 47.1, 46.1, 24.9, 14.1. **HRMS** (ESI-TOF) calcd for $C_{19}H_{18}FOS^+$ ($[M+H]^+$) 313.1057, found 313.1058.

4-(Benzo[d][1,3]dioxol-5-yl)-3-(ethylthio)-2-(4-fluorophenyl)cyclopent-2-enone (2q)



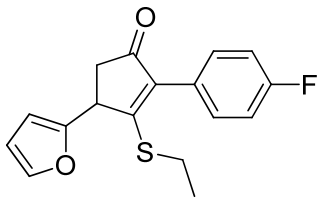
Yellow solid. mp 146-147 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.12 (t, J = 7.5 Hz, 3H), 2.38 (dd, J = 1.5, 18.5 Hz, 1H), 2.55-2.58 (m, 1H), 2.79-2.84 (m, 1H), 3.08 (dd, J = 7.5, 18.0 Hz, 1H), 4.27 (t, J = 6.5 Hz, 1H), 5.97 (d, J = 1.5 Hz, 2H), 6.69-6.74 (m, 2H), 6.79 (d, J = 8.0 Hz, 1H), 7.13 (t, J = 8.0 Hz, 2H), 7.51-7.54 (m, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 201.6, 173.9, 162.2 (d, J = 246.1 Hz, 1C), 148.4, 146.9, 136.9, 135.7, 130.9 (d, J = 8.0 Hz, 2C), 127.1 (d, J = 2.9 Hz, 1C), 120.1, 115.1 (d, J = 21.5 Hz, 2C), 108.8, 106.8, 101.2, 46.8, 46.1, 24.9, 14.1. **HRMS** (ESI-TOF) calcd for $C_{20}H_{18}FO_3S^+$ ($[M+H]^+$) 357.0955, found 357.0954.

4-(4-Chlorophenyl)-3-(ethylthio)-2-(4-fluorophenyl)cyclopent-2-enone (2r)



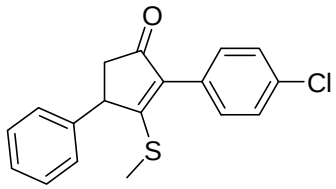
Yellow solid. mp 136-137 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.10 (t, J = 7.5 Hz, 3H), 2.38 (dd, J = 1.5, 18.5 Hz, 1H), 2.46-2.50 (m, 1H), 2.76-2.80 (m, 1H), 3.11 (dd, J = 7.5, 18.5 Hz, 1H), 4.33 (dd, J = 1.5, 7.5 Hz, 1H), 7.11-7.15 (m, 2H), 7.20 (t, J = 7.0 Hz, 2H), 7.36 (t, J = 7.0 Hz, 2H), 7.52-7.54 (m, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 201.3, 173.2, 162.3 (d, J = 247.0 Hz, 1C), 140.5, 137.2, 133.2, 130.9 (d, J = 8.1 Hz, 2C), 129.5 (2C), 128.2 (2C), 126.9 (d, J = 3.4 Hz, 1C), 115.2 (d, J = 21.5 Hz, 2C), 46.4, 45.8, 25.0, 14.0. **HRMS** (ESI-TOF) calcd for $C_{19}H_{17}ClFOS^+$ ($[M+H]^+$) 347.0667, found 367.0664.

3-(Ethylthio)-2-(4-fluorophenyl)-4-(furan-2-yl)cyclopent-2-enone (2s)



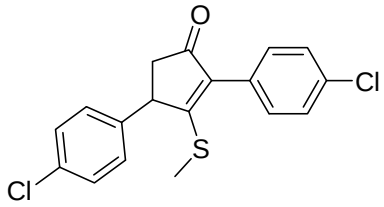
Yellow solid. mp 99-100 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.17 (t, *J* = 7.5 Hz, 3H), 2.64 (dd, *J* = 2.0, 18.0 Hz, 1H), 2.67-2.71 (m, 1H), 2.85-2.89 (m, 1H), 3.02 (dd, *J* = 7.5, 18.0 Hz, 1H), 3.45 (dd, *J* = 2.0, 7.5 Hz, 1H), 6.24 (d, *J* = 3.0 Hz, 1H), 6.36-6.37 (m, 1H), 7.12 (t, *J* = 9.0 Hz, 2H), 7.38 (d, *J* = 1.0 Hz, 1H), 7.47-7.50 (m, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 201.2, 170.7, 162.3 (d, *J* = 246.5 Hz, 1C), 153.9, 142.1, 136.9, 131.0 (d, *J* = 8.1 Hz, 2C), 127.0, 115.2 (d, *J* = 21.5 Hz, 2C), 110.6, 106.3, 42.8, 40.5, 24.9, 14.2. **HRMS** (ESI-TOF) calcd for $C_{17}H_{16}FO_2S^+$ ($[M+H]^+$) 303.0850, found 303.0859.

2-(4-Chlorophenyl)-3-(methylthio)-4-phenylcyclopent-2-enone (2t)



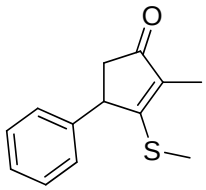
Yellow solid. mp 55-56°C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 2.11 (s, 3H), 2.41 (dd, *J* = 1.5, 18.5 Hz, 1H), 3.13 (dd, *J* = 7.5, 18.5 Hz, 1H), 4.37 (dd, *J* = 1.5, 7.5 Hz, 1H), 7.24 (d, *J* = 7.5 Hz, 2H), 7.30 (t, *J* = 7.5 Hz, 1H), 7.35-7.41 (m, 4H), 7.51 (d, *J* = 7.5 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 201.5, 174.8, 141.6, 136.8, 133.8, 130.3 (2C), 129.5, 129.3 (2C), 128.4 (2C), 127.5, 126.7 (2C), 46.8, 46.1, 13.9. **HRMS** (ESI-TOF) calcd for $C_{18}H_{16}ClOS^+$ ($[M+H]^+$) 315.0605, found 315.0609.

2,4-Bis(4-chlorophenyl)-3-(methylthio)cyclopent-2-enone (2u)



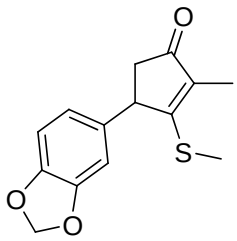
White solid. mp 152-153 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 2.11 (s, 3H), 2.36 (d, *J* = 18.5 Hz, 1H), 3.11 (dd, *J* = 2.5, 18.5 Hz, 1H), 4.34 (d, *J* = 7.0 Hz, 1H), 7.19 (d, *J* = 8.0 Hz, 2H), 7.34 (d, *J* = 8.0 Hz, 2H), 7.40 (d, *J* = 8.5 Hz, 2H), 7.49 (d, *J* = 8.5 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 200.9, 173.9, 140.2, 137.1, 133.9, 133.3, 130.3 (2C), 129.5 (2C), 129.3, 128.4 (2C), 128.1 (2C), 46.1, 45.9, 13.9. **HRMS** (ESI-TOF) calcd for $C_{18}H_{15}Cl_2OS^+$ ($[M+H]^+$) 349.0215, found 349.0213.

2-Methyl-3-(methylthio)-4-phenylcyclopent-2-enone (2v)



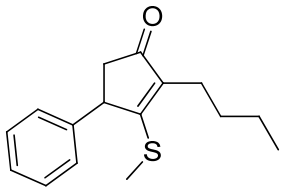
Light yellow solid. mp 79-80 °C **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.85 (s, 3H), 2.11 (s, 3H), 2.25 (dd, *J* = 2.0, 18.5 Hz, 1H), 2.98 (dd, *J* = 7.5, 18.5 Hz, 1H), 4.24-4.26 (m, 1H), 7.17 (q, *J* =7.0 Hz, 2H), 7.25-7.33 (m, 1H), 7.32-7.35 (m, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 203.3, 172.4, 142.0, 135.6, 129.1 (2C), 127.3, 126.8 (2C), 46.9, 45.8, 13.4, 8.7. **HRMS** (ESI-TOF) calcd for $C_{13}H_{15}OS^+$ ($[M+H]^+$) 219.0838, found 219.0837.

4-(Benzo[d][1,3]dioxol-5-yl)-2-methyl-3-(methylthio)cyclopent-2-enone (2w)



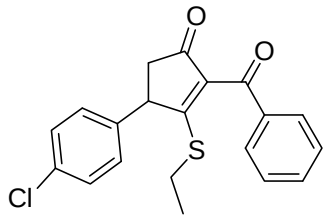
Light yellow solid. mp 111-112 °C **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.83 (s, 3H), 2.17 (s, 3H), 2.24 (dd, *J* = 1.0, 18.0 Hz, 1H), 2.94 (dd, *J* = 7.0, 18.5 Hz, 1H), 4.17 (d, *J* = 7.0 Hz, 1H), 5.96 (d, *J* = 1.5 Hz, 2H), 6.60 (d, *J* =1.5 Hz, 1H), 6.65 (q, *J* = 8.0 Hz, 1H), 6.76 (d, *J* = 8.0 Hz, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 203.1, 172.3, 148.4, 146.7, 135.8, 135.6, 120.1,108.6, 106.8, 101.1, 46.5, 45.8, 13.4, 8.6. **HRMS** (ESI-TOF) calcd for $C_{14}H_{15}O_3S^+$ ($[M+H]^+$) 263.0736, found 263.0731.

2-Butyl-3-(methylthio)-4-phenylcyclopent-2-enone (2x)



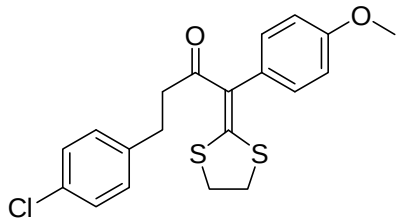
Light yellow oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 0.95 (s, *J* = 7.0 Hz, 3H), 1.26-1.43 (m, 2H), 1.49 (q, *J* = 7.5 Hz, 2H), 2.09 (s, 3H), 2.23-2.31 (m, 2H), 2.35-2.40 (m, 1H) 2.96 (dd, *J* = 7.0, 18.0 Hz, 1H), 4.24 (d, *J* = 7.0 Hz, 1H), 7.16 (d, *J* = 7.5 Hz, 2H), 7.26 (t, *J* =7.5 Hz, 1H), 7.33 (t, *J* = 7.5 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 203.1, 172.2, 142.1, 140.4, 129.2 (2C), 127.2, 126.7 (2C), 46.7, 45.9, 29.3, 23.6, 22.8, 13.9, 13.3. **HRMS** (ESI-TOF) calcd for $C_{16}H_{21}OS^+$ ($[M+H]^+$) 261.1308, found 261.1304.

2-Benzoyl-4-(4-chlorophenyl)-3-(ethylthio)cyclopent-2-enone (2y)



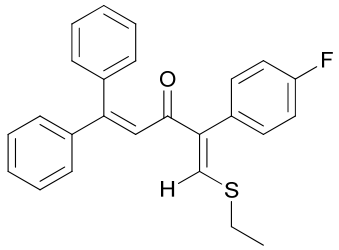
Yellow solid. mp 142-143 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.10 (t, *J* = 7.0 Hz, 3H), 2.45 (dd, *J* = 2.0, 18.5 Hz, 1H), 2.52-2.56 (m, 1H), 2.75-2.79 (m, 1H), 3.16 (dd, *J* = 8.0, 18.0 Hz, 1H), 4.39 (dd, *J* = 2.0, 8.0 Hz, 1H), 7.21 (dd, *J* = 7.0, 6.5 Hz, 2H), 7.36-7.39 (m, 2H), 7.49 (t, *J* = 7.5 Hz, 2H), 7.59 (dd, *J* = 2.0, 8.0 Hz, 1H), 7.85 (dd, *J* = 2.0, 8.0 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 199.3, 192.0, 184.1, 139.7, 136.9, 136.6, 133.7, 133.6, 129.6 (2C), 129.5 (2C), 128.5 (2C), 128.4 (2C), 48.0, 46.2, 26.2, 13.5. **HRMS** (ESI-TOF) calcd for $C_{20}H_{18}ClO_2S^+$ ($[M+H]^+$) 357.0711, found 357.0719.

4-(4-Chlorophenyl)-1-(1,3-dithiolan-2-ylidene)-1-(4-methoxyphenyl)butan-2-one(2aa')



Yellowish liquid. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 2.49 (t, *J* = 7.5 Hz, 2H), 2.84 (t, *J* = 7.5 Hz, 2H), 3.21 (t, *J* = 7.0 Hz, 2H), 3.46 (t, *J* = 7.0 Hz, 2H), 3.84 (s, 3H), 6.92 (d, *J* = 8.5 Hz, 2H), 6.98 (d, *J* = 8.5 Hz, 2H), 7.09 (d, *J* = 8.5 Hz, 2H), 7.16 (d, *J* = 8.0 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 194.7, 159.3, 143.4, 140.1, 132.1, 131.5, 130.9 (2C), 129.8 (2C), 128.3 (2C), 126.0, 114.4 (2C), 55.2, 41.9, 39.8, 33.5, 29.8. **HRMS** (ESI-TOF) calcd for $C_{20}H_{20}ClO_2S_2^+$ ($[M+H]^+$) 391.0588, found 391.0585.

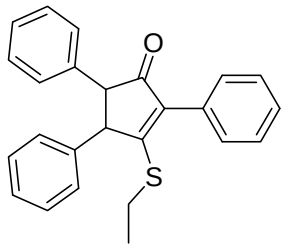
5-(Ethylthio)-4-(4-fluorophenyl)-1,1-diphenylpenta-1,4-dien-3-one (2'ab)



Light yellow solid. mp 128-129 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.32 (t, *J* = 7.5 Hz, 3H), 2.79 (q, *J* = 7.5 Hz, 2H), 6.66 (s, 1H), 7.05-7.13 (m, 4H), 7.20-7.22 (m, 2H), 7.29-7.31 (m, 2H), 7.35-7,40 (m, 6H), 7.78(s, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 189.5, 162.1 (d, *J* = 246.0 Hz, 1C), 152.1, 148.5, 141.0, 139.1, 136.4, 134.9, 131.2 (d, *J* = 8.1 Hz, 2C), 129.6 (2C), 129.0, 128.4 (2C), 128.3

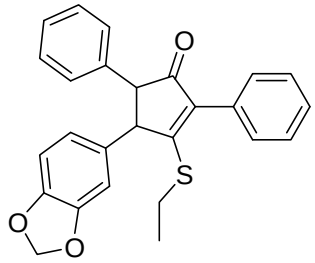
(2C), 128.2 (2C), 127.8, 124.8, 115.2 (d, J = 21.5 Hz, 2C), 29.0, 15.4. **HRMS** (ESI-TOF) calcd for $C_{25}H_{22}FOS^+$ ($[M+H]^+$) 389.1370, found 389.1374.

3-(Ethylthio)-2,4,5-triphenylcyclopent-2-enone(2ac)



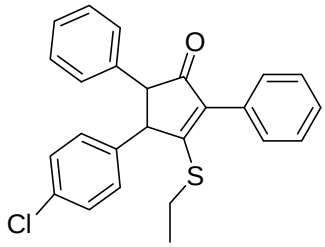
Lightyellow liquid. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.06 (t, J = 7.5 Hz, 3H), 2.44-2.48 (m, 1H), 2.75-2.79 (m, 1H), 3.55 (d, J = 2.0 Hz, 1H), 4.31 (d, J = 2.0 Hz, 1H), 7.17 (d, J = 7.5 Hz, 2H), 7.24-7.39 (m, 9H), 7.44 (t, J = 7.5 Hz, 2H), 7.61 (d, J = 7.5 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 201.1, 173.3, 141.4, 139.6, 137.6, 131.2, 129.4 (2C), 129.2 (2C), 129.0 (2C), 128.7, 128.2 (2C), 127.6, 127.5 (2C), 127.2, 126.9 (2C), 63.2, 57.4, 25.1, 14.1. **HRMS** (ESI-TOF) calcd for $C_{25}H_{23}OS^+$ ($[M+H]^+$) 371.1464, found 371.1460.

4-(Benzo[d][1,3]dioxol-5-yl)-3-(ethylthio)-2,5-diphenylcyclopent-2-enone(2ad)



Yellow solid. mp 149-150 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.11 (t, J = 7.5 Hz, 3H), 2.53-2.57 (m, 1H), 2.79-2.83 (m, 1H), 3.52 (d, J = 2.0 Hz, 1H), 4.22 (d, J = 2.0 Hz, 1H), 5.98 (d, J = 2.0 Hz, 2H), 6.70 (t, J = 1.5 Hz, 2H), 6.80 (d, J = 8.0 Hz, 1H), 7.17 (d, J = 7.0 Hz, 2H), 7.24-7.37 (m, 4H), 7.45 (t, J = 8.0 Hz, 2H), 7.59 (t, J = 7.0 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 201.1, 173.2, 148.5, 147.1, 139.6, 137.6, 135.2, 131.2, 129.2 (2C), 129.0 (2C), 128.2 (3C), 127.5 (2C), 127.2, 120.3, 108.9, 106.9, 101.2, 63.2, 57.2, 25.1, 14.2. **HRMS** (ESI-TOF) calcd for $C_{26}H_{23}O_3S^+$ ($[M+H]^+$) 415.1362, found 415.1362.

4-(4-Chlorophenyl)-3-(ethylthio)-2,5-diphenylcyclopent-2-enone(2ae)



Lightyellow liquid. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 1.09 (t, *J* = 7.5 Hz, 3H), 2.44-2.48 (m, 1H), 2.74-2.78 (m, 1H), 3.50 (d, *J* = 2.0 Hz, 1H), 4.28 (d, *J* = 2.0 Hz, 1H), 7.16 (d, *J* = 7.5 Hz, 2H), 7.19 (d, *J* = 8.0 Hz, 2H), 7.29 (t, *J* = 7.5 Hz, 1H), 7.34-7.38 (m, 5H), 7.45 (d, *J* = 7.5 Hz, 2H), 7.59 (d, *J* = 7.5 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 200.8, 172.5, 139.9, 139.3, 137.9, 133.4, 131.0, 129.6 (2C), 129.2 (2C), 129.1 (2C), 128.3, 128.3 (2C), 128.2 (2C), 127.5 (2C), 127.4, 63.1, 56.8, 25.2, 14.1. **HRMS** (ESI-TOF) calcd for $C_{25}H_{22}ClOS^+$ ($[M+H]^+$) 405.1074, found 405.1078.

IV. Crystal data and ORTEP drawing of compound 2a

Crystal data for **2a**: $C_{20}H_{20}O_2S$, colorless, *M* = 324.42, monoclinic, space group *P*21/c, *a* = 19.0155(8) Å, *b* = 8.2100(3) Å, *c* = 11.6450(5) Å, *V* = 1735.83(12) Å^3, α = 90.00, β = 107.291(4), γ = 90.00, Z = 4, *T* = 293(2) K, *F*000 = 688, 6642 reflections collected, 3048 unique with *R*(int) = 0.0206, R_1 = 0.0427, wR_2 = 0.1047 ($I > 2\sigma(I)$). CCDC 901005 (**2a**) contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre *via* www.ccdc.cam.uk/data_request/cif.

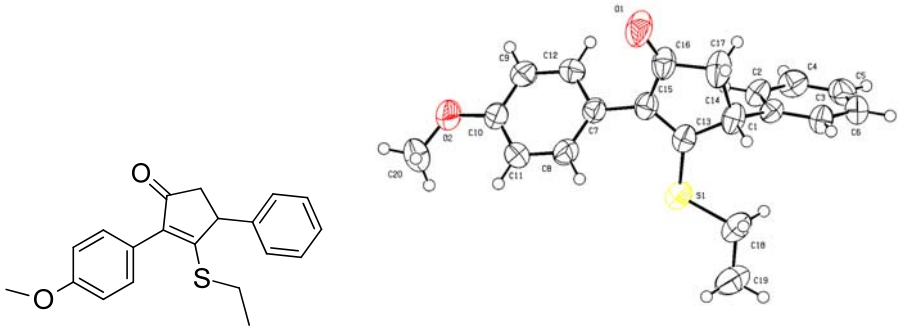


Fig. ORTEP diagram of **2a**.

V. References

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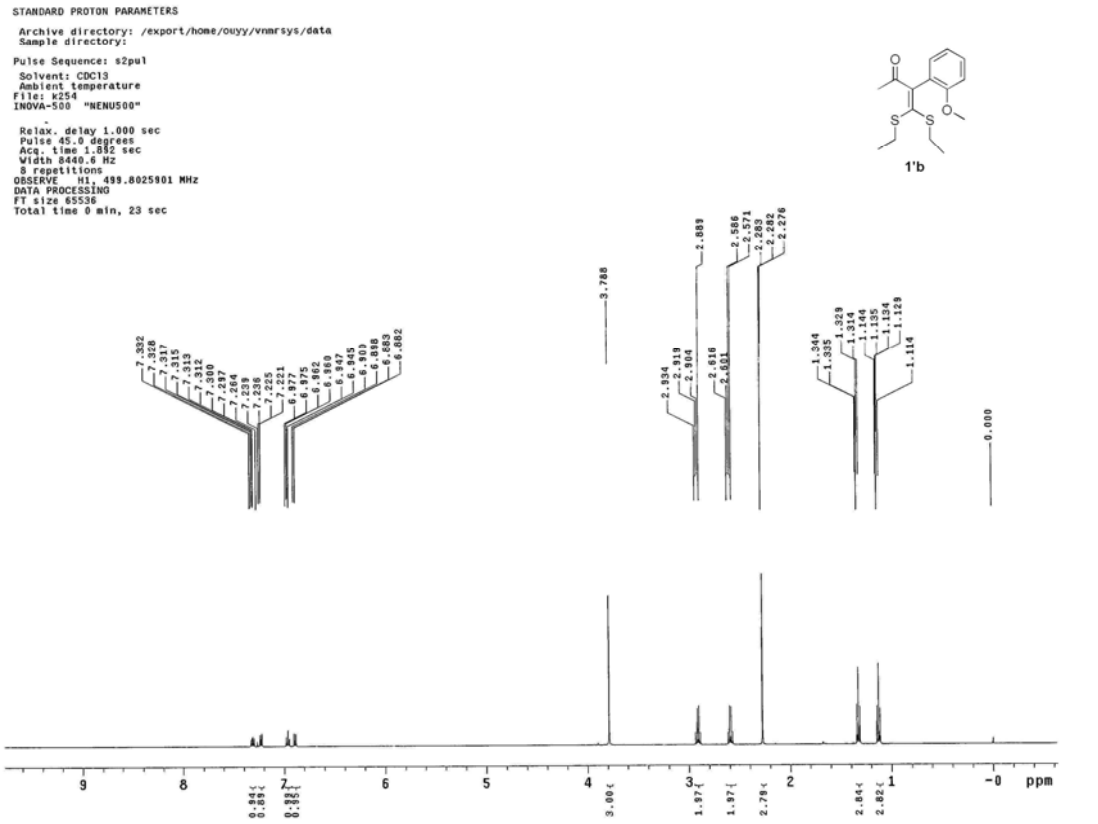
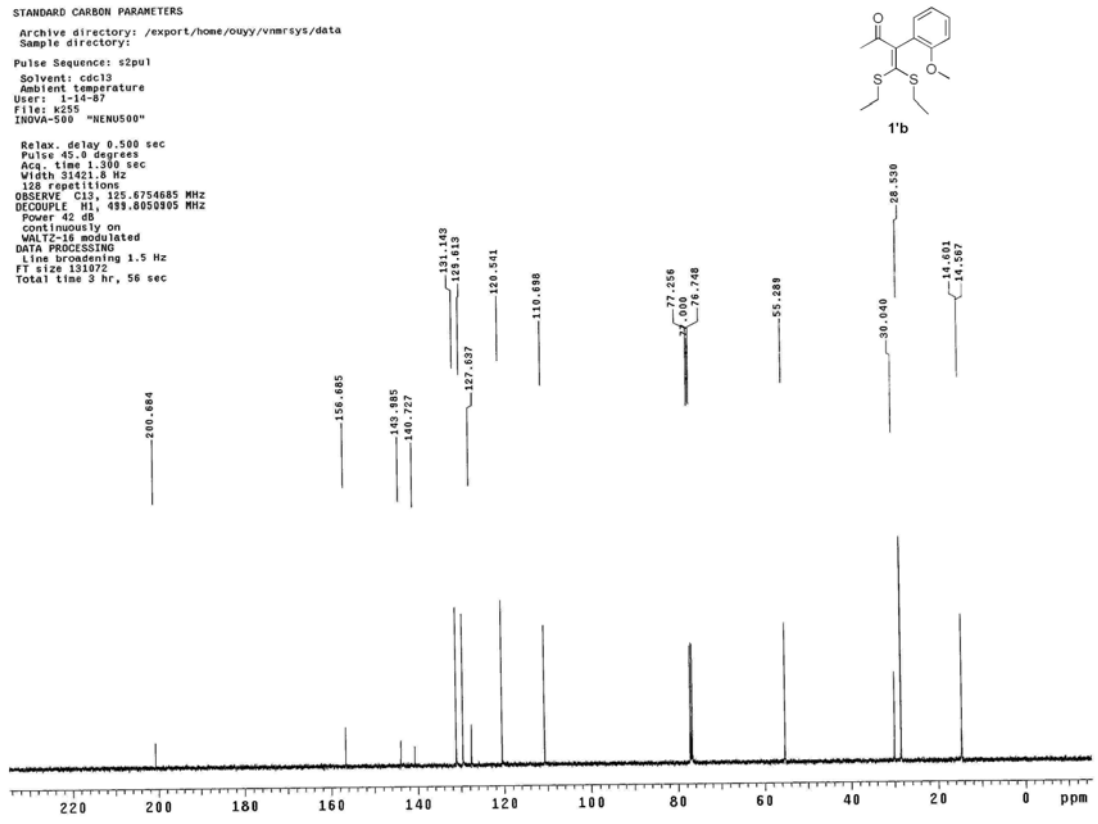
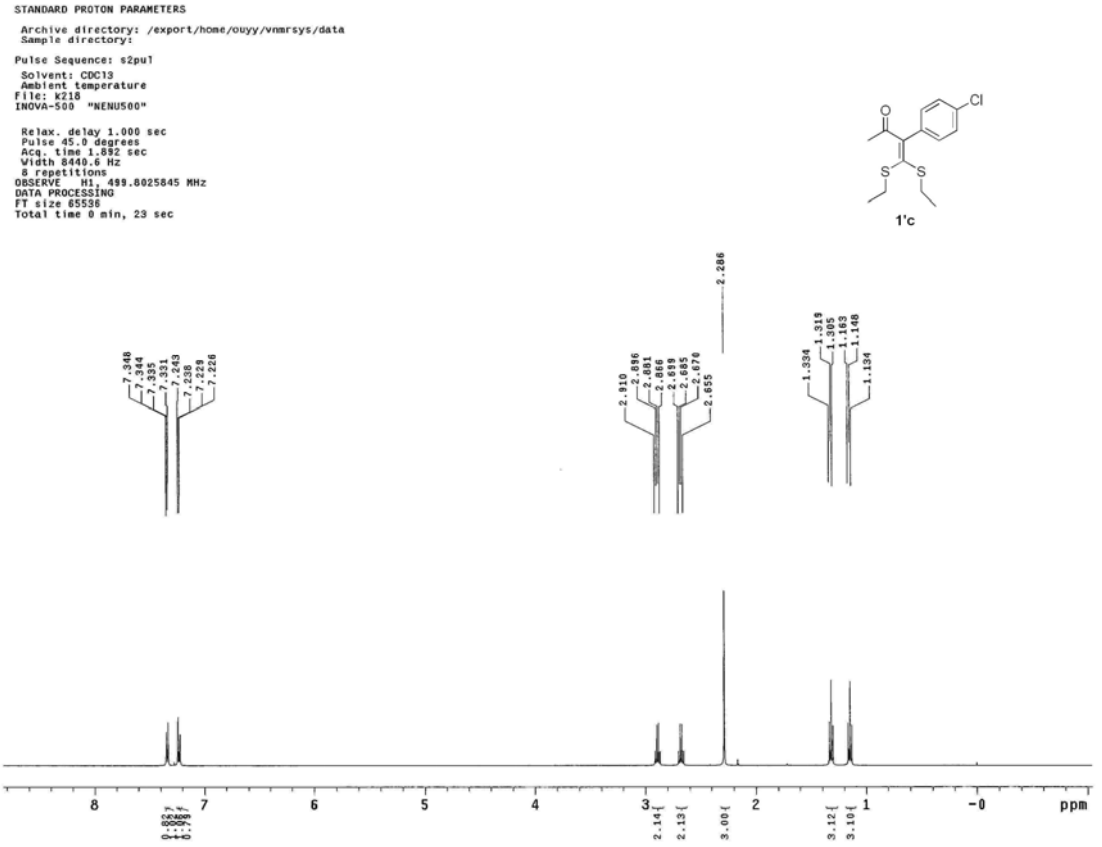
VI. Copies of ^{1}H NMR and ^{13}C NMR spectra of compounds 1′, **1** and **2**



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Ambient temperature
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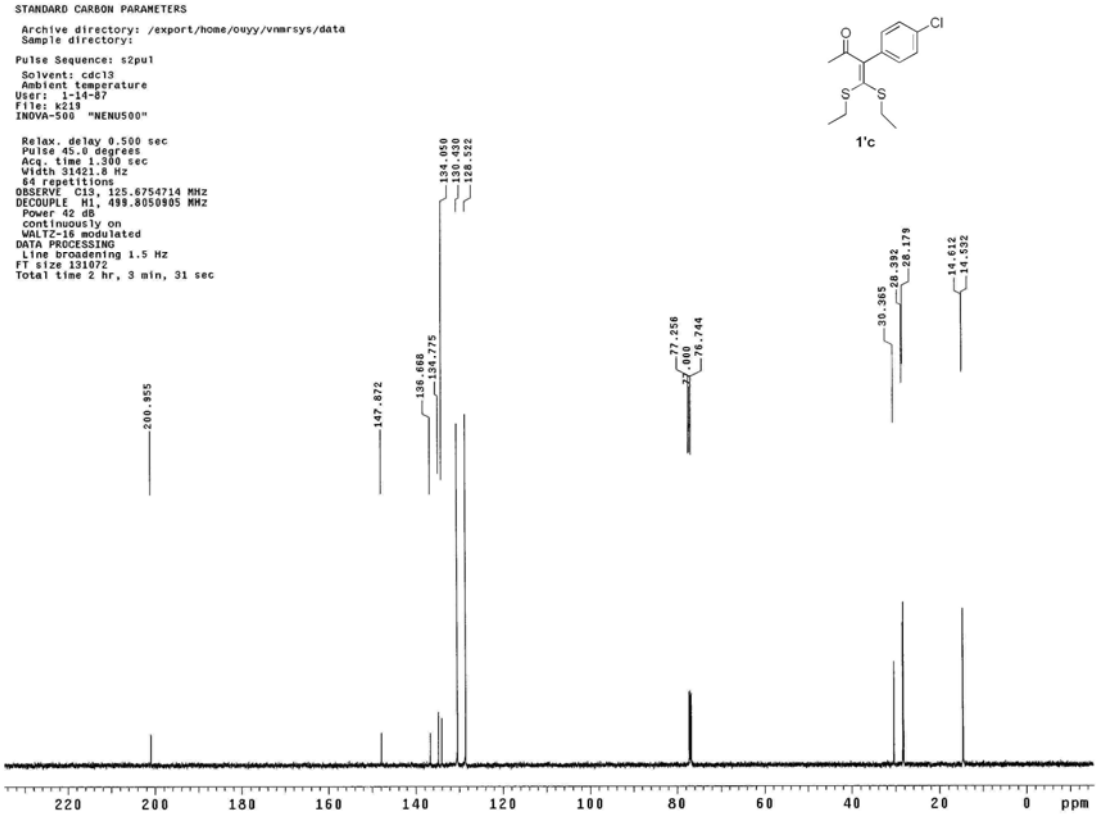
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8440.6 Hz
8 repetitions
OBSERVE H1, 499.8025845 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
1'c
7.348
7.344
7.335
7.331
7.243
7.238
7.228
7.226
2.910
2.886
2.881
2.866
2.685
2.670
2.655
2.286
1.334
1.319
1.305
1.163
1.148
1.134
8
7
6
5
4
3
2
1
-0
ppm
2.14
2.13
3.00
3.12
3.10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File: k219
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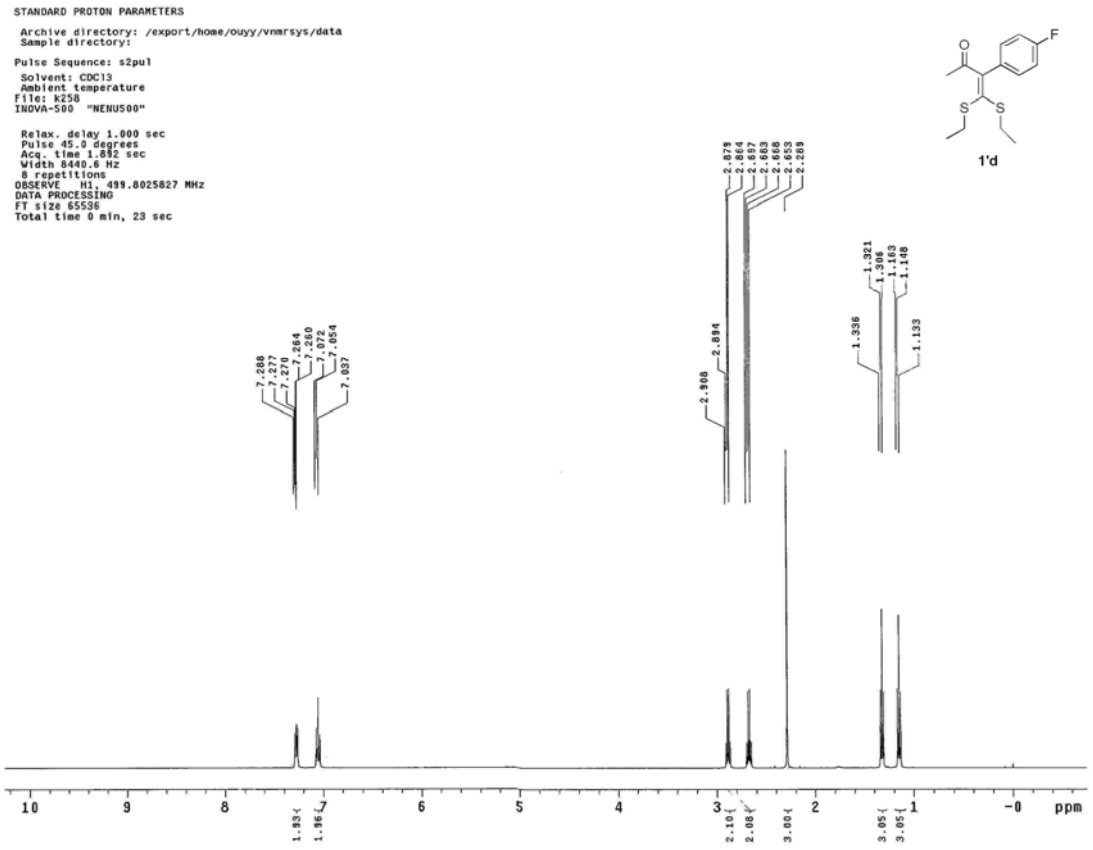
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
64 repetitions
OBSERVE C13, 125.6754714 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec
1'c
200.955
147.872
136.668
134.775
134.050
130.430
128.522
77.256
77.000
76.744
30.365
28.392
28.179
14.612
14.532
220
200
180
160
140
120
100
80
60
40
20
0
ppm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Ambient temperature
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Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.882 sec
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8 repetitions
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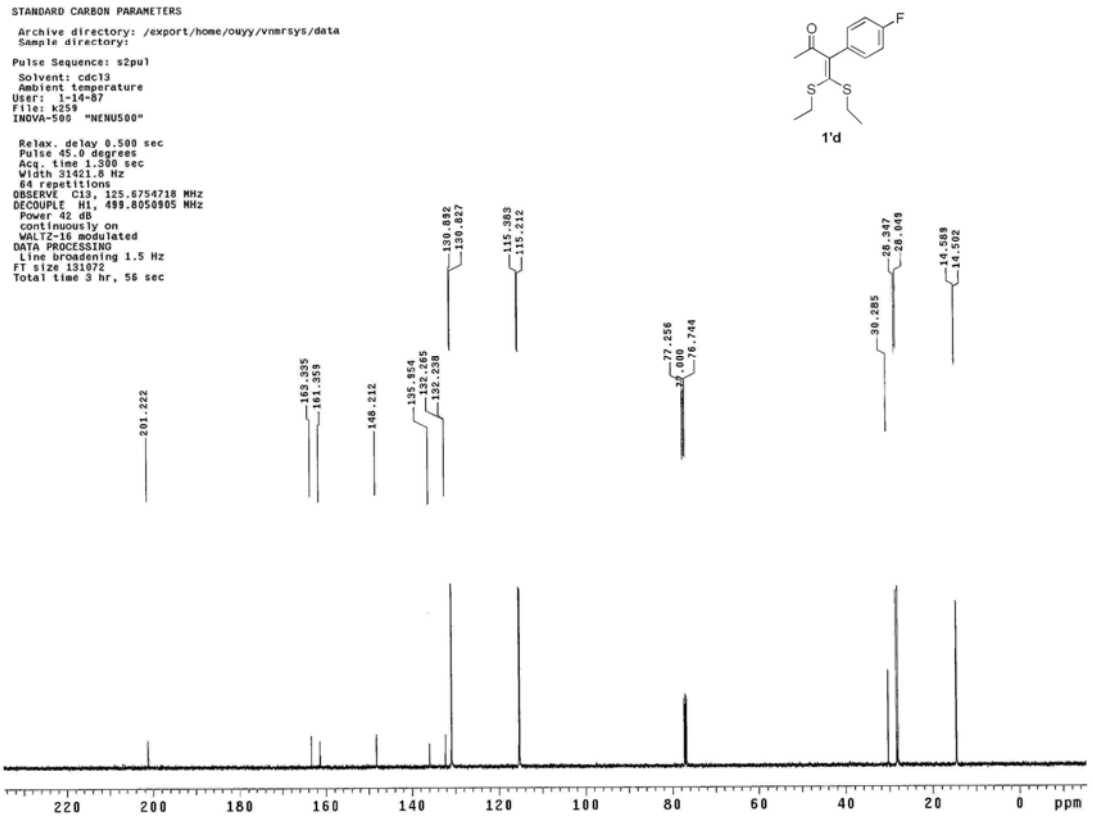
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
1'd
ppm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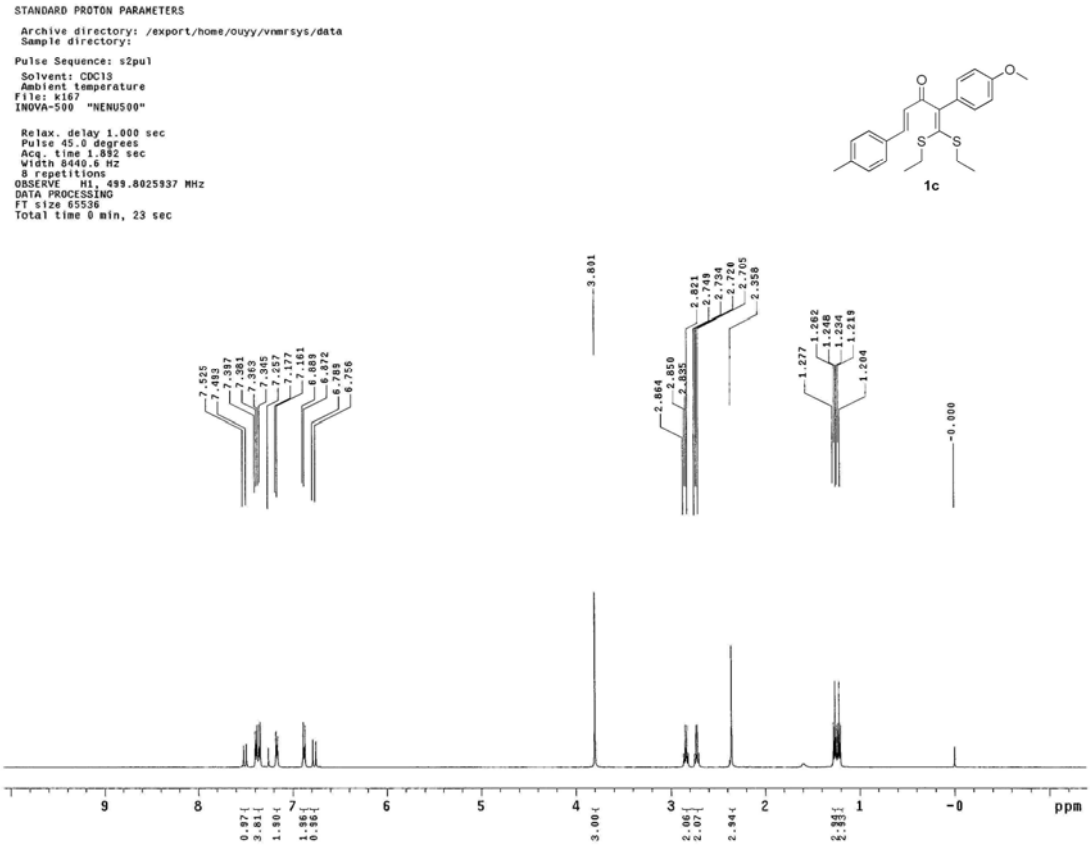
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: k259
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
64 repetitions
OBSERVE C13, 125.6754718 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
1'd
ppm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Sample directory:
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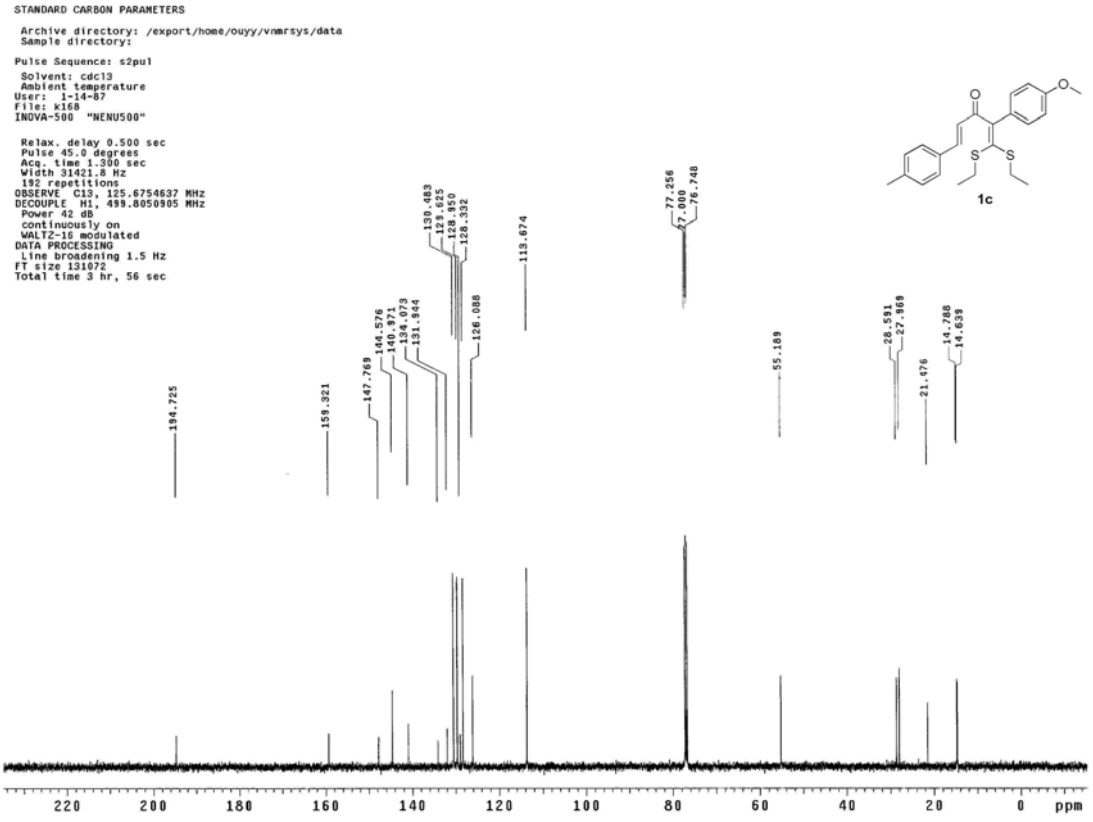
Ambient temperature
File: k167
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8440.6 Hz
8 repetitions
OBSERVE H1, 499.8025937 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
1c
7.525
7.493
7.387
7.381
7.363
7.345
7.257
7.177
7.161
6.809
6.672
6.789
6.756
3.891
2.864
2.850
2.835
2.821
2.749
2.734
2.720
2.705
2.358
1.277
1.262
1.248
1.234
1.219
1.204
-0.000
9
8
7
6
5
4
3
2
1
-0
ppm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Sample directory:
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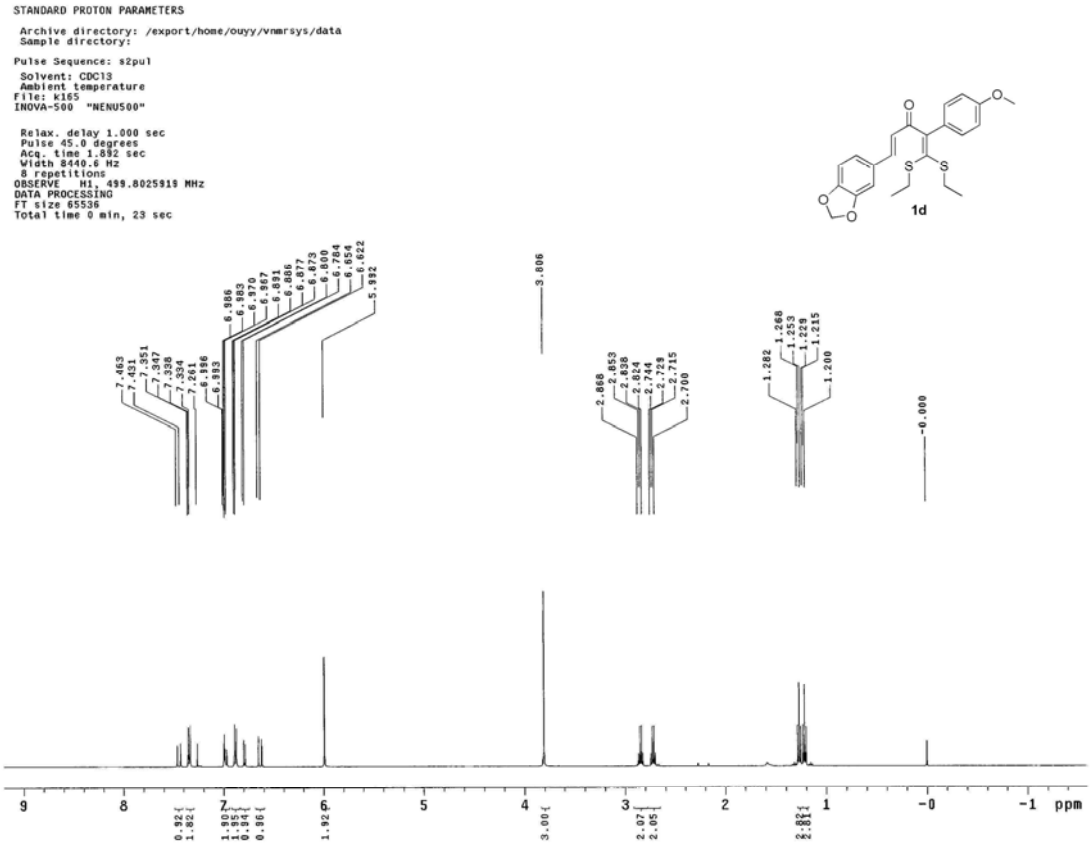
Ambient temperature
User: 1-14-87
File: k168
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
192 repetitions
OBSERVE C13, 125.6754637 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
1c
194.725
159.321
147.769
144.576
140.971
134.073
131.944
130.483
129.625
128.950
128.332
126.088
113.674
77.256
77.000
76.748
55.189
28.591
27.969
21.476
14.788
14.639
220
200
180
160
140
120
100
80
60
40
20
0
ppm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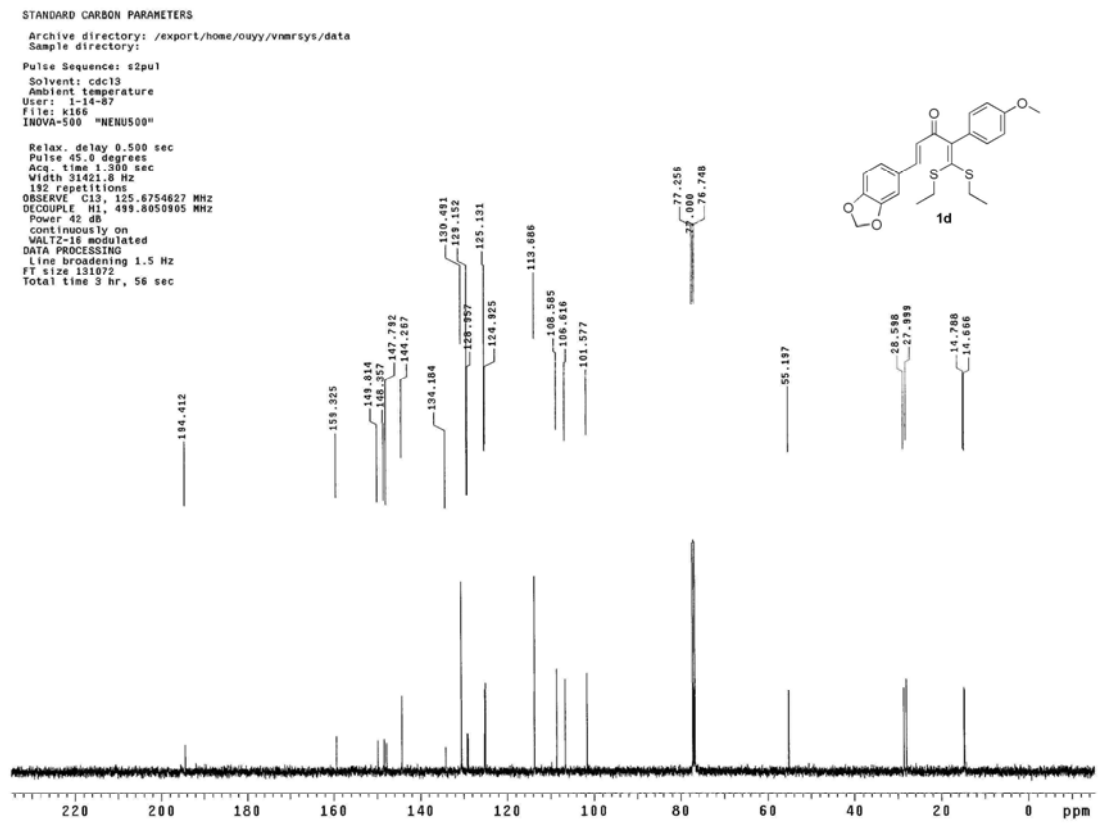
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: k165
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8440.6 Hz
8 repetitions
OBSERVE H1, 499.8025918 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
1d
ppm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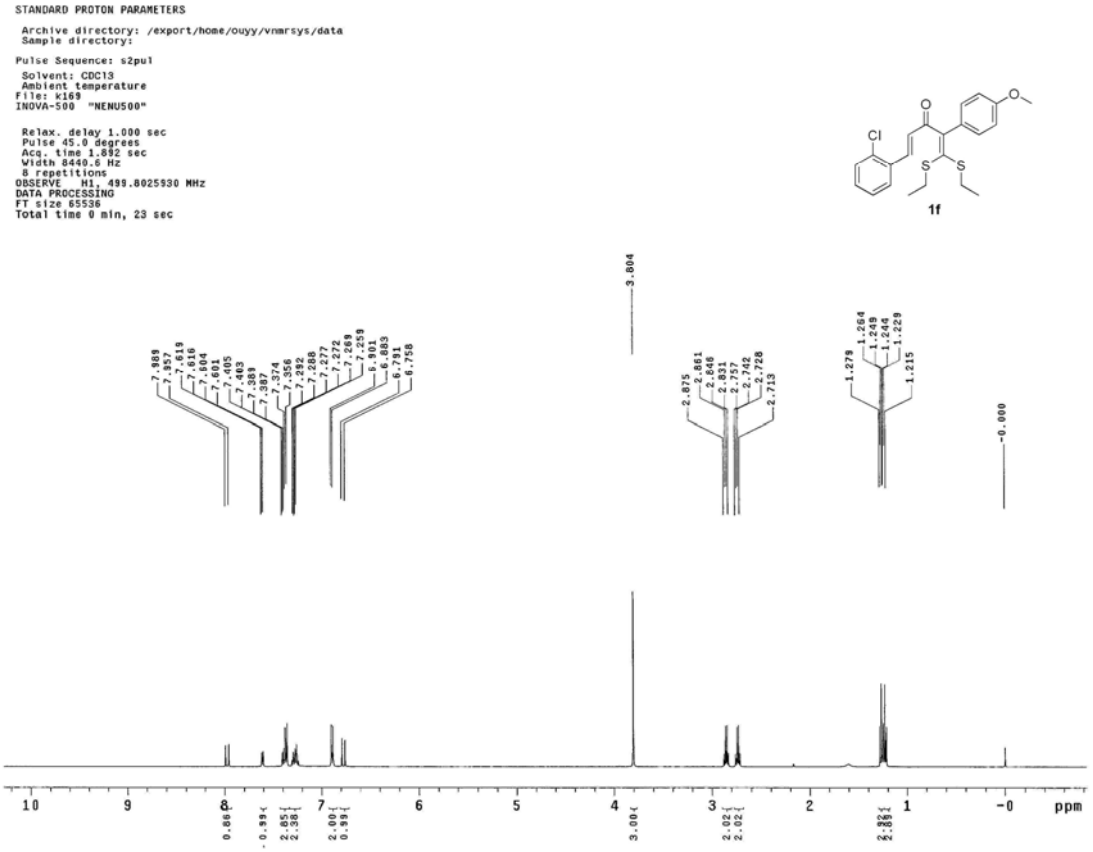
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: k166
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
192 repetitions
OBSERVE C13, 125.6754627 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
1d
ppm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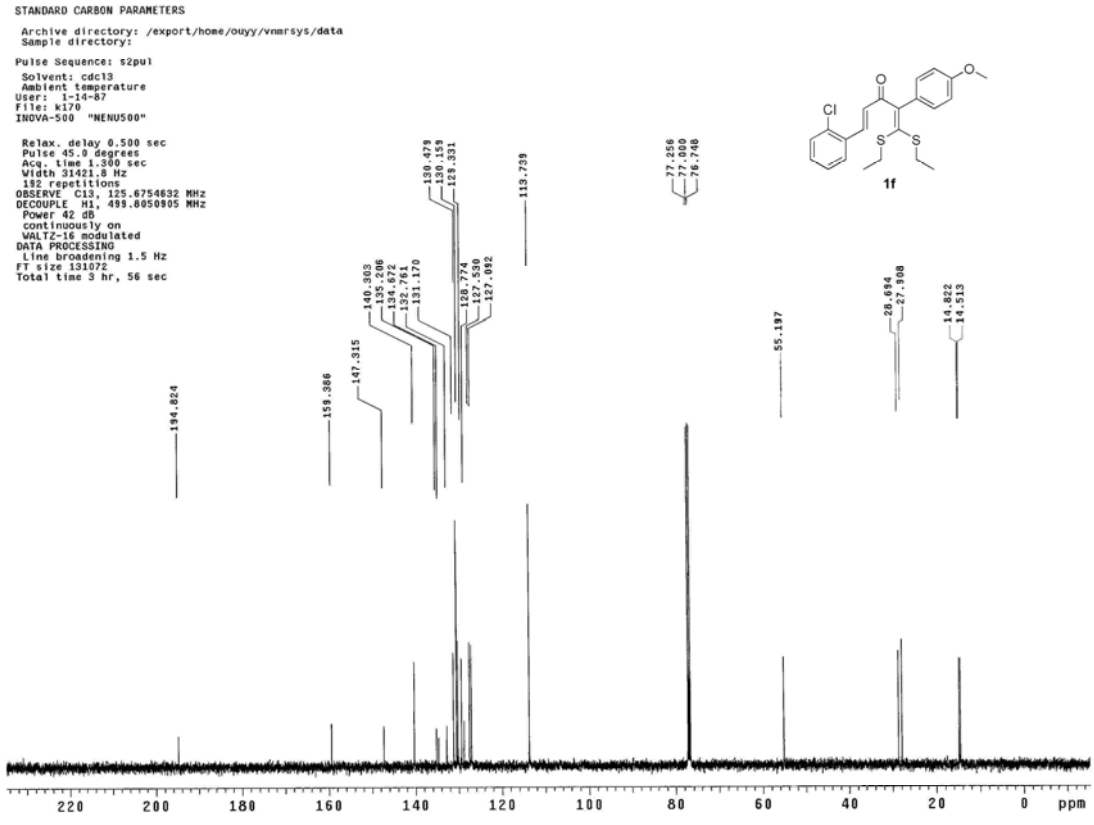
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: k169
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8440.6 Hz
8 repetitions
OBSERVE H1, 499.8025930 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
1f
ppm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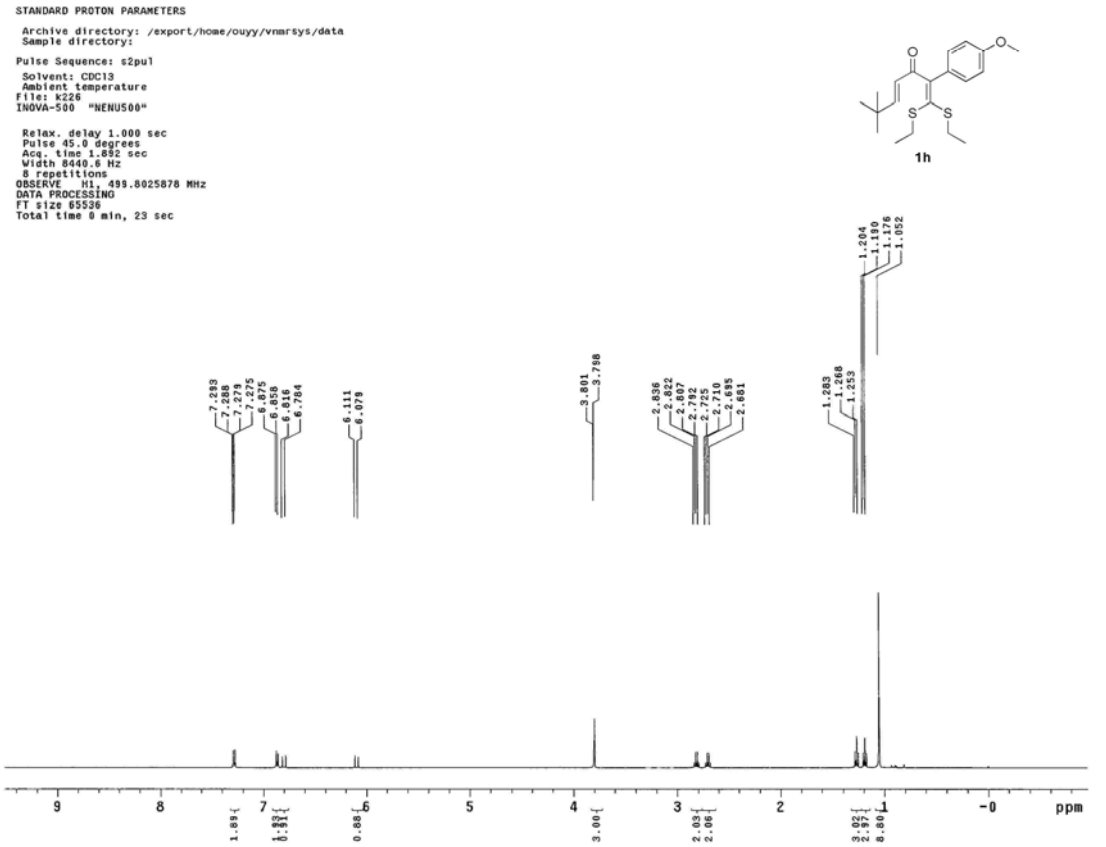
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: k170
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
182 repetitions
OBSERVE C13, 125.6754632 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
1f
ppm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Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: k226
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8440.6 Hz
8 repetitions
OBSERVE H1, 499.8025878 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
1h
7.293
7.288
7.279
7.275
6.875
6.855
6.816
6.784
6.111
6.079
3.801
3.798
2.838
2.822
2.807
2.792
2.725
2.710
2.695
2.681
1.283
1.268
1.253
1.204
1.190
1.176
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1.89
1.03
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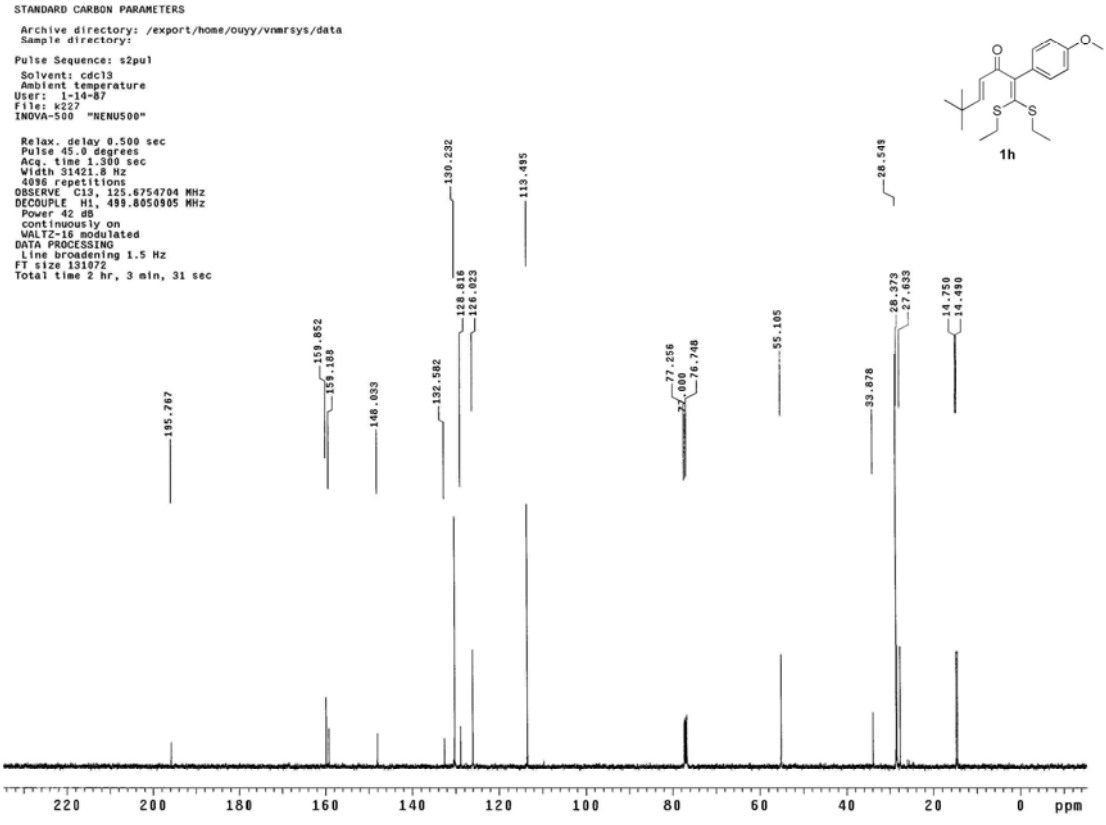
2.03
2.06
3.02
2.97
8.80
ppm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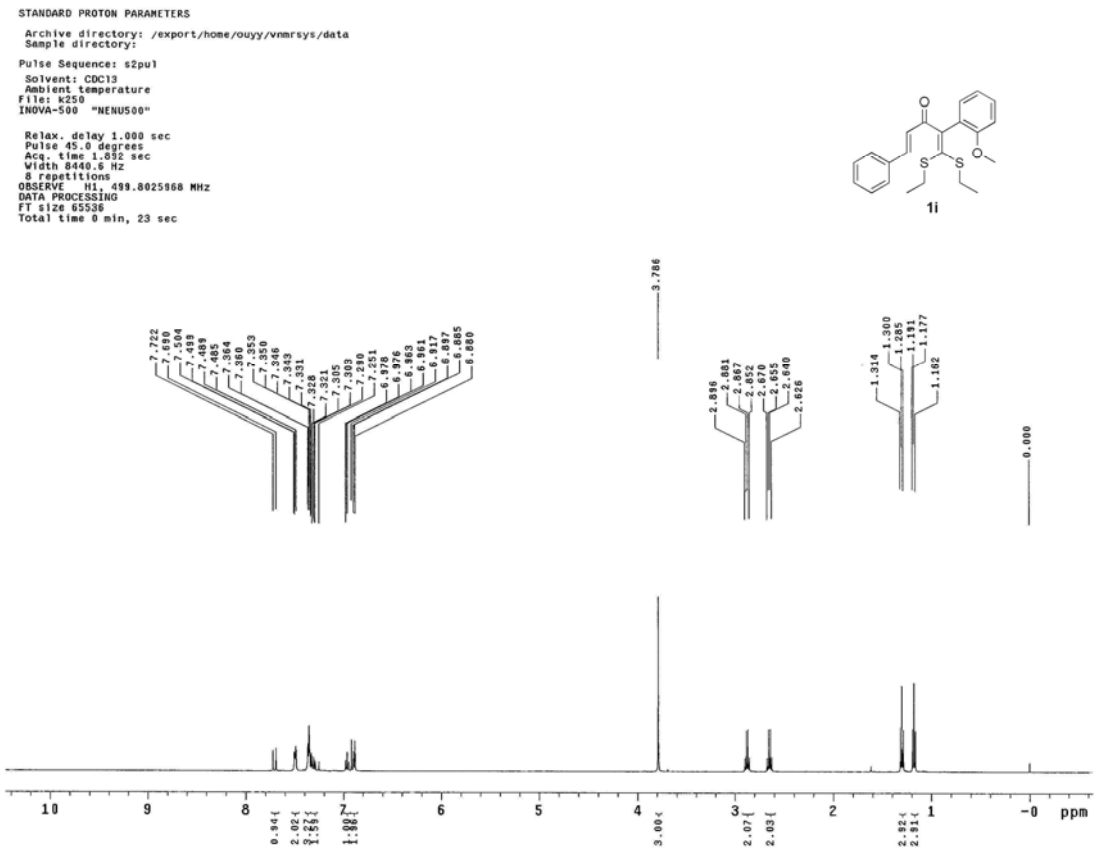
File: k227
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
4096 repetitions
OBSERVE C13, 125.6754704 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec
1h
195.767
159.852
159.106
148.033
132.582
130.232
128.816
126.023
113.495
77.256
77.000
76.748
55.105
33.878
28.548
28.373
27.633
14.750
14.490
220
200
180
160
140
120
100
80
60
40
20
0
ppm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Ambient temperature
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Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
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8 repetitions
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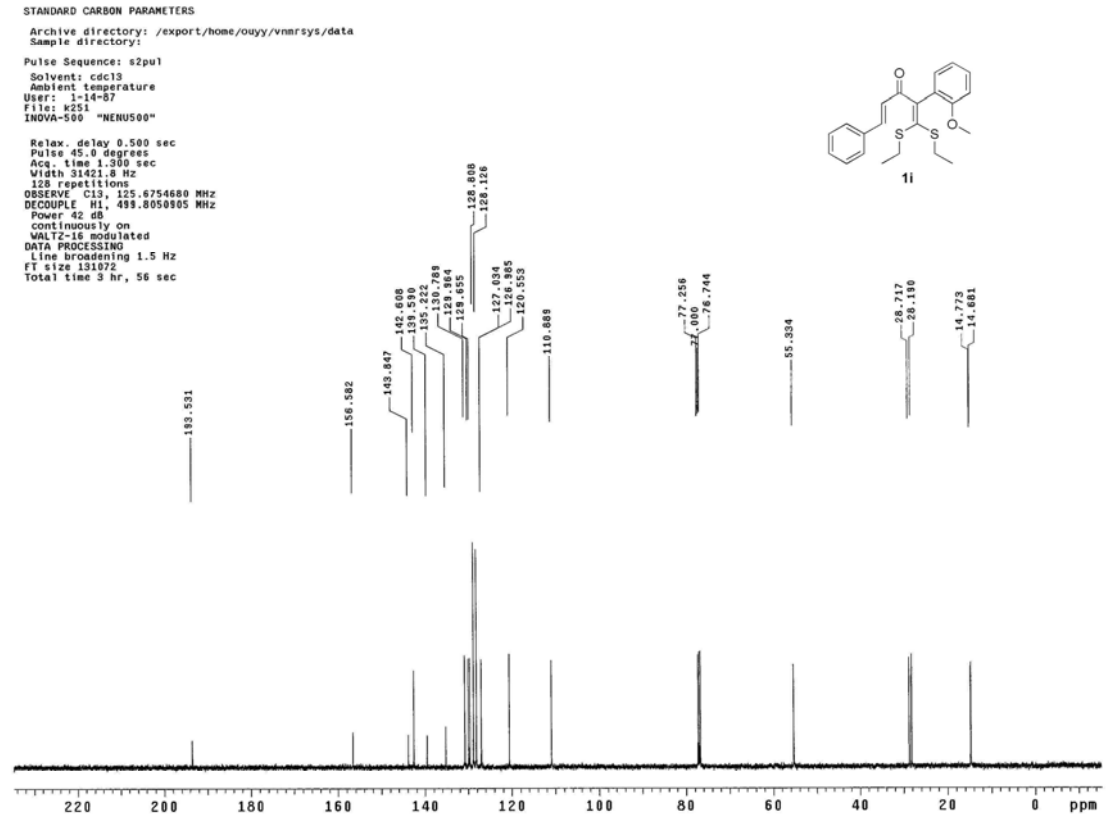
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
1i
ppm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Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: k251
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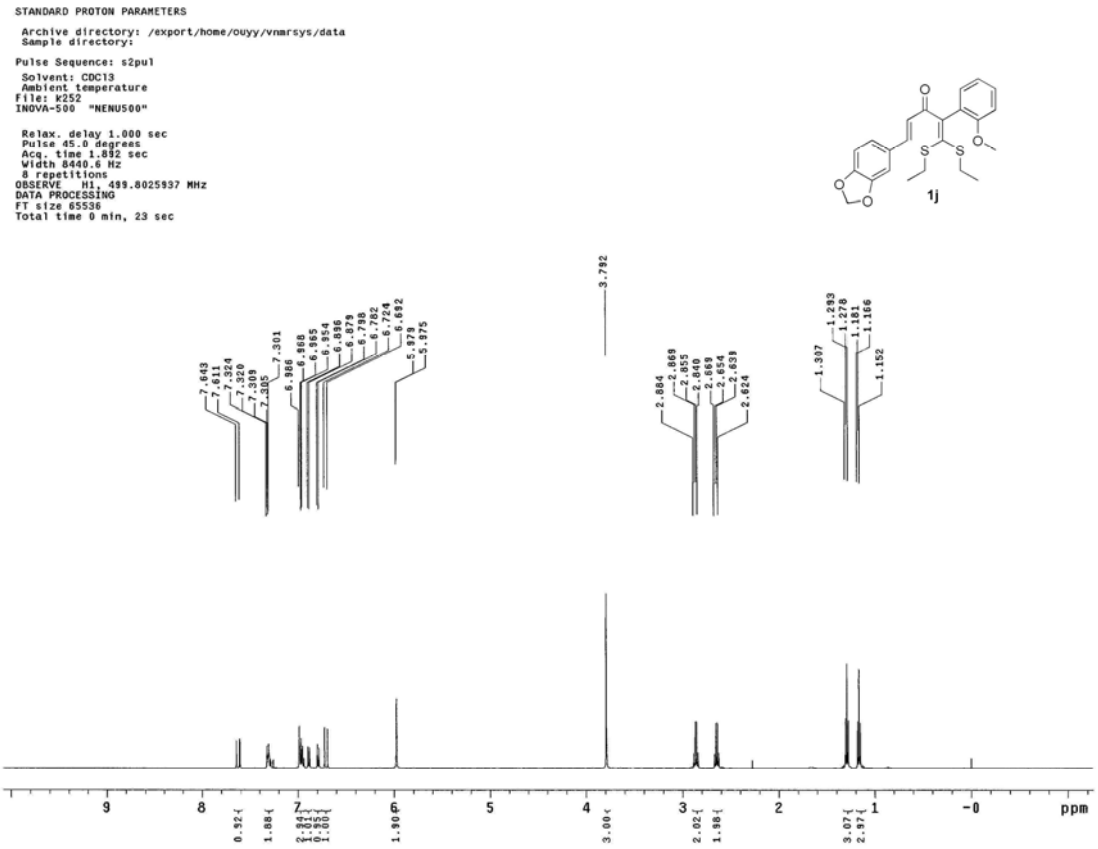
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
128 repetitions
OBSERVE C13, 125.6754680 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
1i
ppm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Ambient temperature
File: k252
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.882 sec
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8 repetitions
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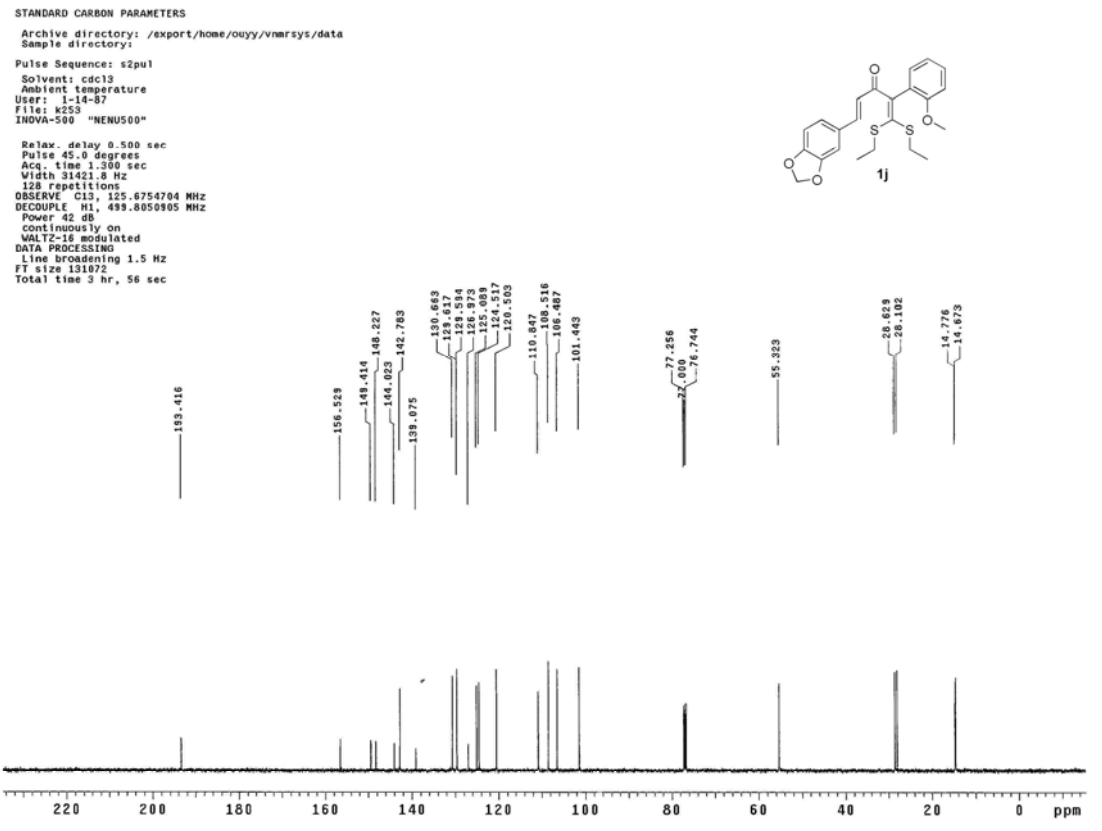
Total time 0 min, 23 sec
1j
ppm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Sample directory:
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Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: k253
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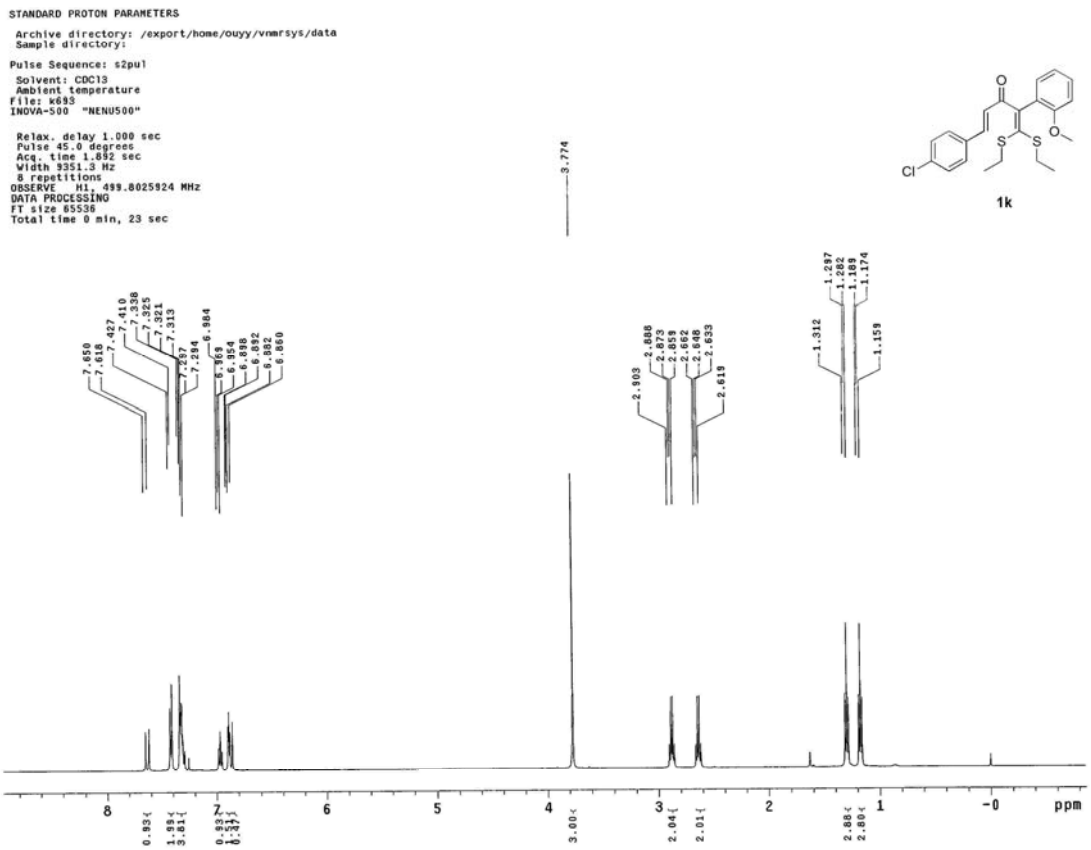
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
128 repetitions
OBSERVE C13, 125.6754704 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
1j
ppm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Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: k693
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Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
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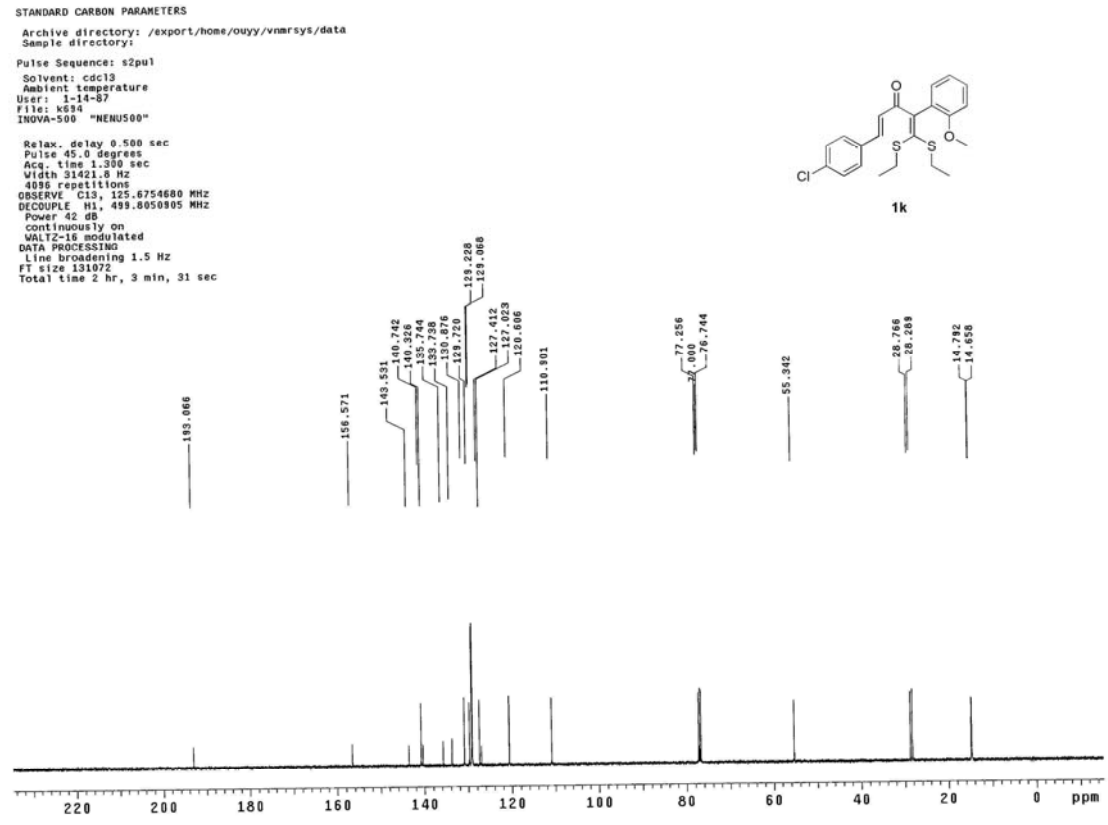
8 repetitions
OBSERVE H1, 499.8025924 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
1k
ppm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Sample directory:
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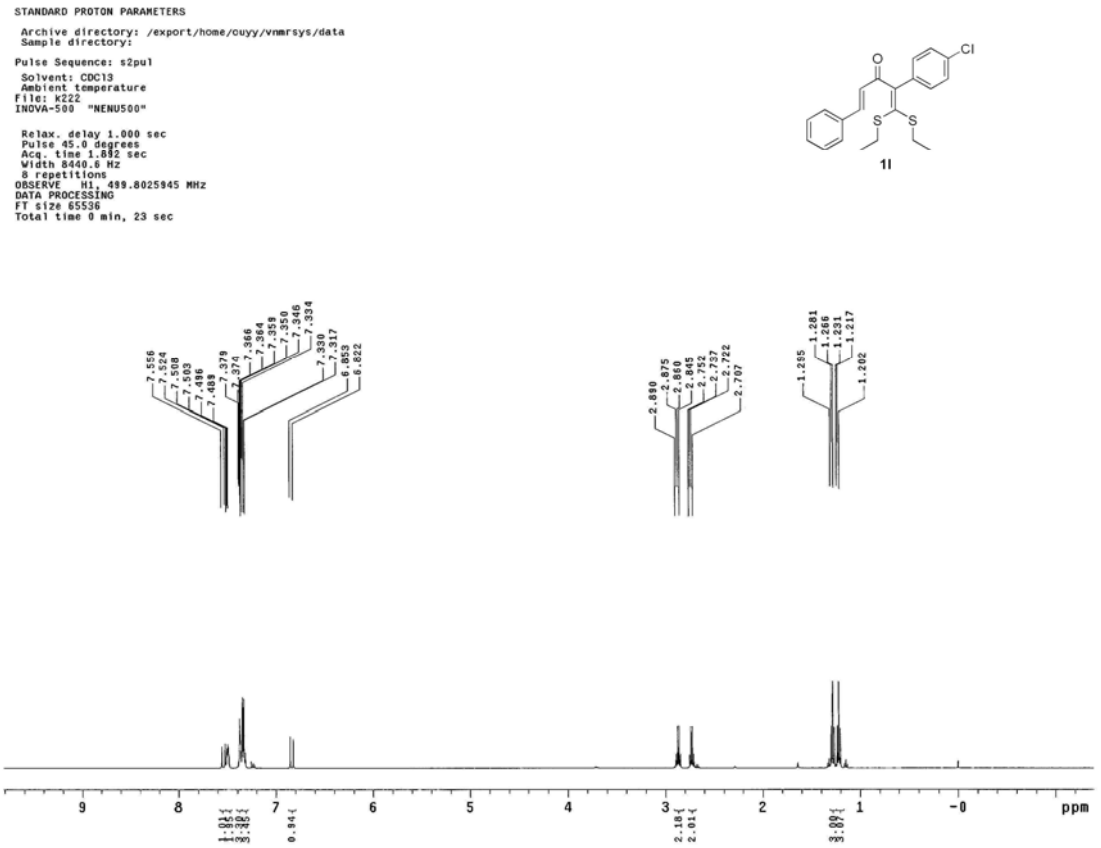
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: k694
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
4096 repetitions
OBSERVE C13, 125.6754680 MHz
DECOUPLE H1, 499.8050805 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec
1k
ppm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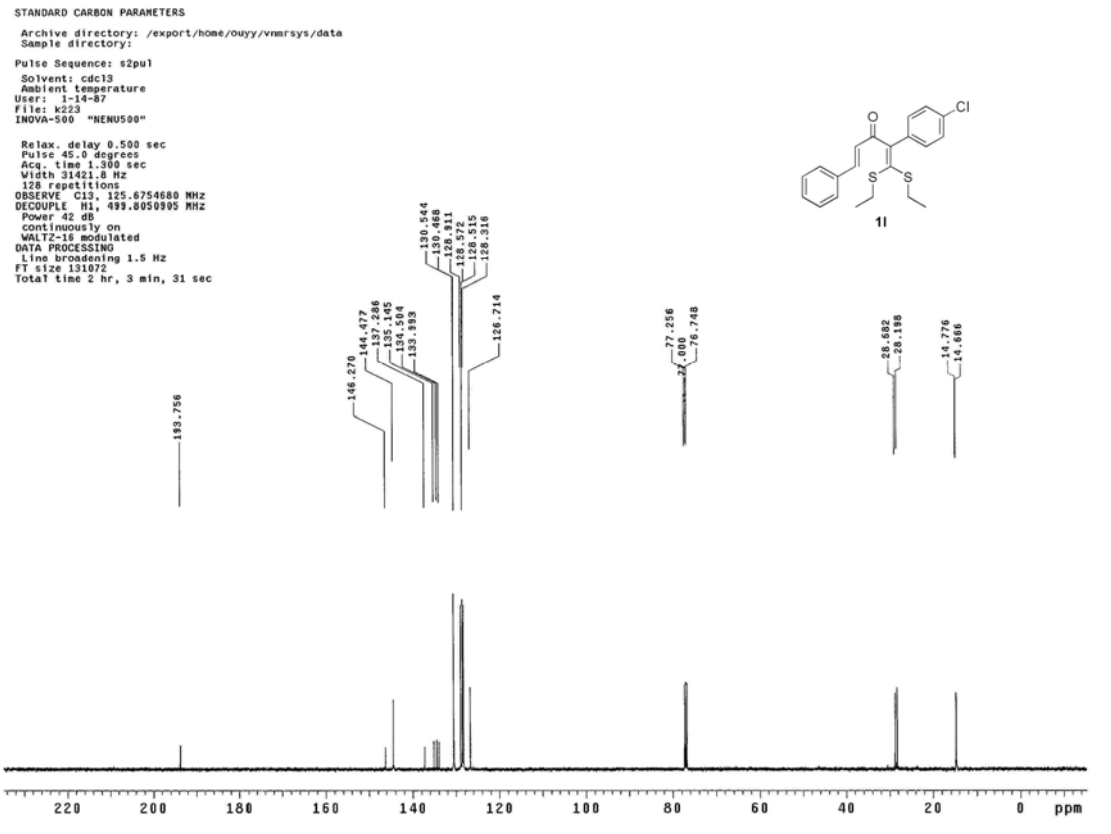
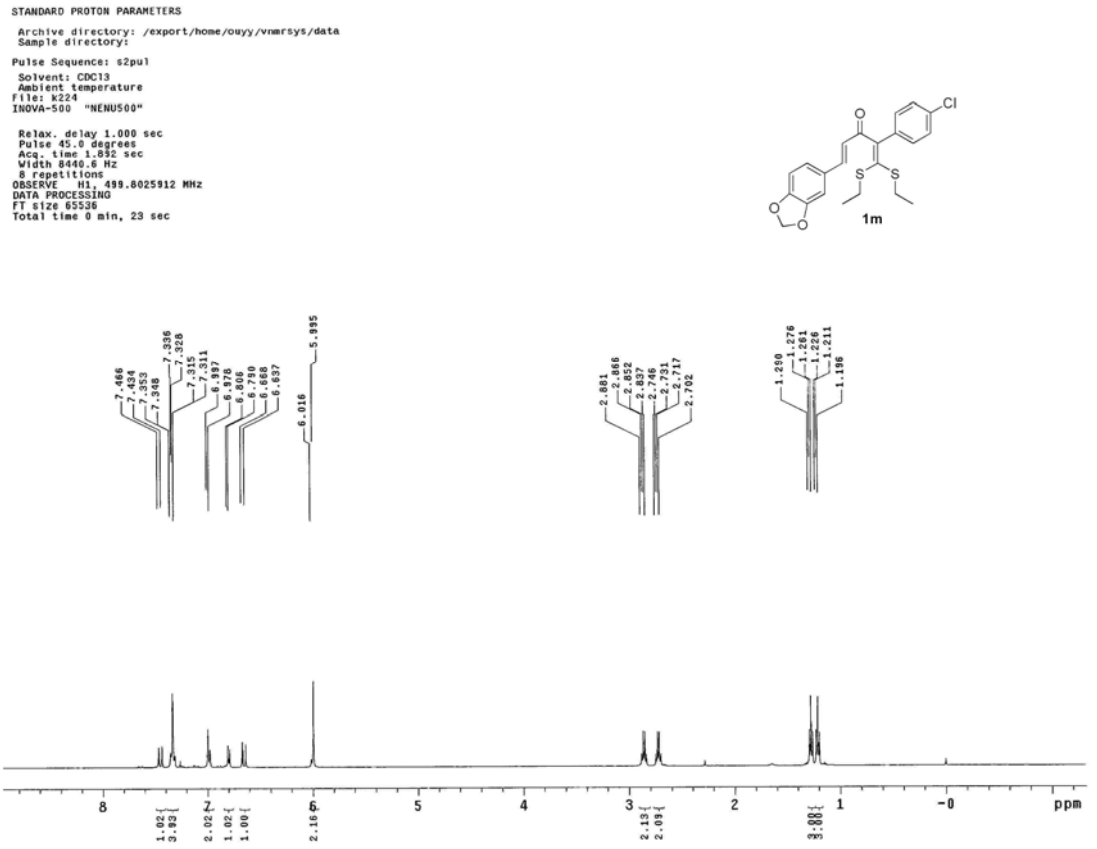
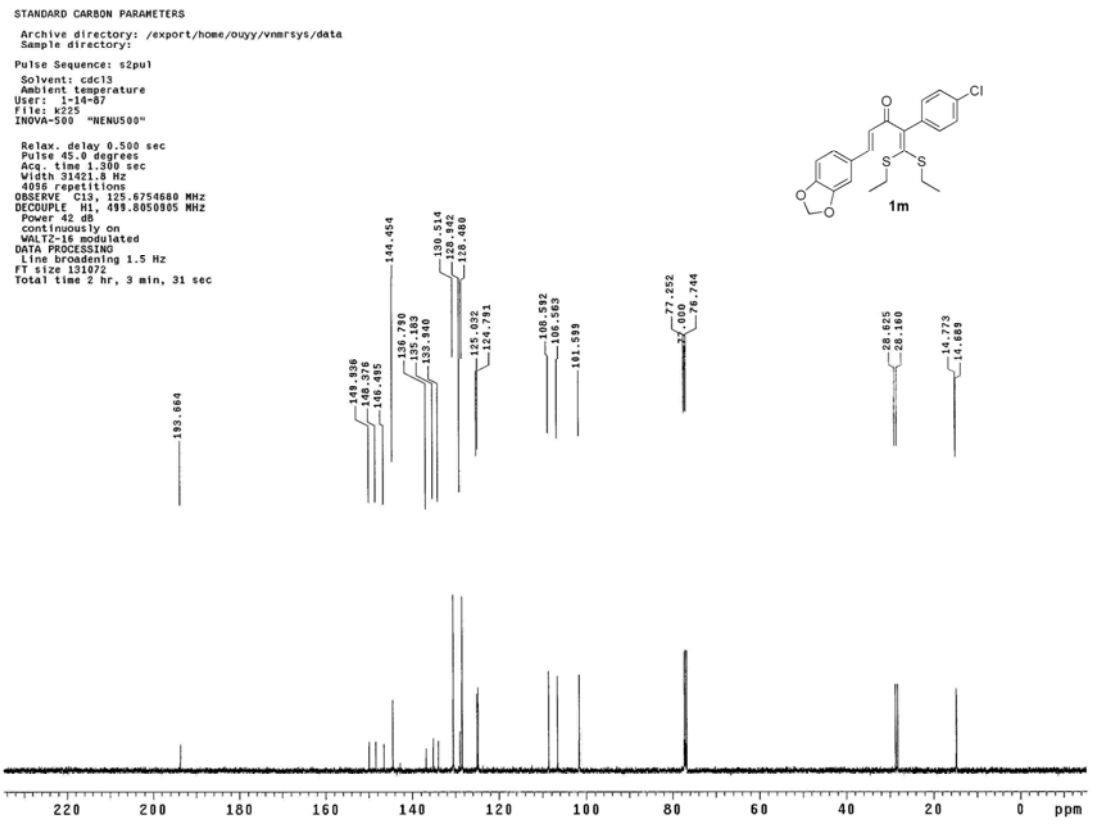
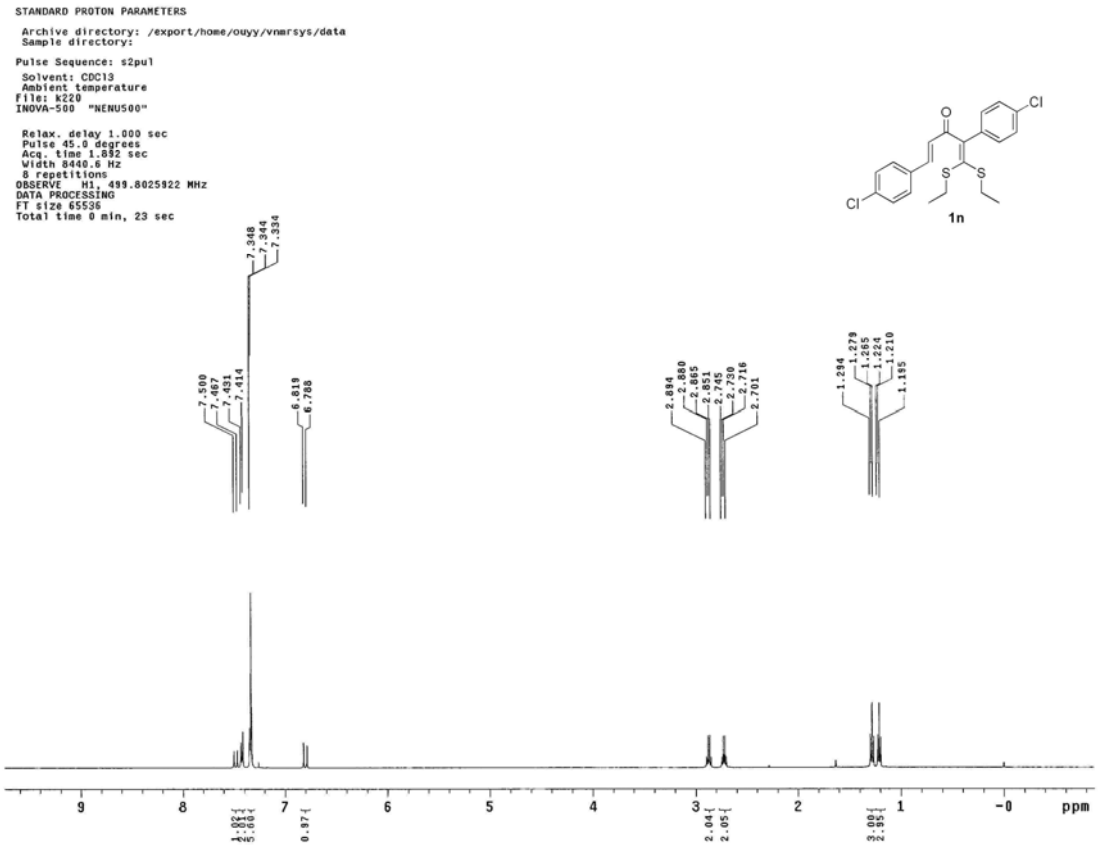
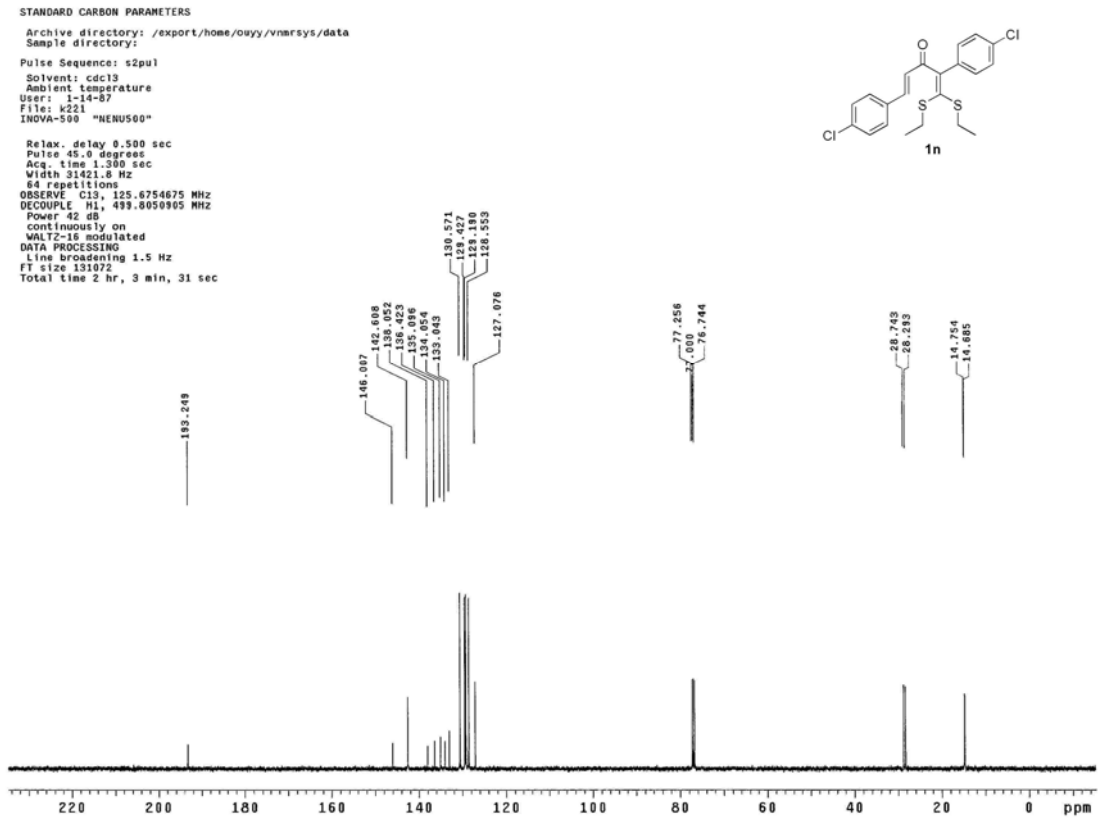
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: k222
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.882 sec
Width 8440.6 Hz
8 repetitions
OBSERVE H1, 499.8025945 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
1l
ppm

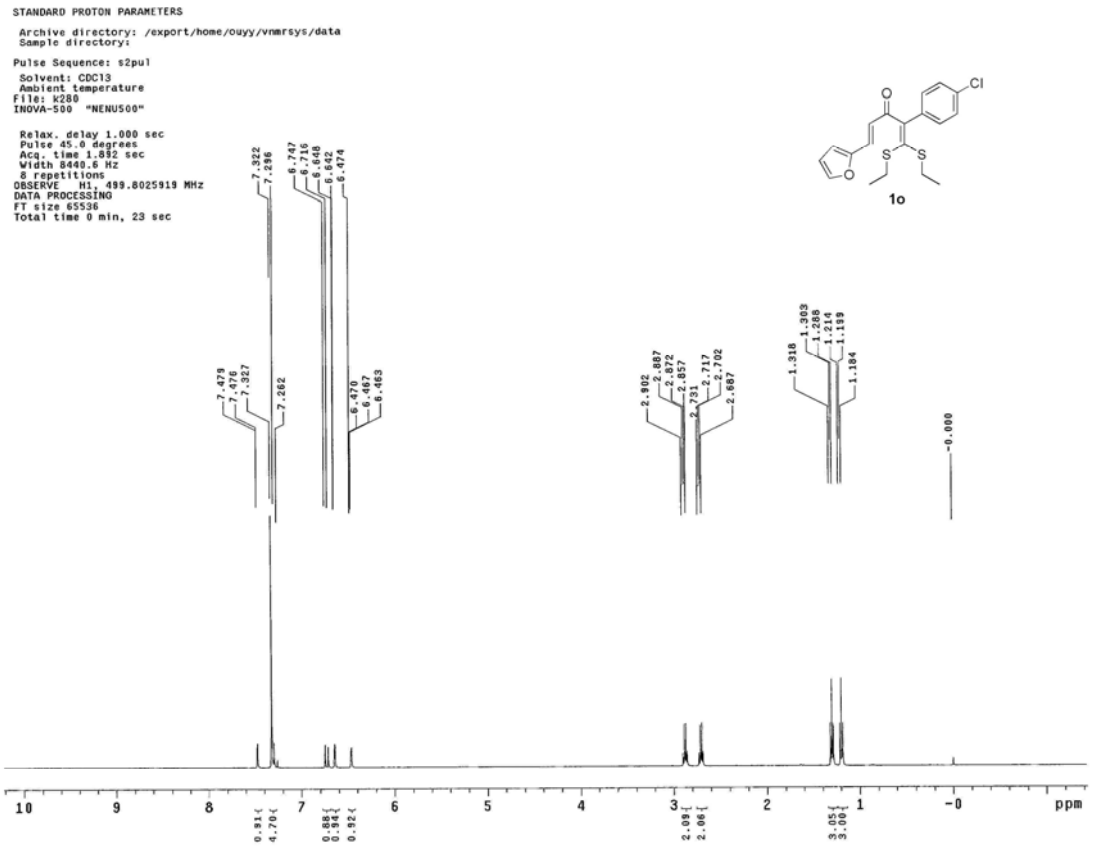

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: k223
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
128 repetitions
OBSERVE C13, 125.6754680 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec
1l
ppm

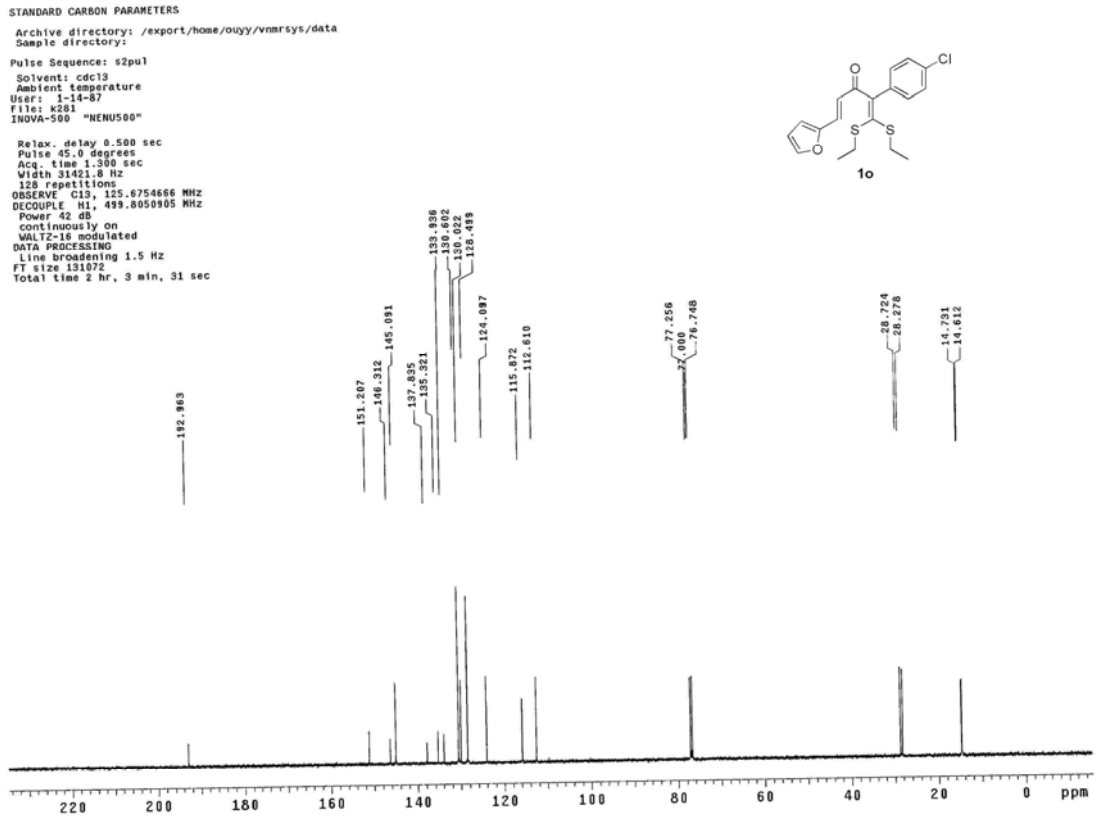

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: k224
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.832 sec
Width 8440.6 Hz
8 repetitions
OBSERVE H1, 499.8025912 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
1m
ppm

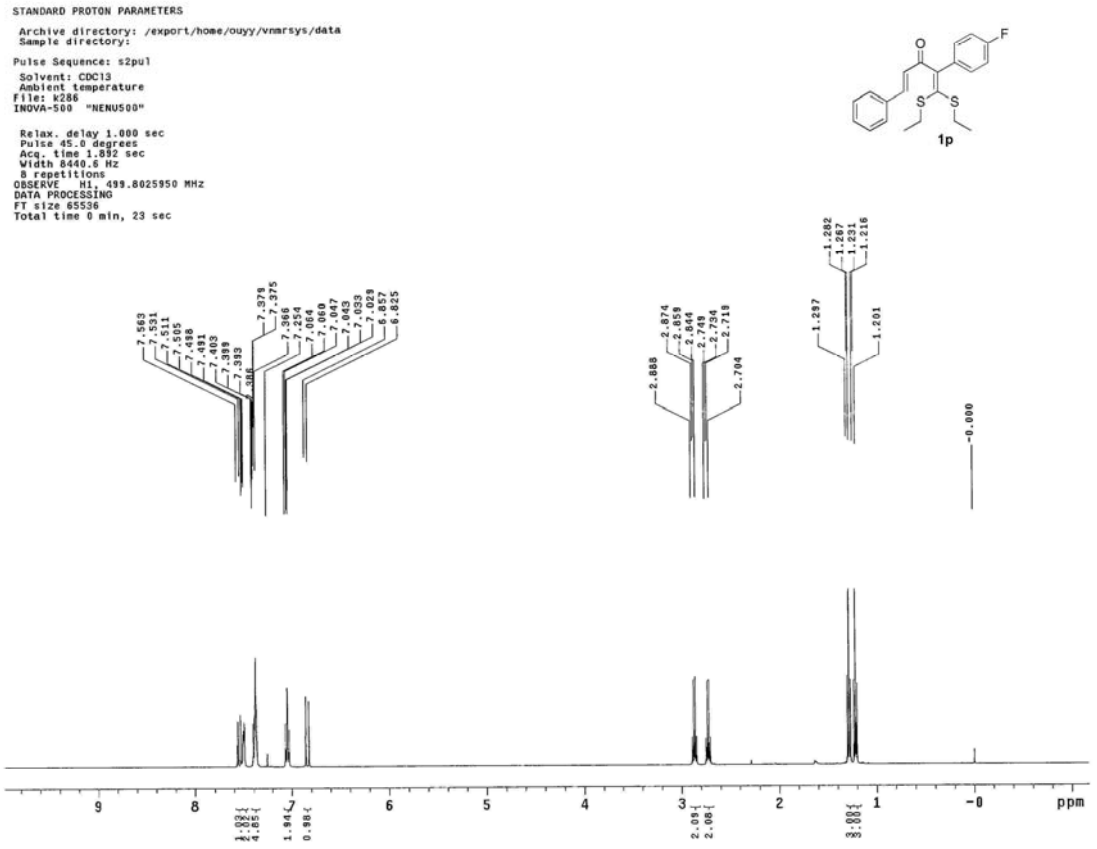

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: k225
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
4096 repetitions
OBSERVE C13, 125.6754680 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec
1m
ppm

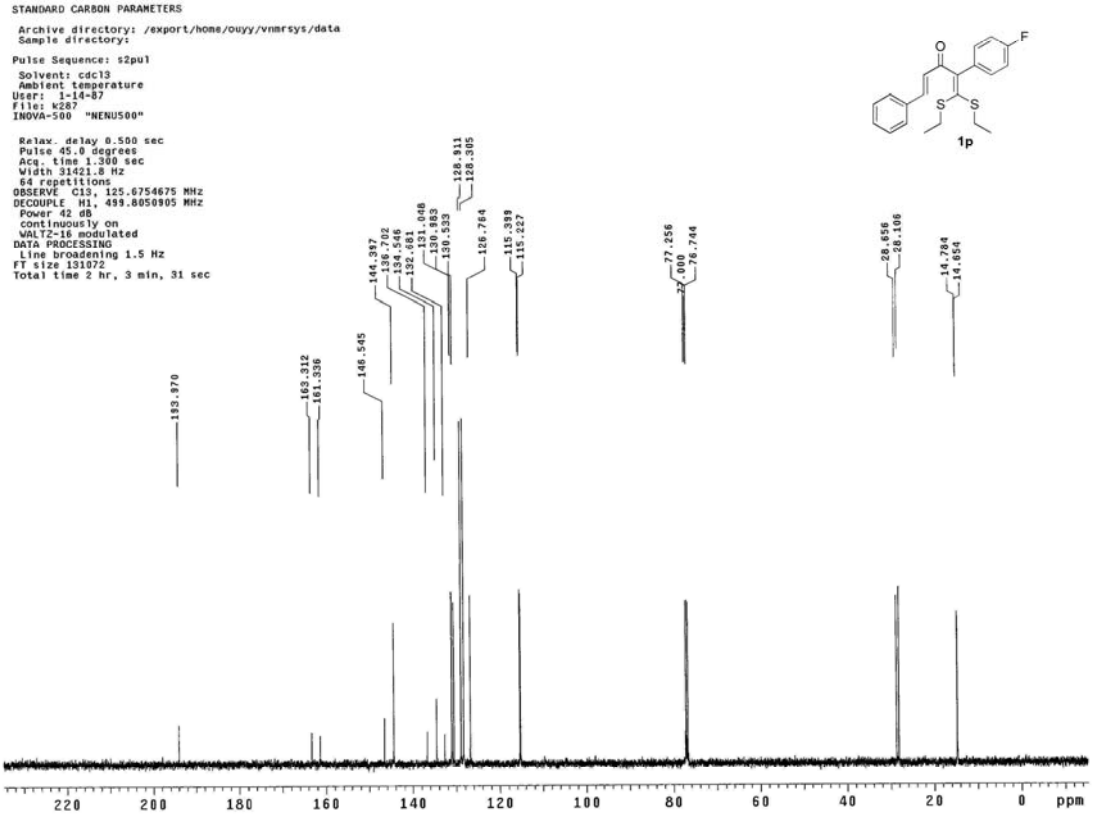

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: k220
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.882 sec
Width 8440.6 Hz
8 repetitions
OBSERVE H1, 499.8025922 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
1n
ppm

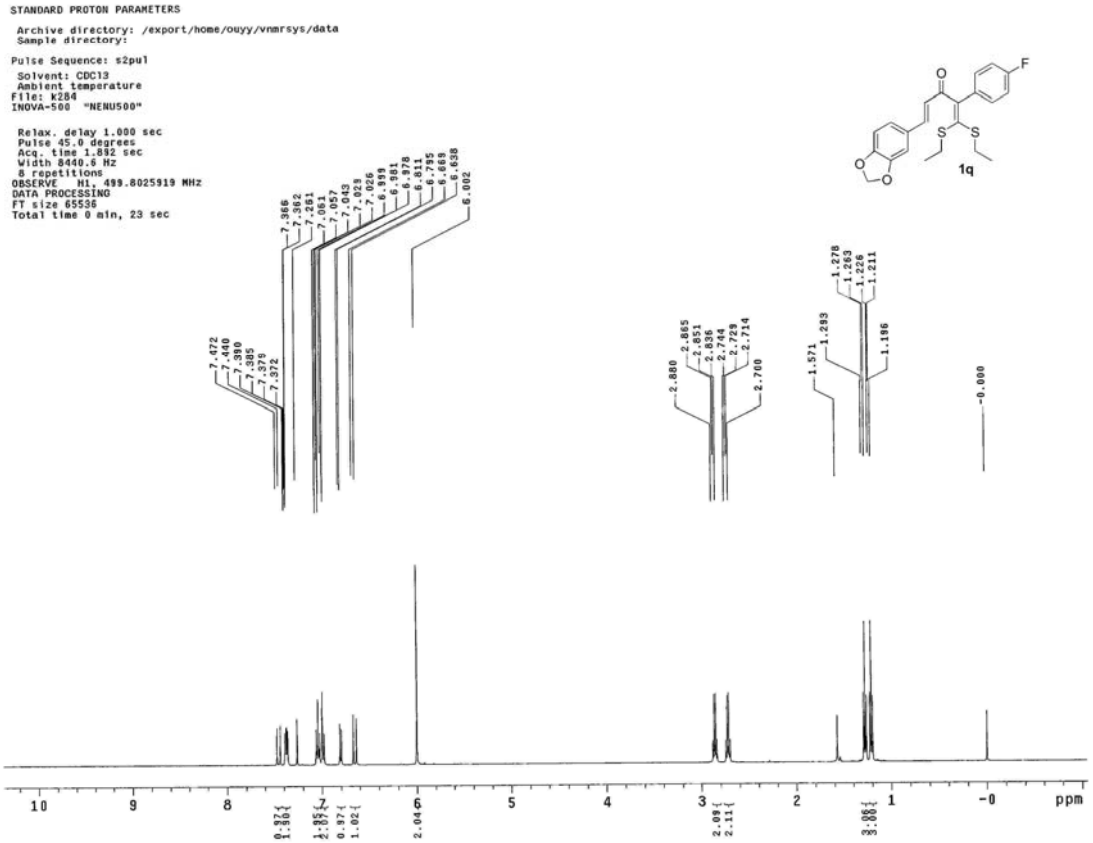

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: k221
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
64 repetitions
OBSERVE C13, 125.6754675 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec
1n
ppm

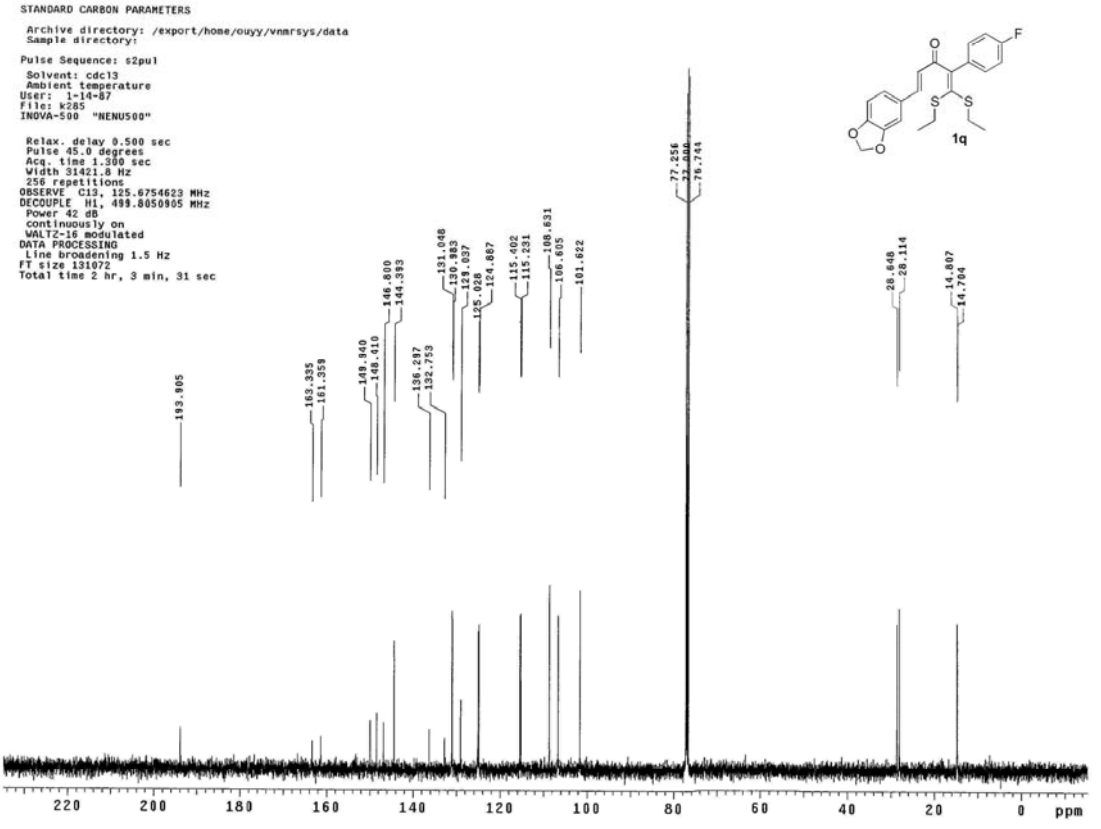

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: k280
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8440.6 Hz
8 repetitions
OBSERVE H1, 499.8025919 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
1o
ppm

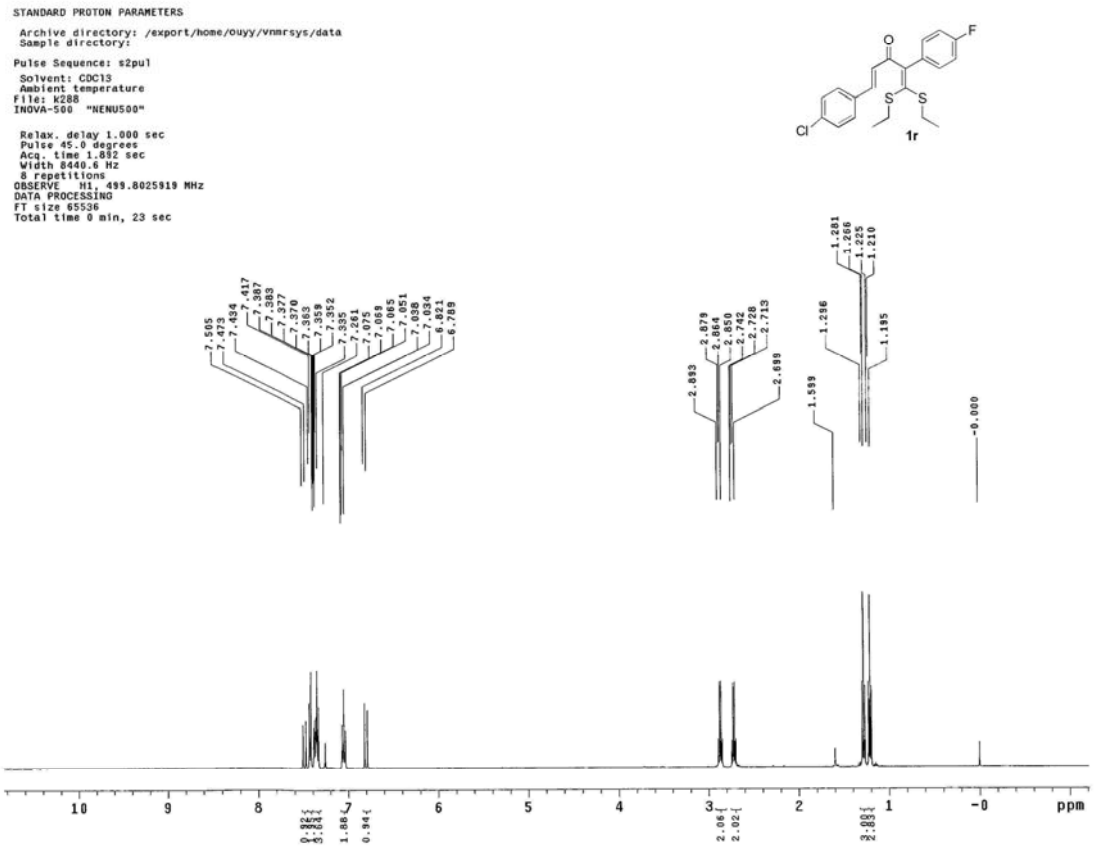

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: k281
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
128 repetitions
OBSERVE C13, 125.6754666 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously On
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec
1o
ppm

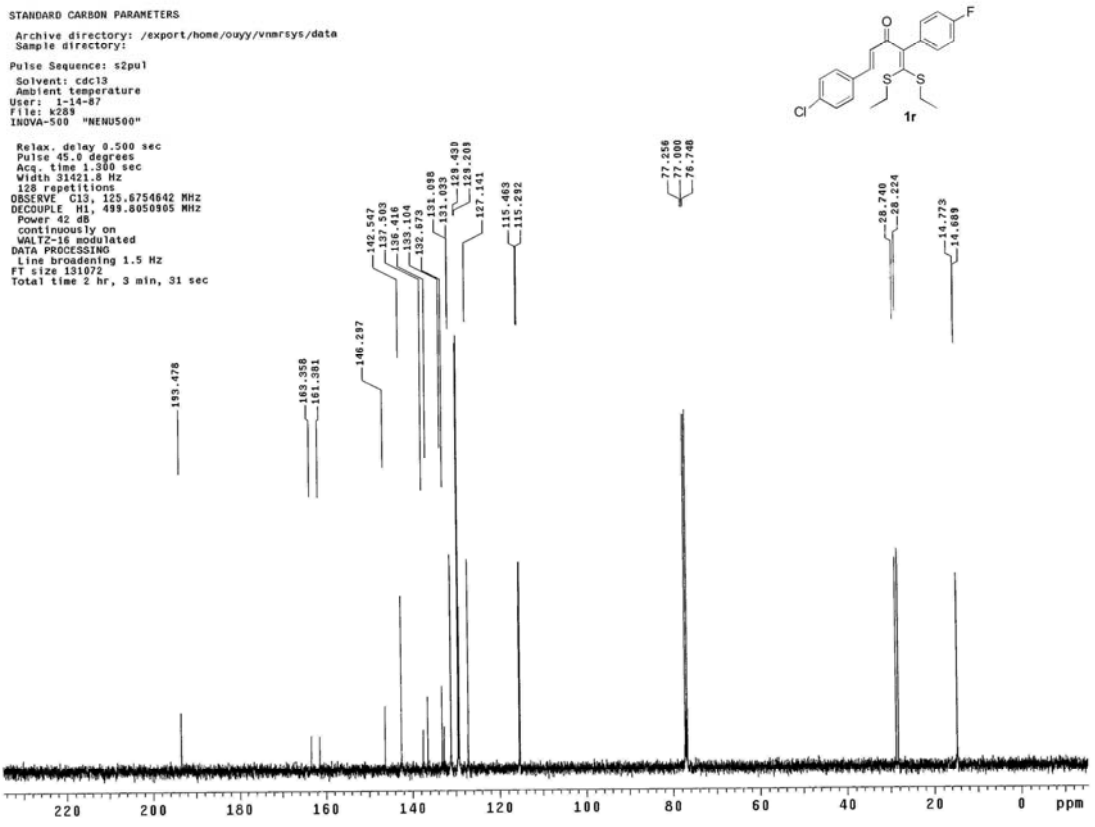

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: k286
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8440.6 Hz
8 repetitions
OBSERVE H1, 499.8025950 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
1p
ppm

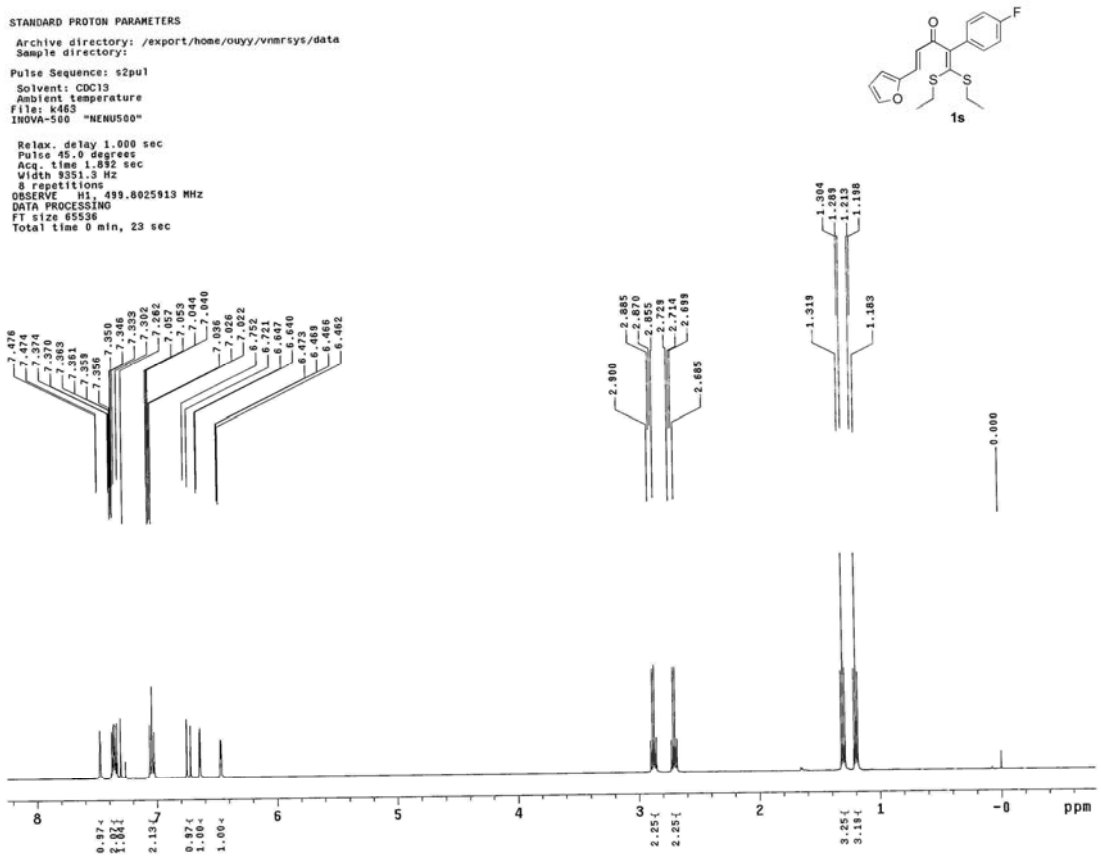

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: k287
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
64 repetitions
OBSERVE C13, 125.6754675 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec
1p
ppm

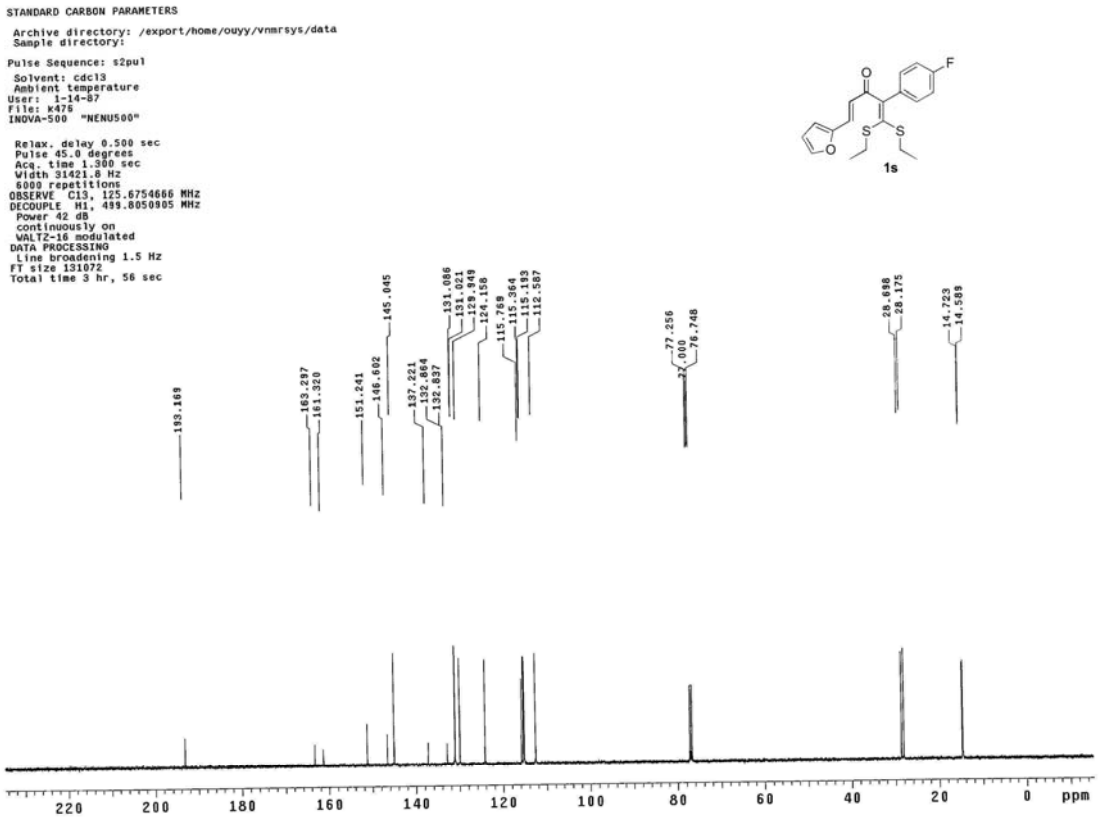

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: k284
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.882 sec
Width 8440.6 Hz
8 repetitions
OBSERVE H1, 499.8025919 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
1q
ppm

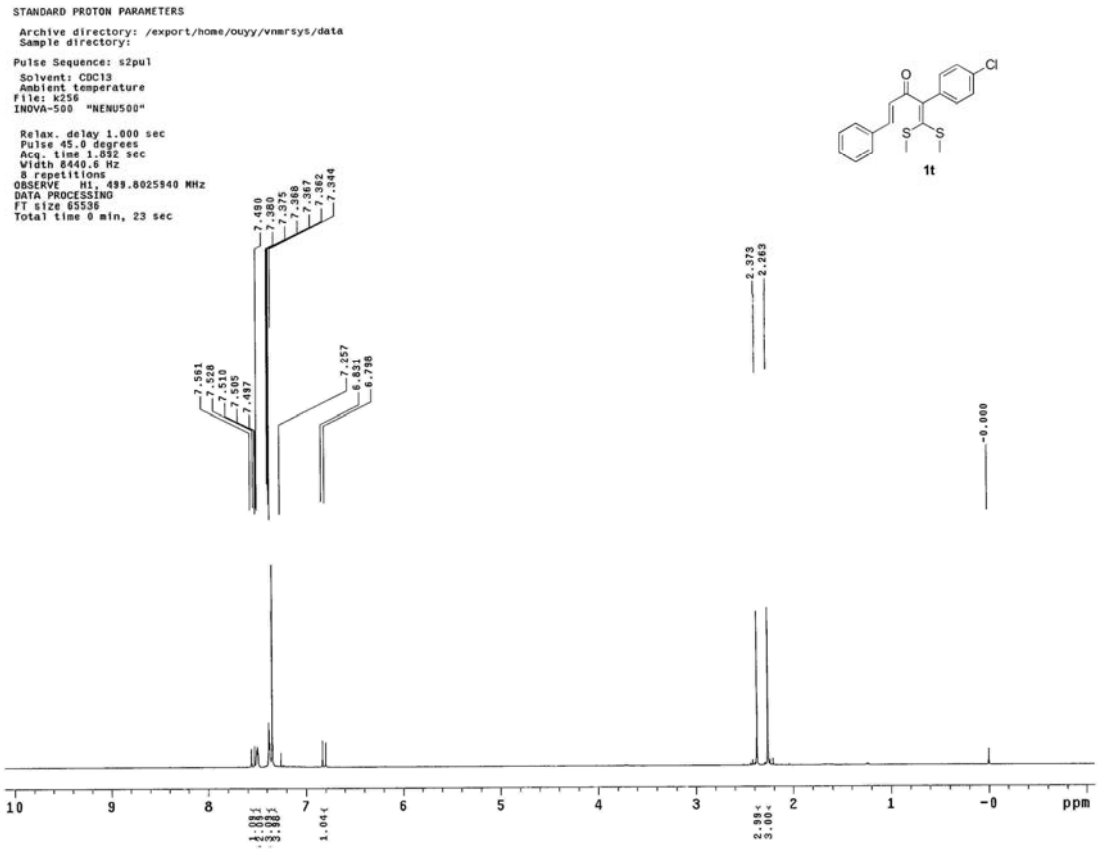

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: k285
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
256 repetitions
OBSERVE C13, 125.6754623 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec
1q
ppm

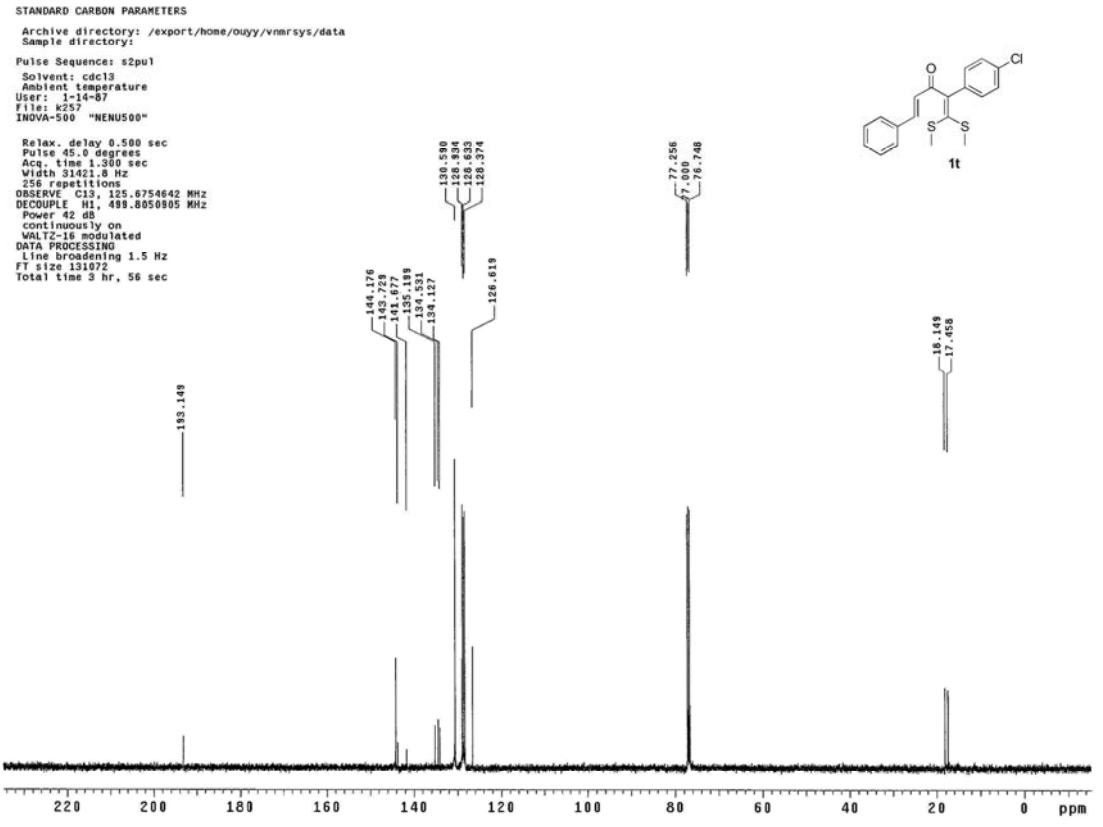

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: k288
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8440.6 Hz
8 repetitions
OBSERVE H1, 499.8025919 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
1r
ppm

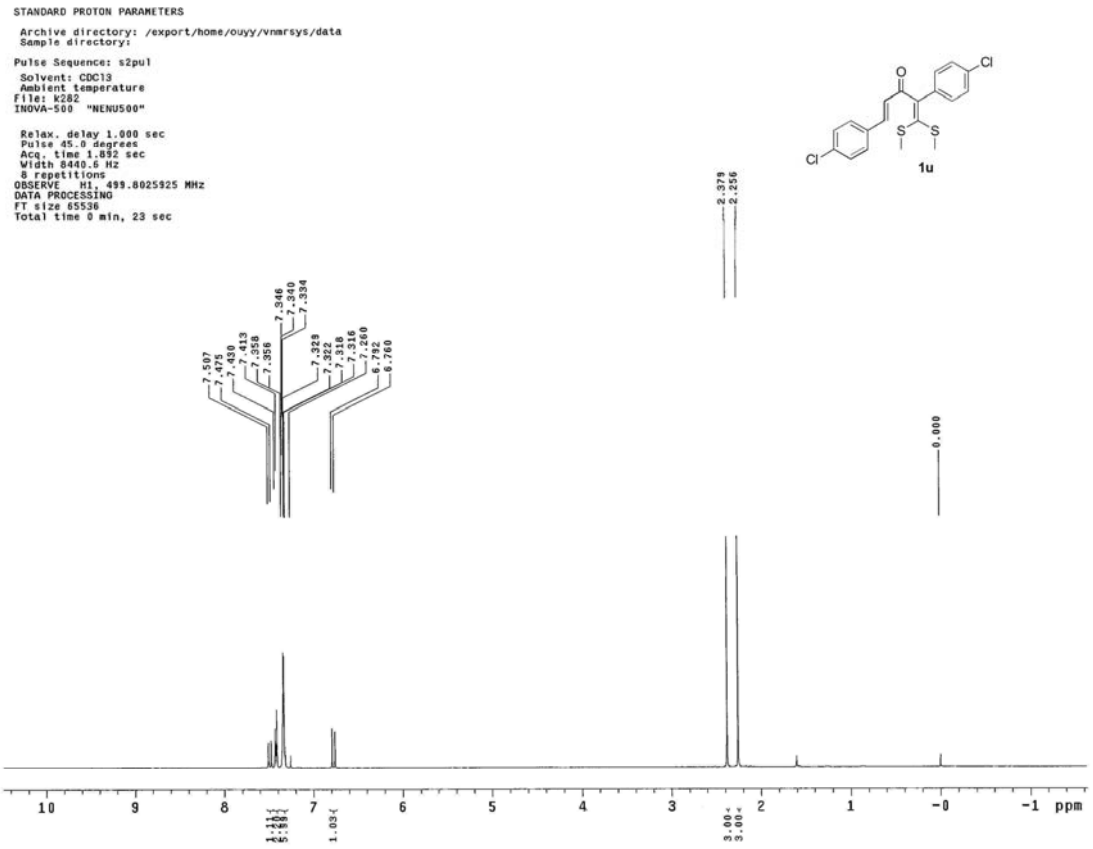

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: k288
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
128 repetitions
OBSERVE C13, 125.6754642 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec
1r
ppm

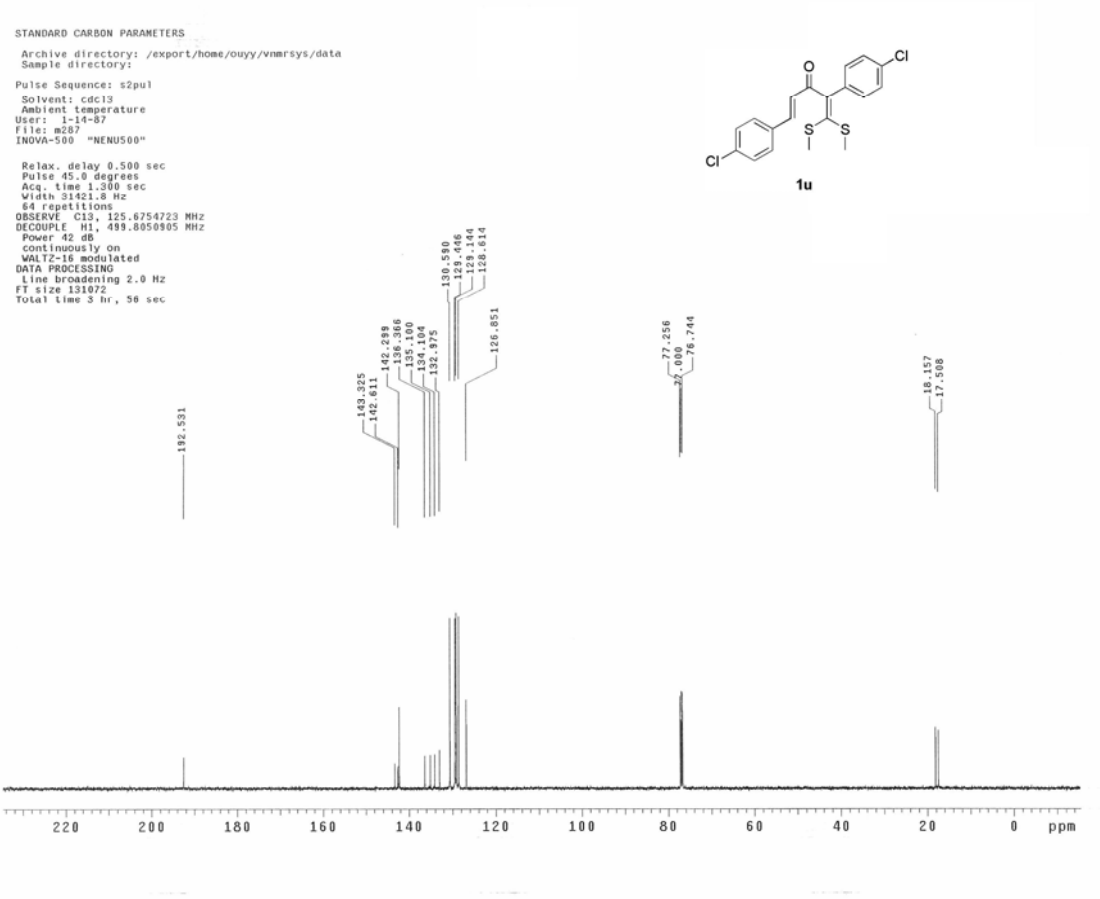

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: k463
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 9351.3 Hz
8 repetitions
OBSERVE H1, 499.8025913 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
1s
ppm

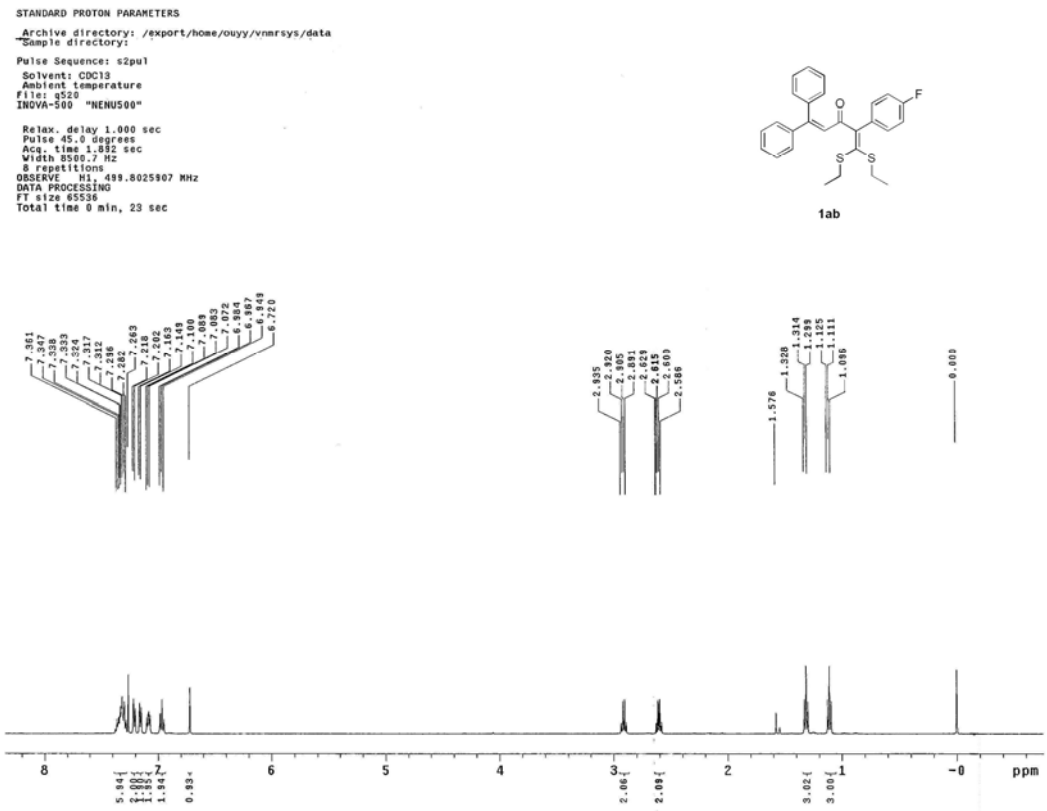

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: k476
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
6000 repetitions
OBSERVE C13, 125.6754666 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
1s
ppm

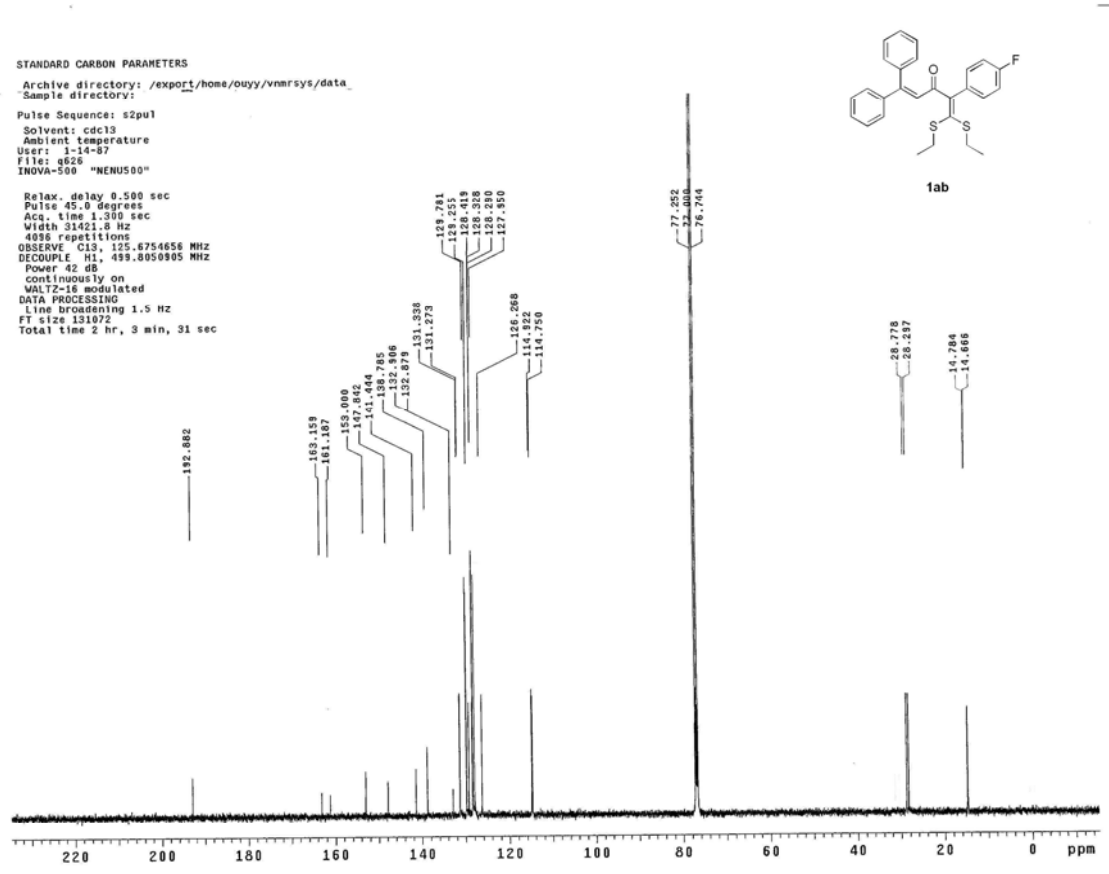

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: k256
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8440.6 Hz
8 repetitions
OBSERVE H1, 499.8025840 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
1t
ppm

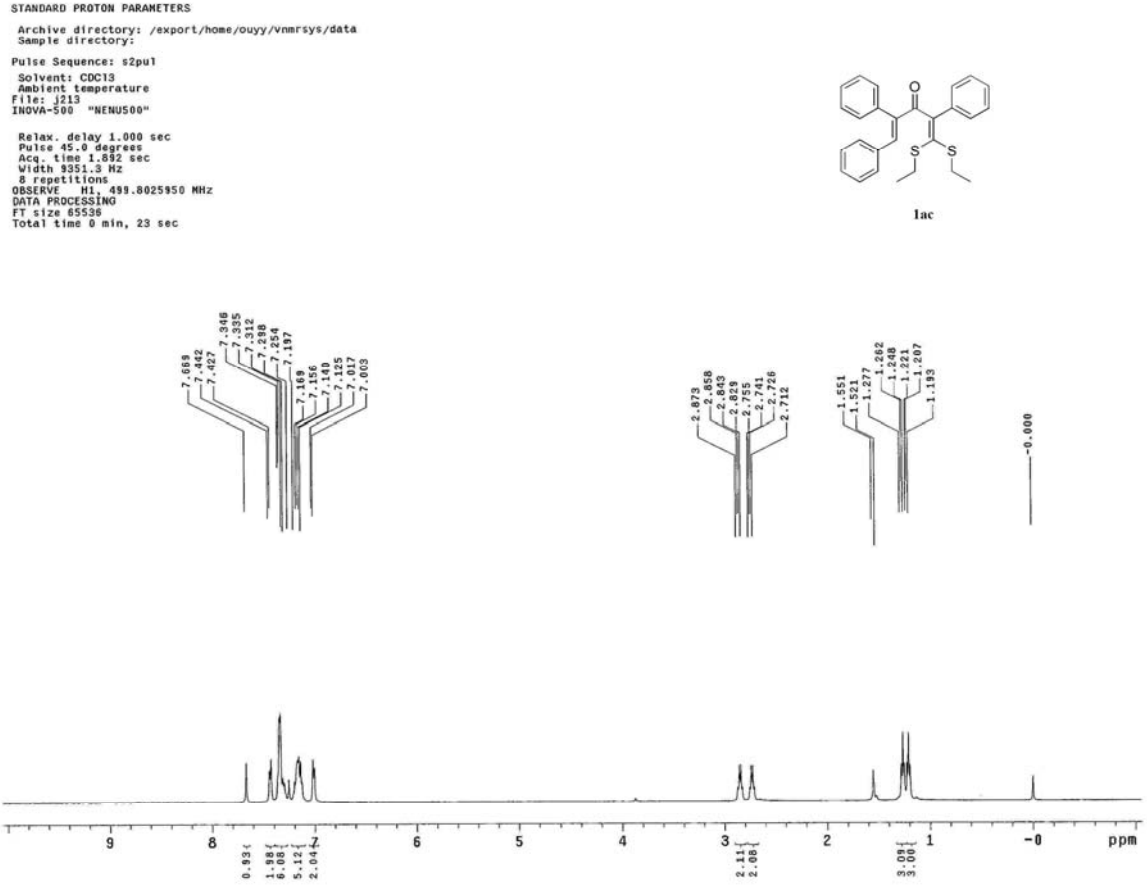

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: k257
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
256 repetitions
OBSERVE C13, 125.6754642 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
1t
ppm

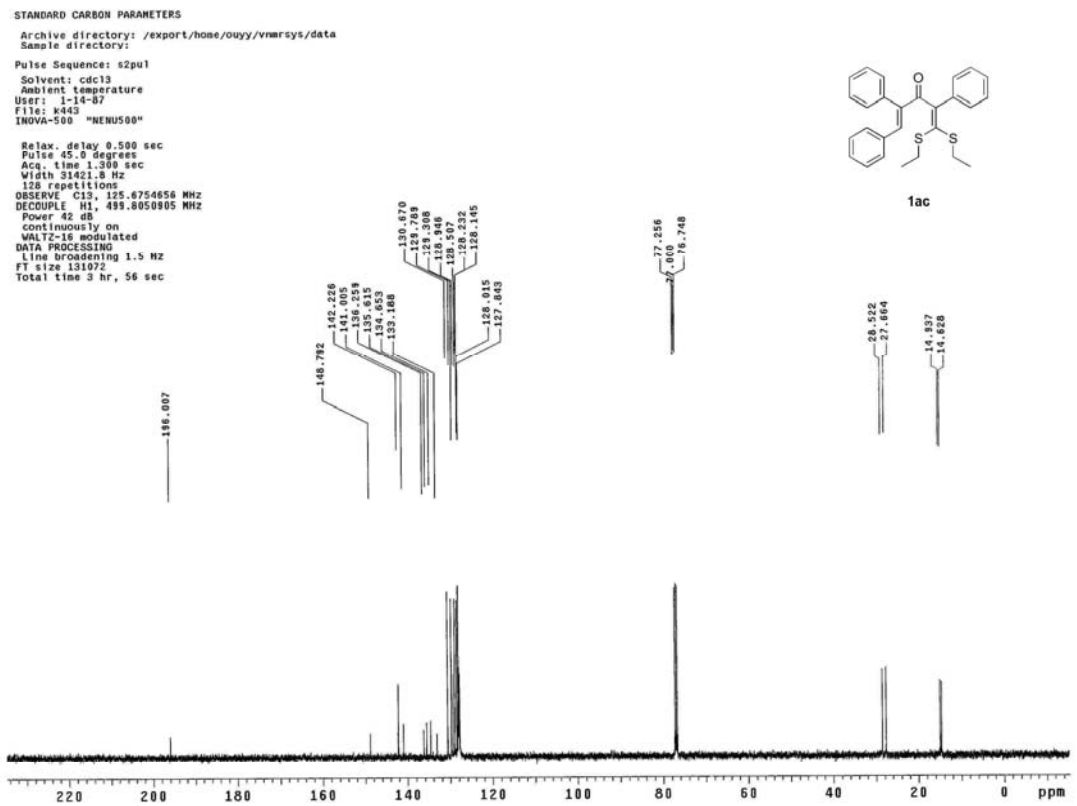

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: k282
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8440.6 Hz
8 repetitions
OBSERVE H1, 499.8025925 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
1u
7.507
7.475
7.430
7.413
7.358
7.356
7.346
7.340
7.334
7.329
7.322
7.318
7.316
7.260
6.782
6.760
2.379
2.256
0.000
1.03
3.00
3.00
10
9
8
7
6
5
4
3
2
1
-0
-1
ppm

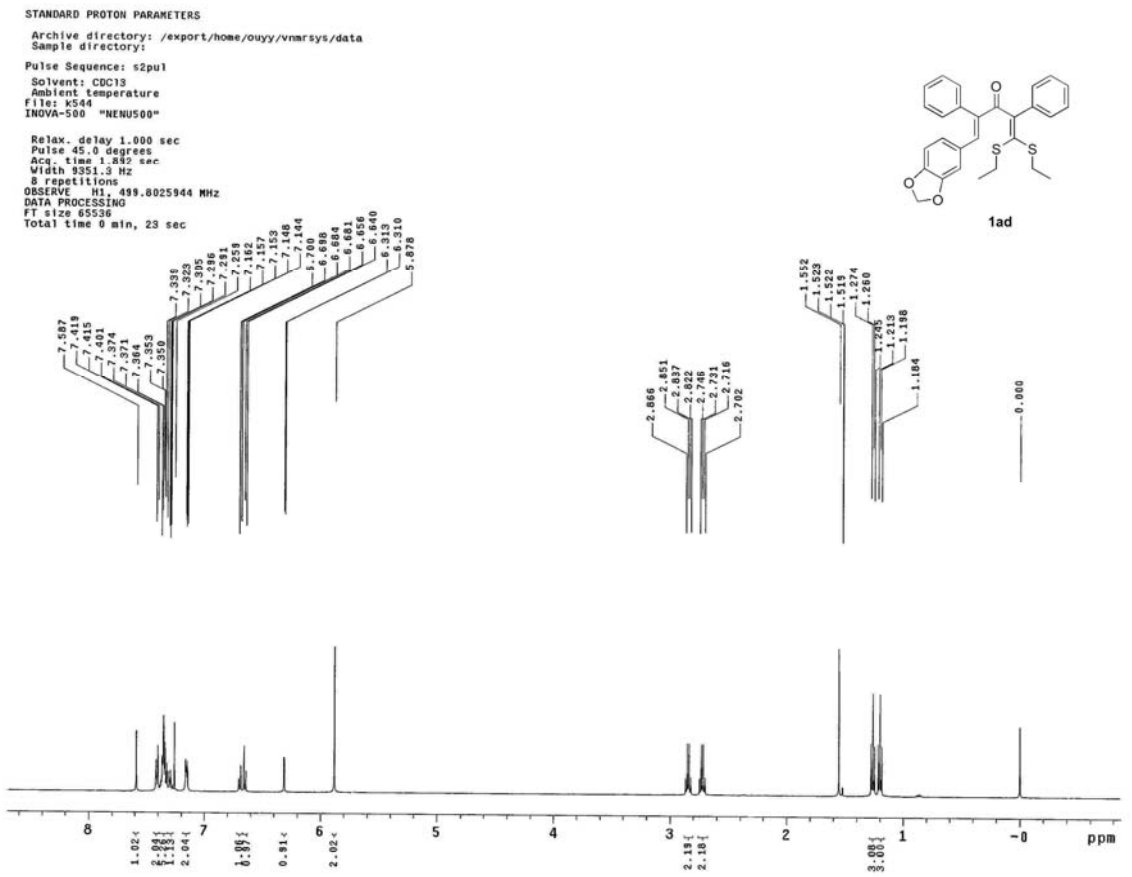

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: m287
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
64 repetitions
OBSERVE C13, 125.6754723 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 131072
Total time 3 hr, 56 sec
1u
192.531
143.325
142.611
142.289
136.366
135.100
134.104
132.975
130.590
129.446
129.144
128.614
126.851
77.256
77.000
76.744
18.157
17.508
220
200
180
160
140
120
100
80
60
40
20
0
ppm

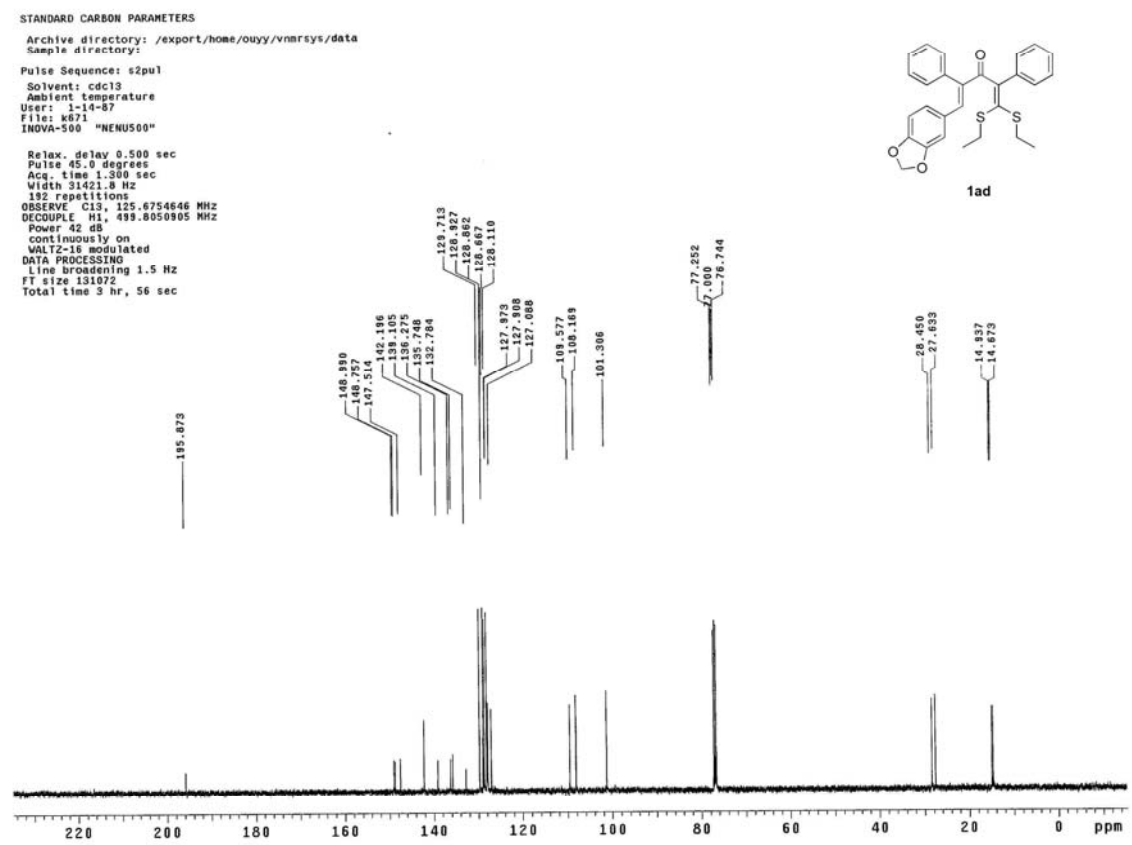

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: q520
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.882 sec
Width 8500.7 Hz
8 repetitions
OBSERVE H1, 499.8025907 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
1ab
ppm

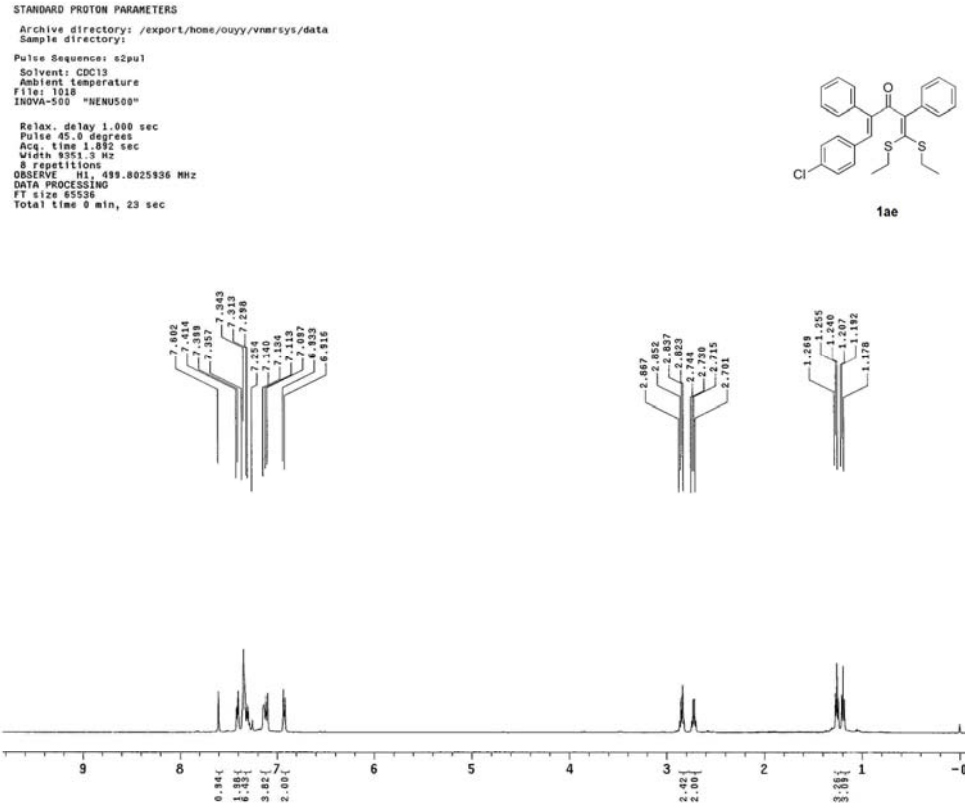

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: q626
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
4096 repetitions
OBSERVE C13, 125.6754656 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec
1ab
ppm

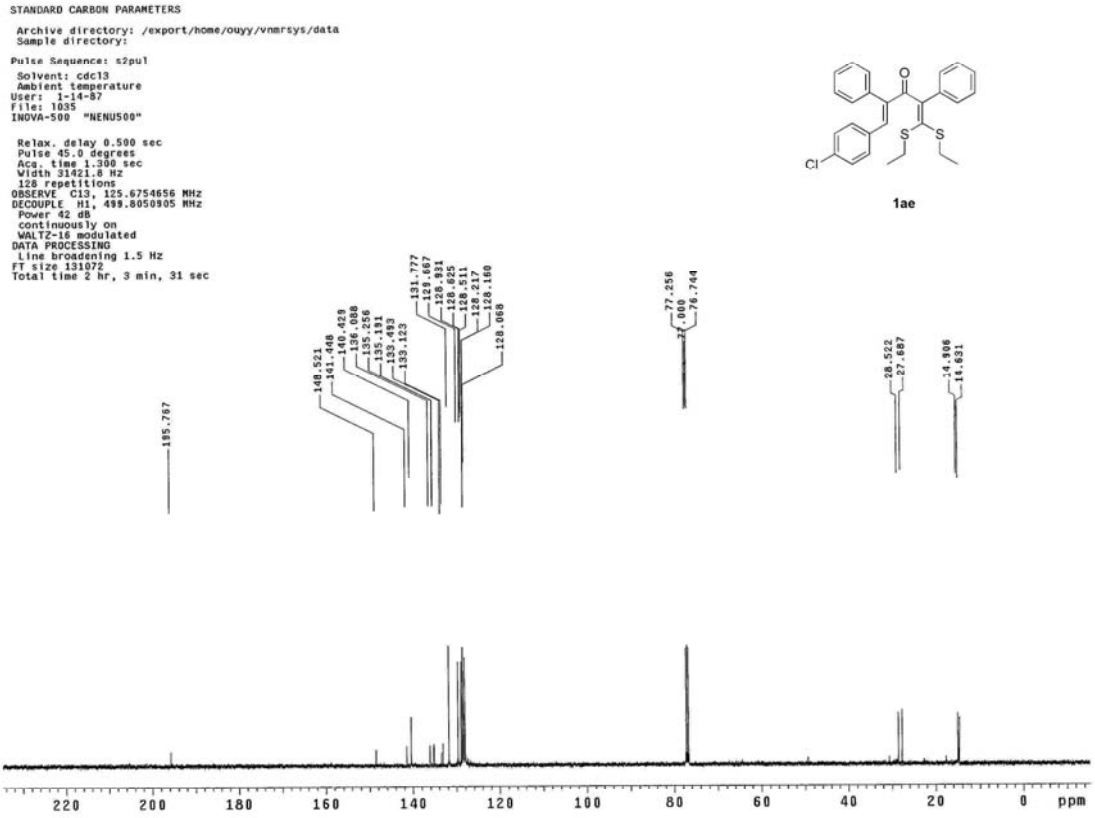

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: j213
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 9351.3 Hz
8 repetitions
OBSERVE H1, 499.8025950 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
1ac
ppm

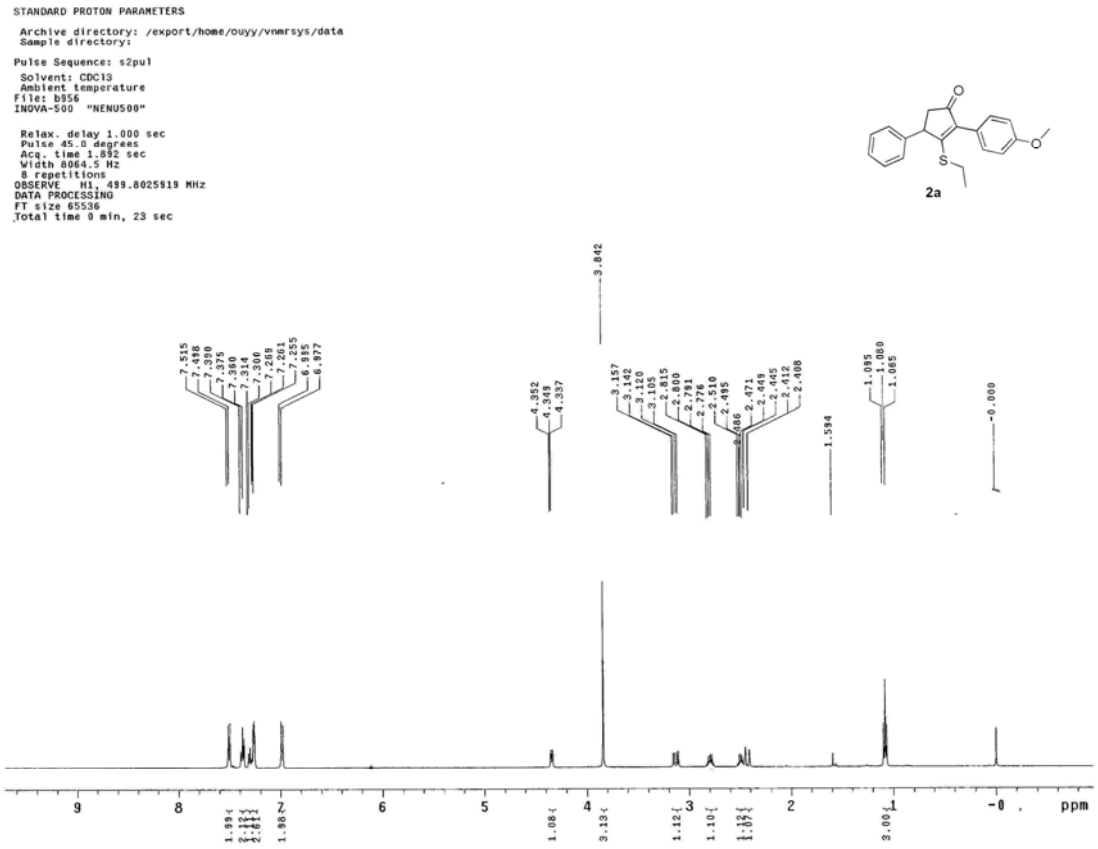

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: k443
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
128 repetitions
OBSERVE C13, 125.6754656 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
1ac
ppm

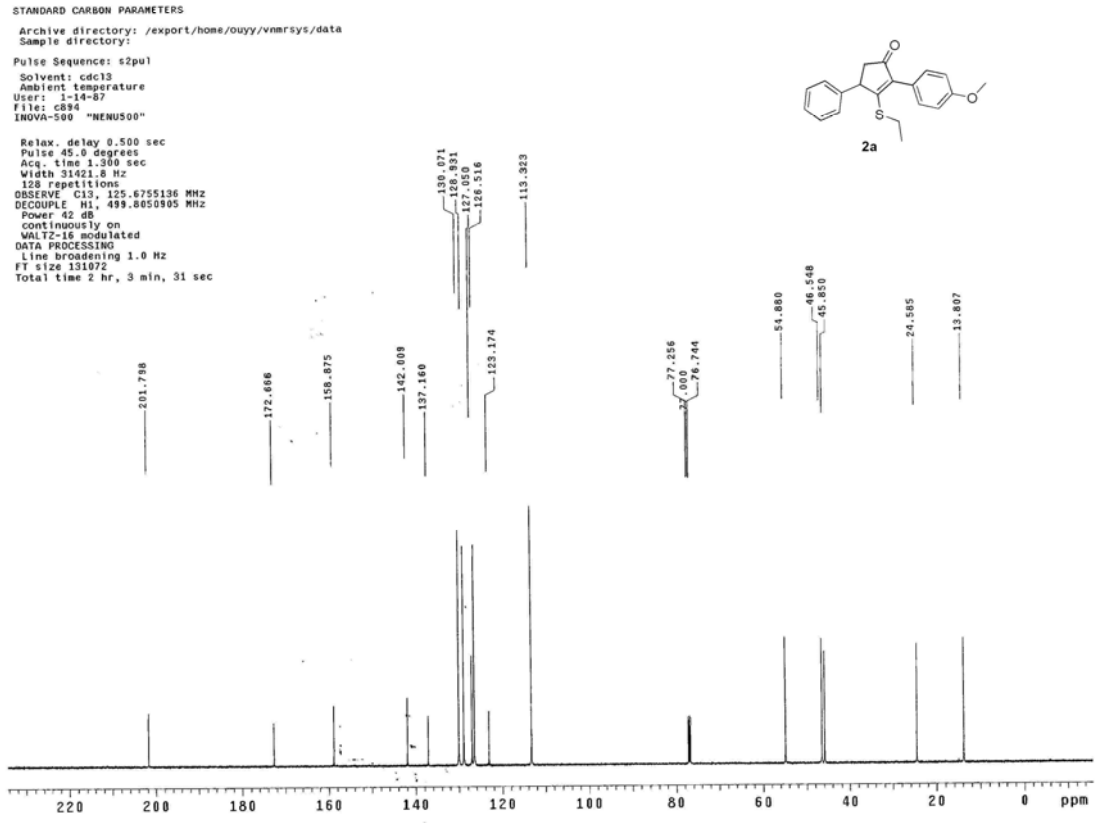

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: k544
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.882 sec
Width 9351.3 Hz
8 repetitions
OBSERVE H1, 499.8025944 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
1ad
ppm

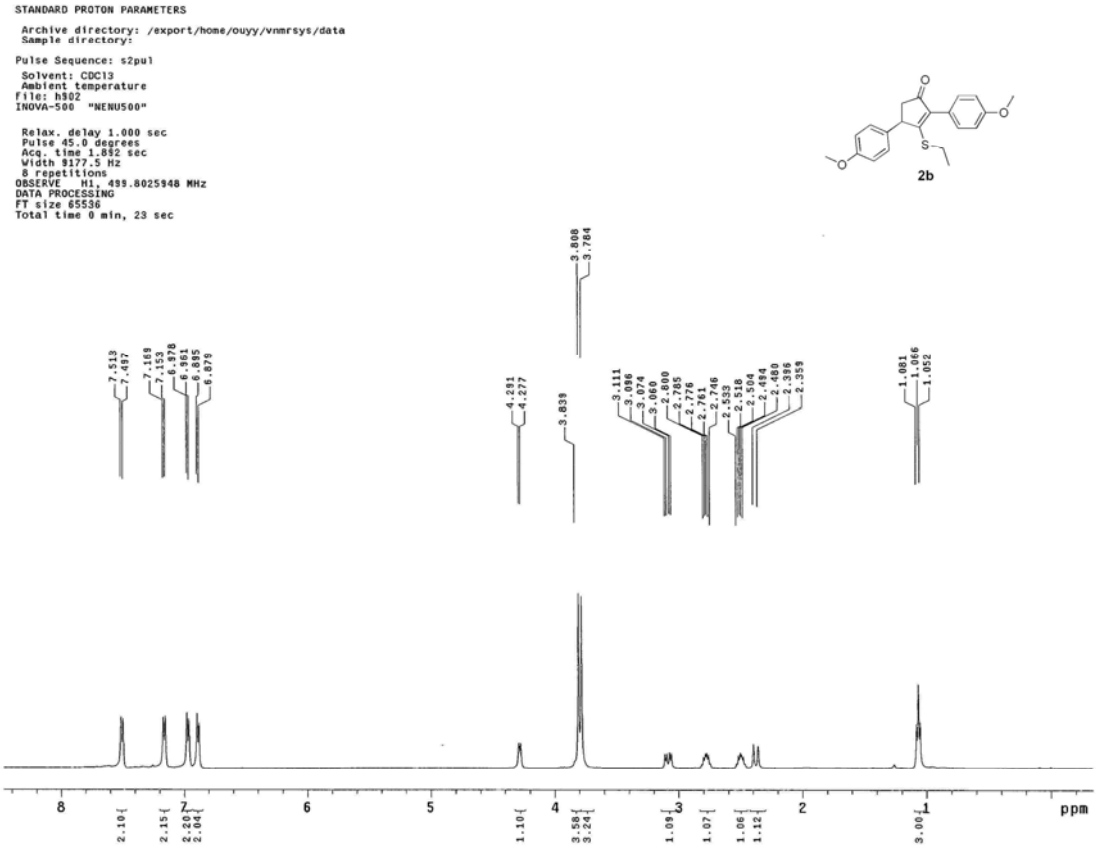

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: k671
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
192 repetitions
OBSERVE C13, 125.6754646 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
1ad
ppm

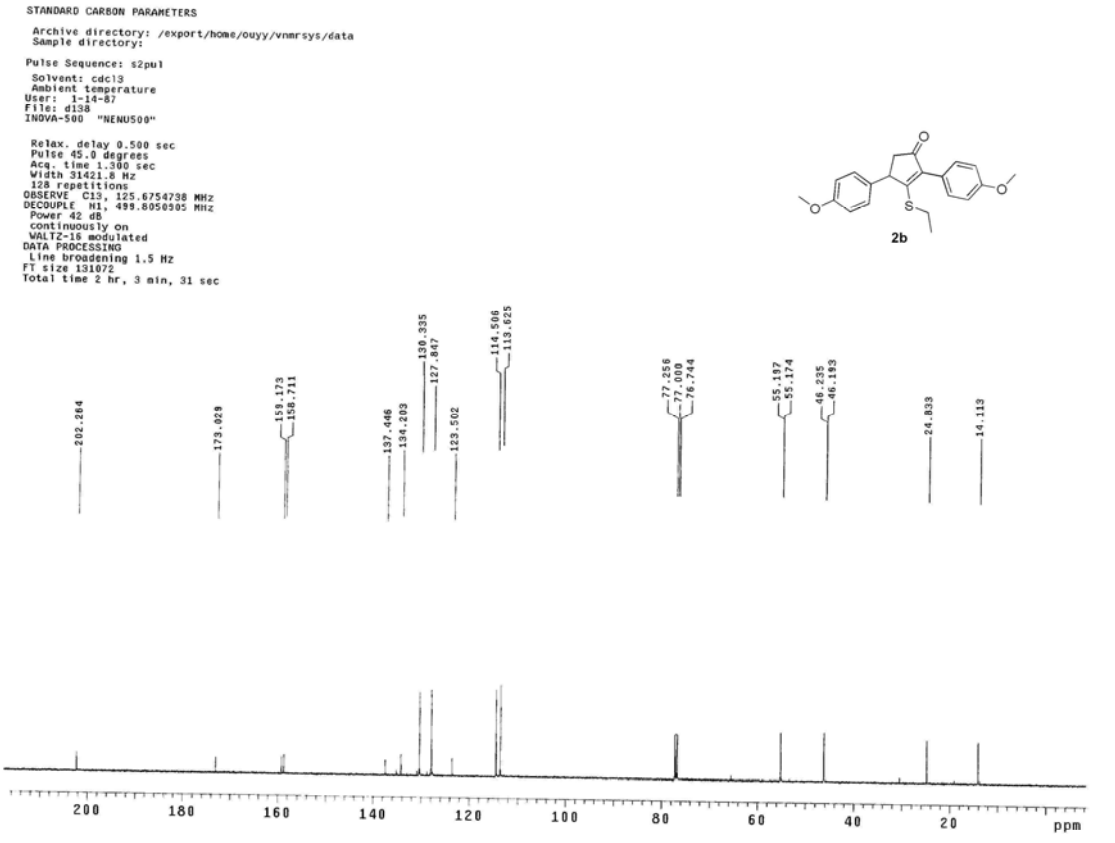

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: 1018
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 9351.3 Hz
8 repetitions
OBSERVE H1, 499.8025936 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
1ae
ppm

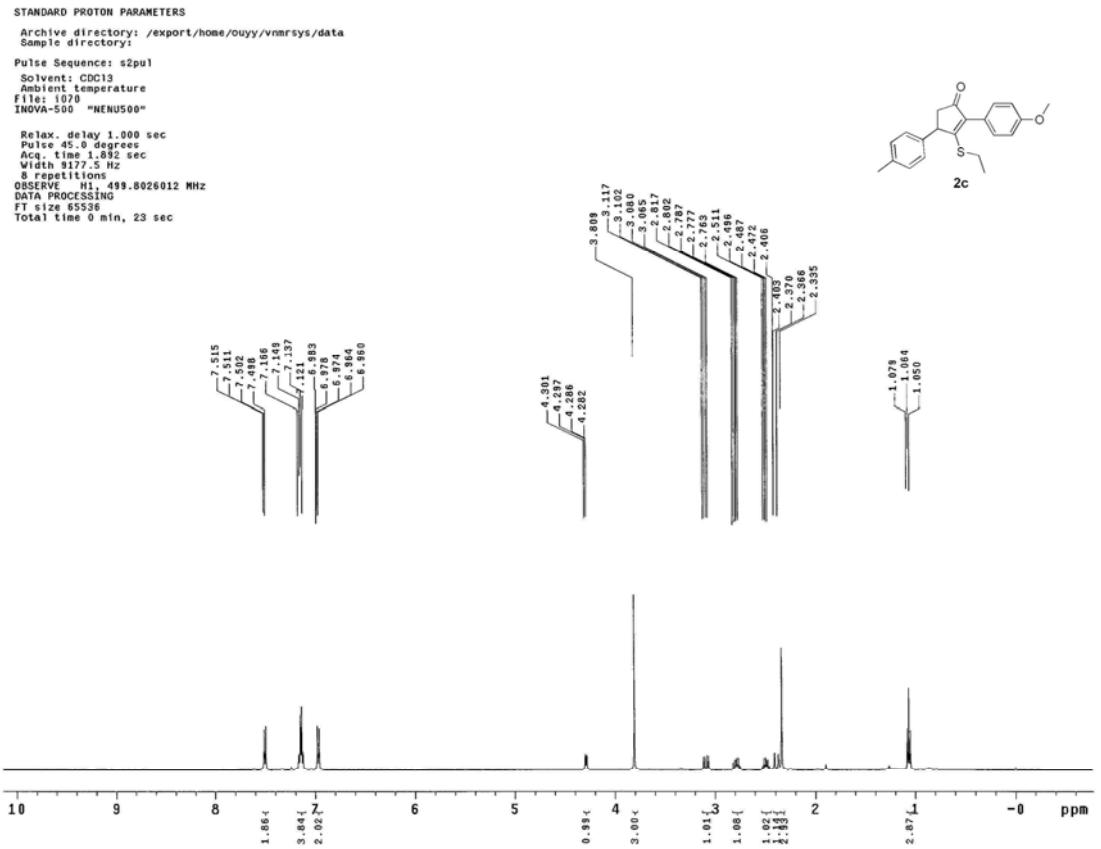

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: 1035
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
128 repetitions
OBSERVE C13, 125.6754656 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec
1ae
ppm

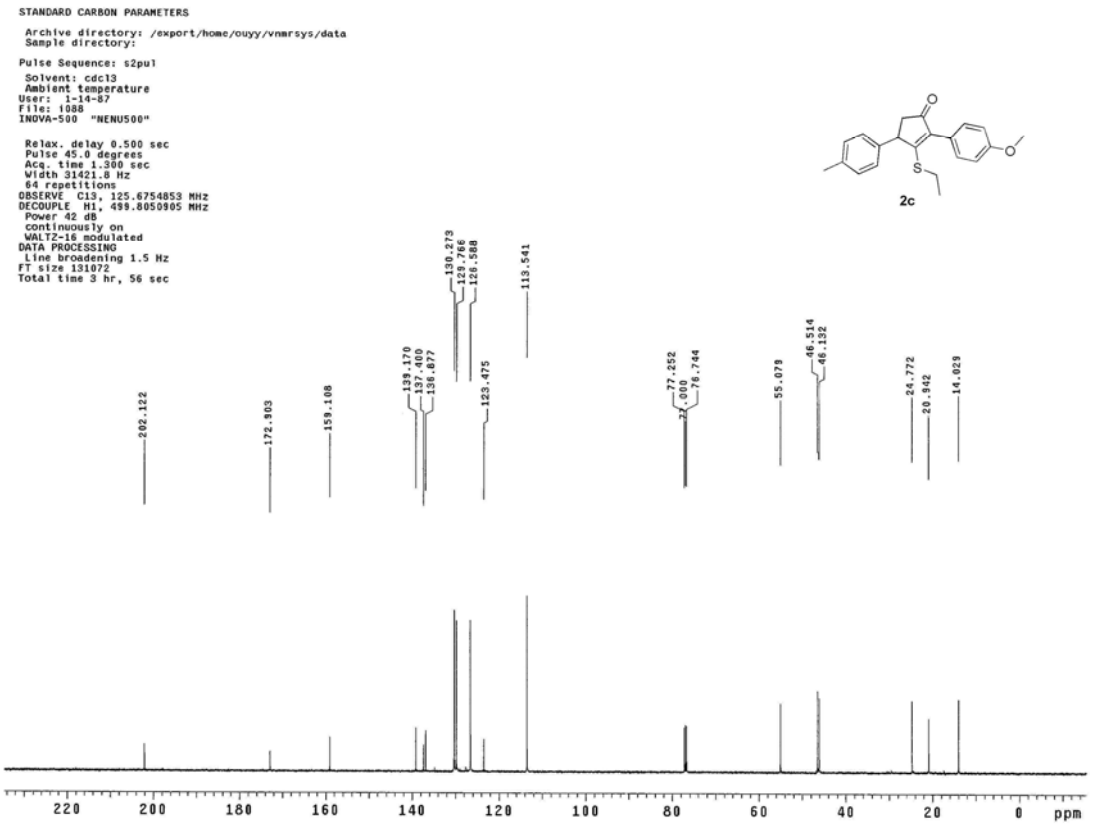

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: b956
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8064.5 Hz
8 repetitions
OBSERVE H1, 499.8025919 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
2a
ppm

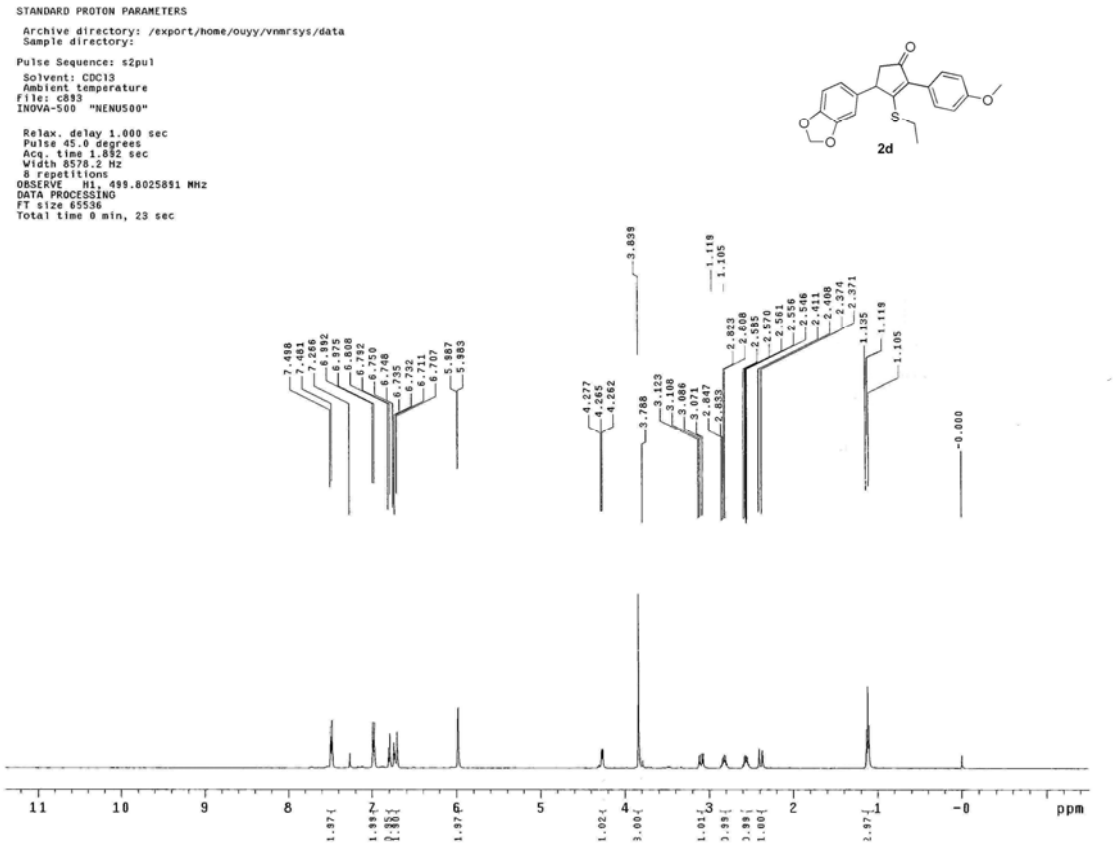

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: c894
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
128 repetitions
OBSERVE C13, 125.6755136 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec
2a
ppm

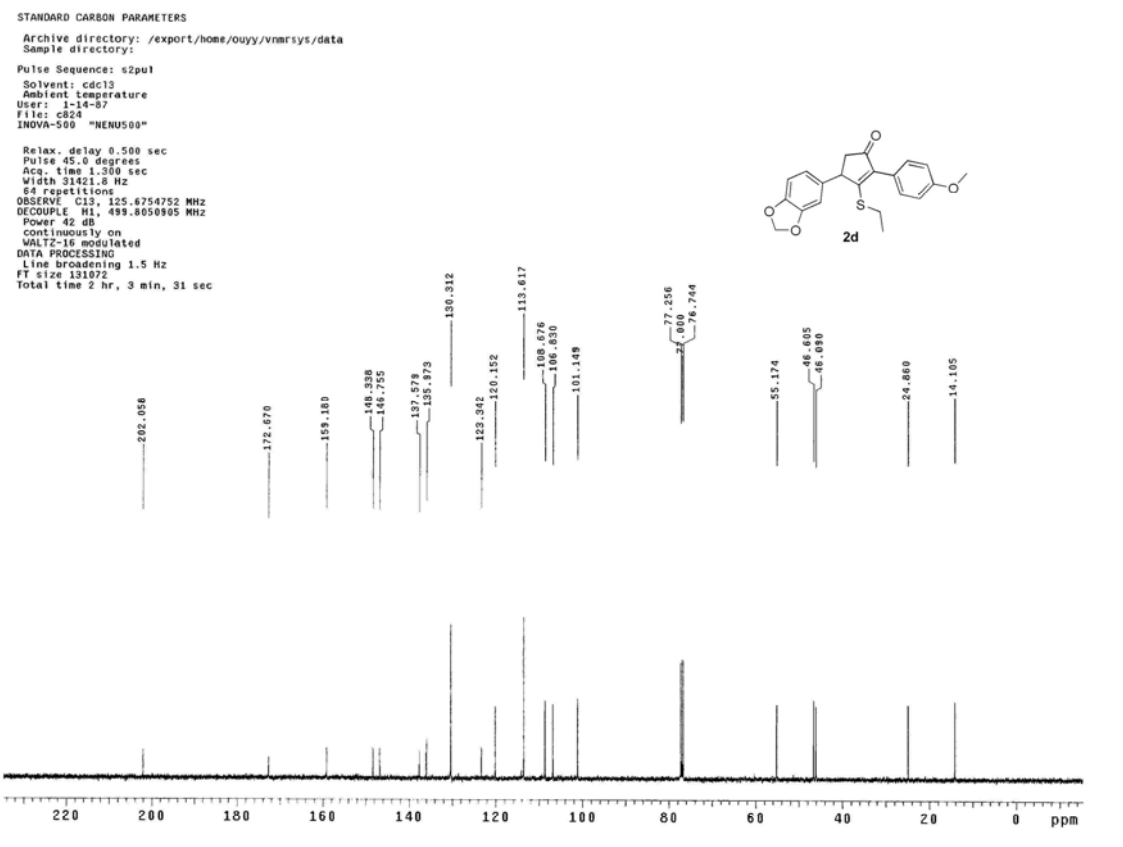

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: h802
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.882 sec
Width 8177.5 Hz
8 repetitions
OBSERVE H1, 499.8025948 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
2b
7.513
7.497
7.169
7.153
6.897
6.881
6.885
6.879
4.291
4.277
3.839
3.808
3.784
3.111
3.096
3.074
3.060
2.800
2.785
2.776
2.761
2.746
2.533
2.518
2.504
2.494
2.480
2.396
2.359
1.081
1.066
1.052
ppm

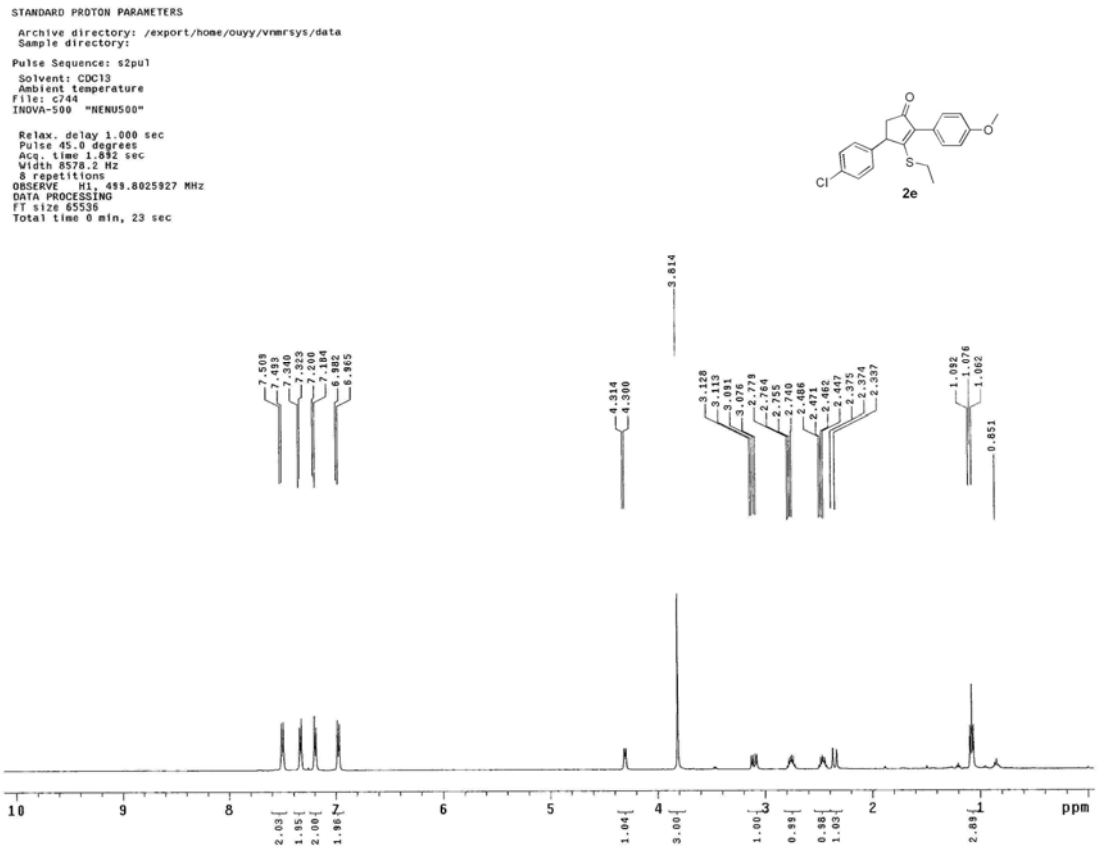

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: d138
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
128 repetitions
OBSERVE C13, 125.6754738 MHz
DECOUPLE H1, 499.8050305 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec
2b
202.264
173.029
159.173
158.711
137.446
134.203
130.335
127.847
123.502
114.506
113.625
77.256
77.000
76.744
55.197
55.174
46.235
46.193
24.833
14.113
ppm

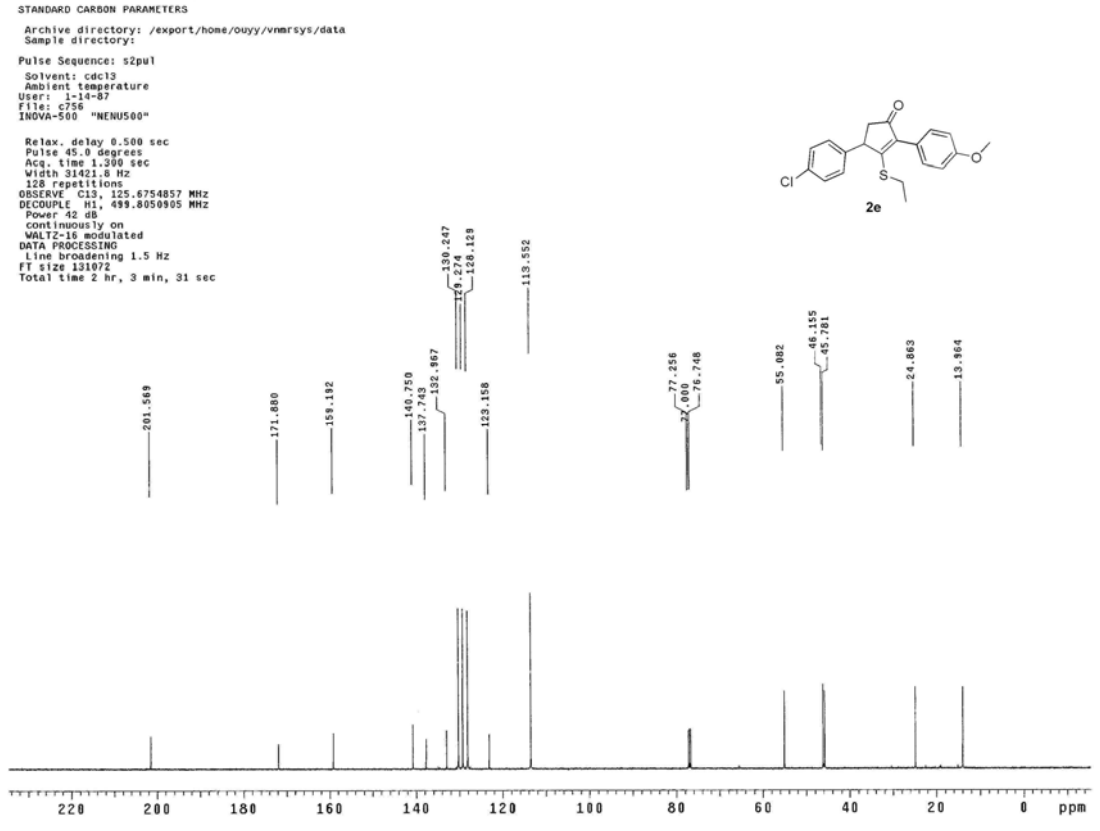

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: 1070
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 9177.5 Hz
8 repetitions
OBSERVE H1, 499.8026012 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
2c
ppm

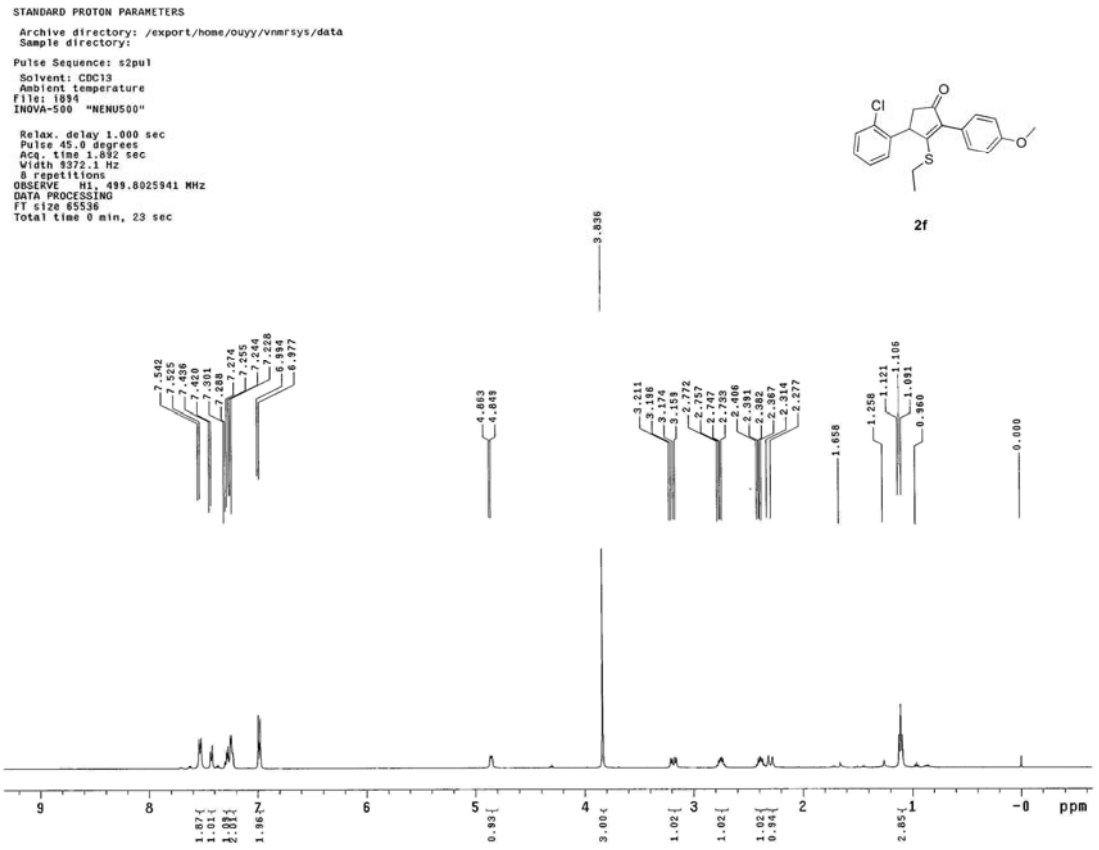

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: 1088
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
64 repetitions
OBSERVE C13, 125.6754853 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
2c
ppm

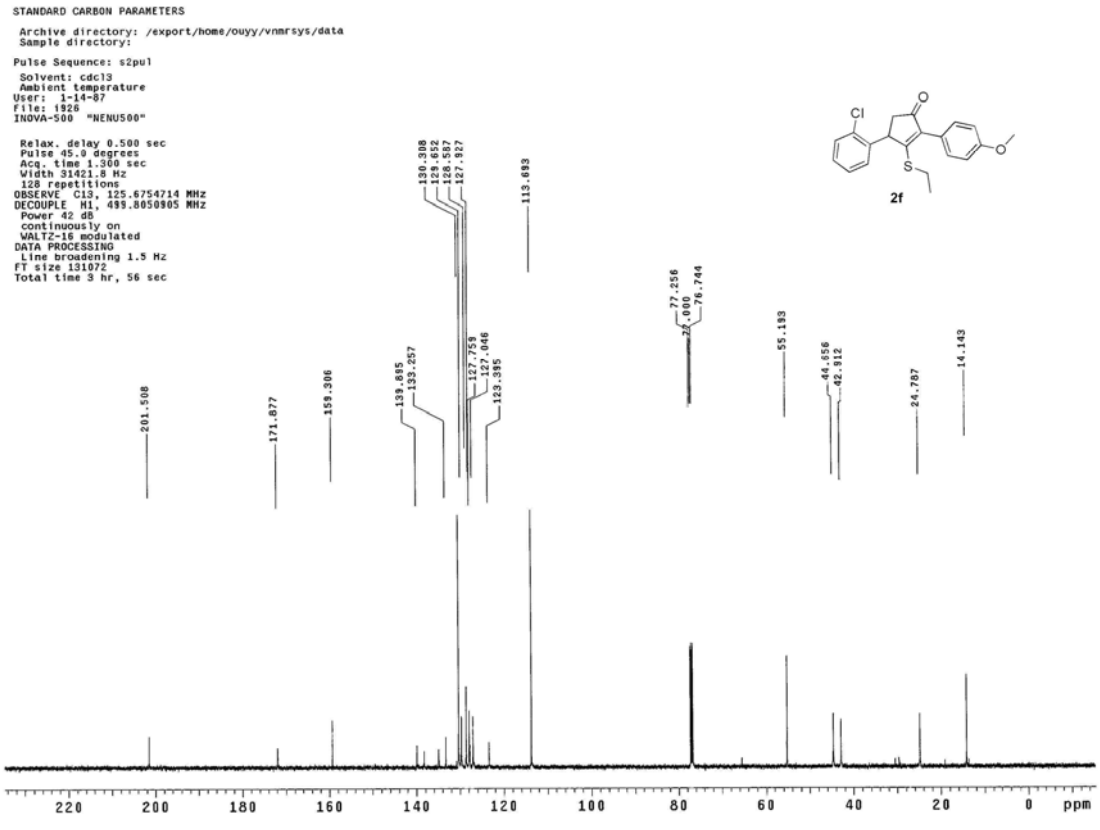

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: c893
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.882 sec
Width 8578.2 Hz
8 repetitions
OBSERVE H1, 499.8025851 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
2d
ppm


STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: c824
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
64 repetitions
OBSERVE C13, 125.6754752 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec
2d
ppm

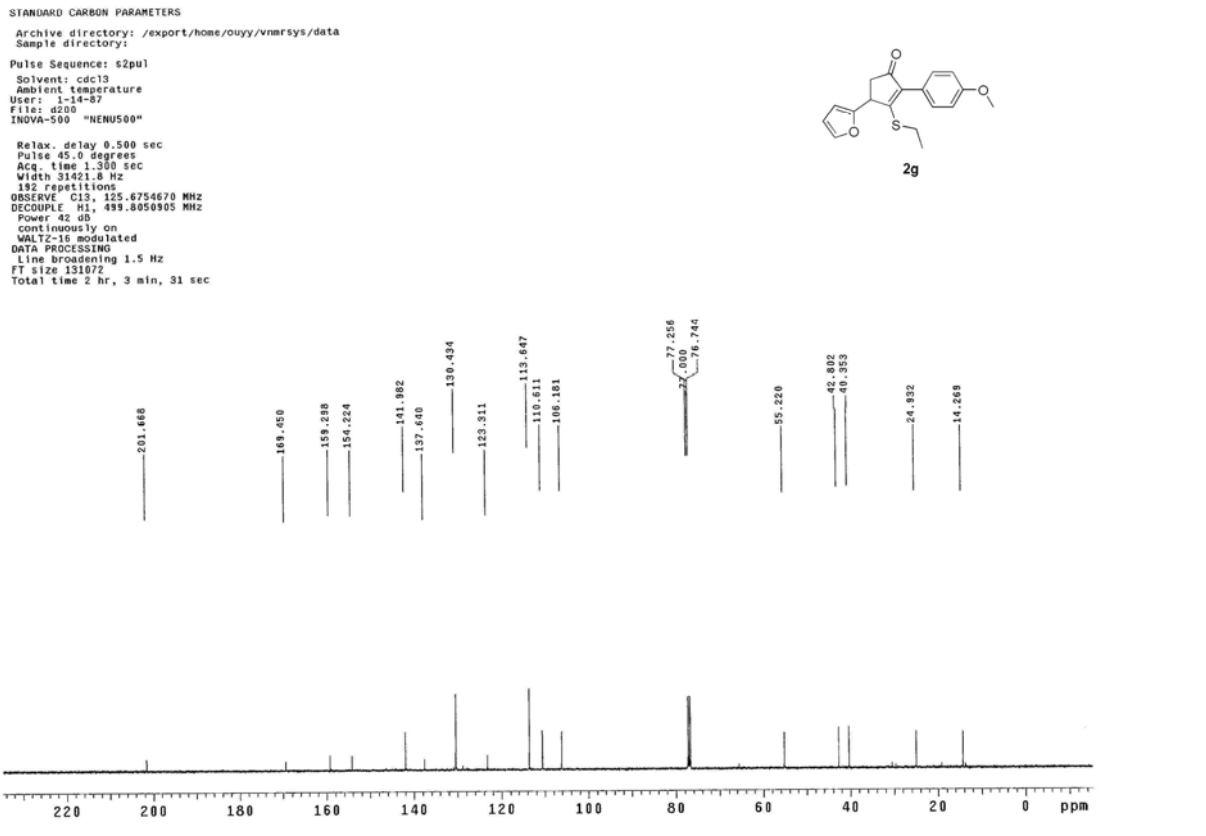

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: c744
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.882 sec
Width 8578.2 Hz
8 repetitions
OBSERVE H1, 499.8025927 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
2e
ppm

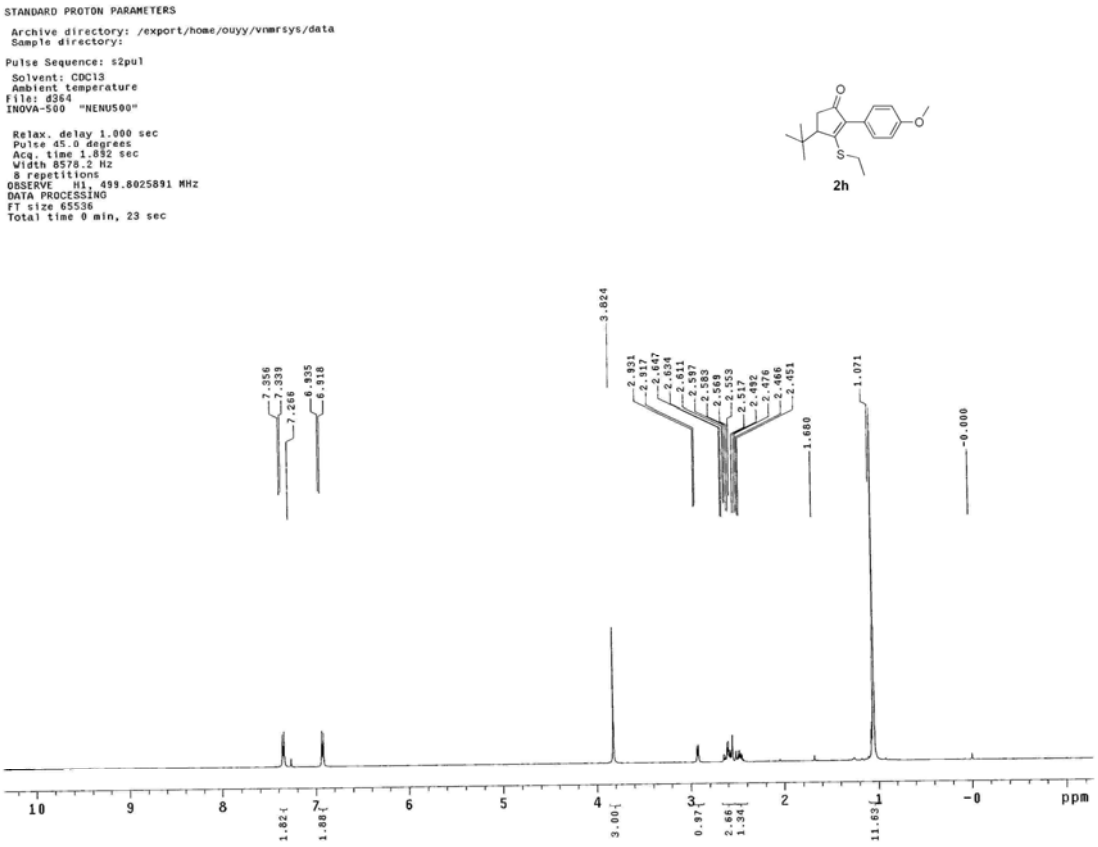

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: c756
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
128 repetitions
OBSERVE C13, 125.6754857 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec
2e
ppm

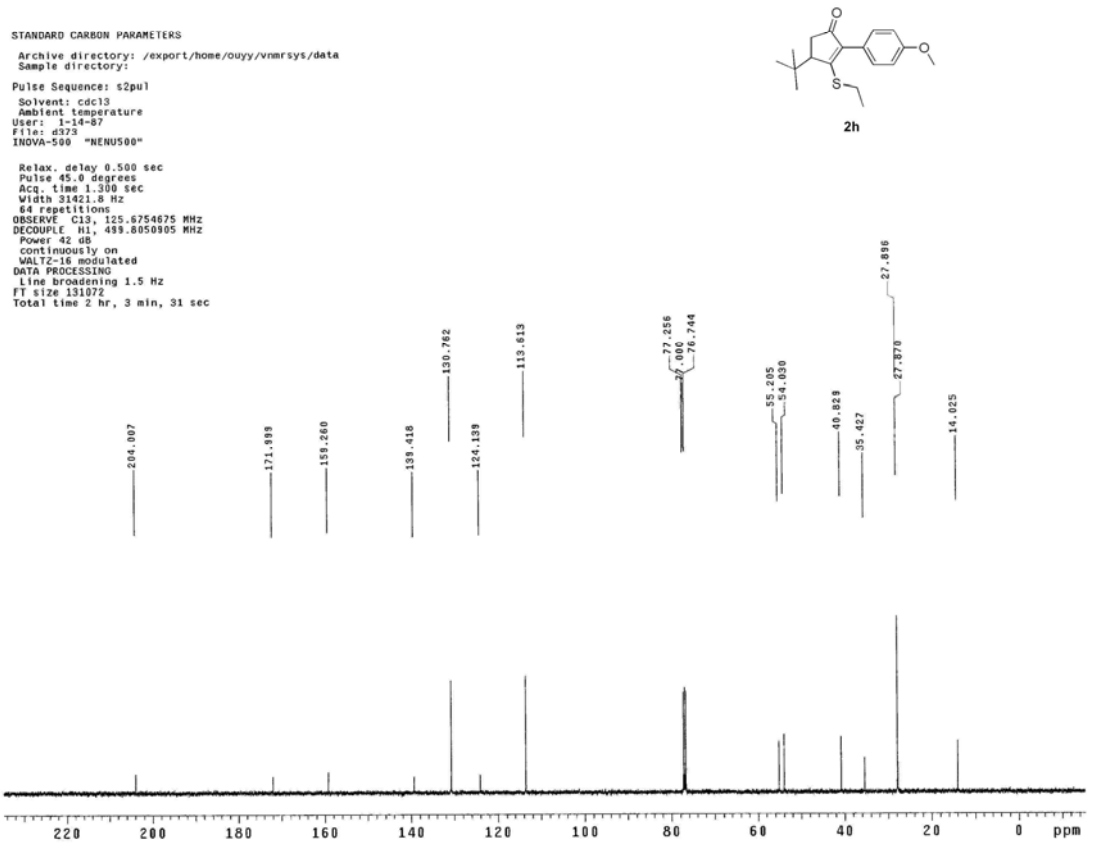

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: i894
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8372.1 Hz
8 repetitions
OBSERVE H1, 499.8025941 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
2f
ppm

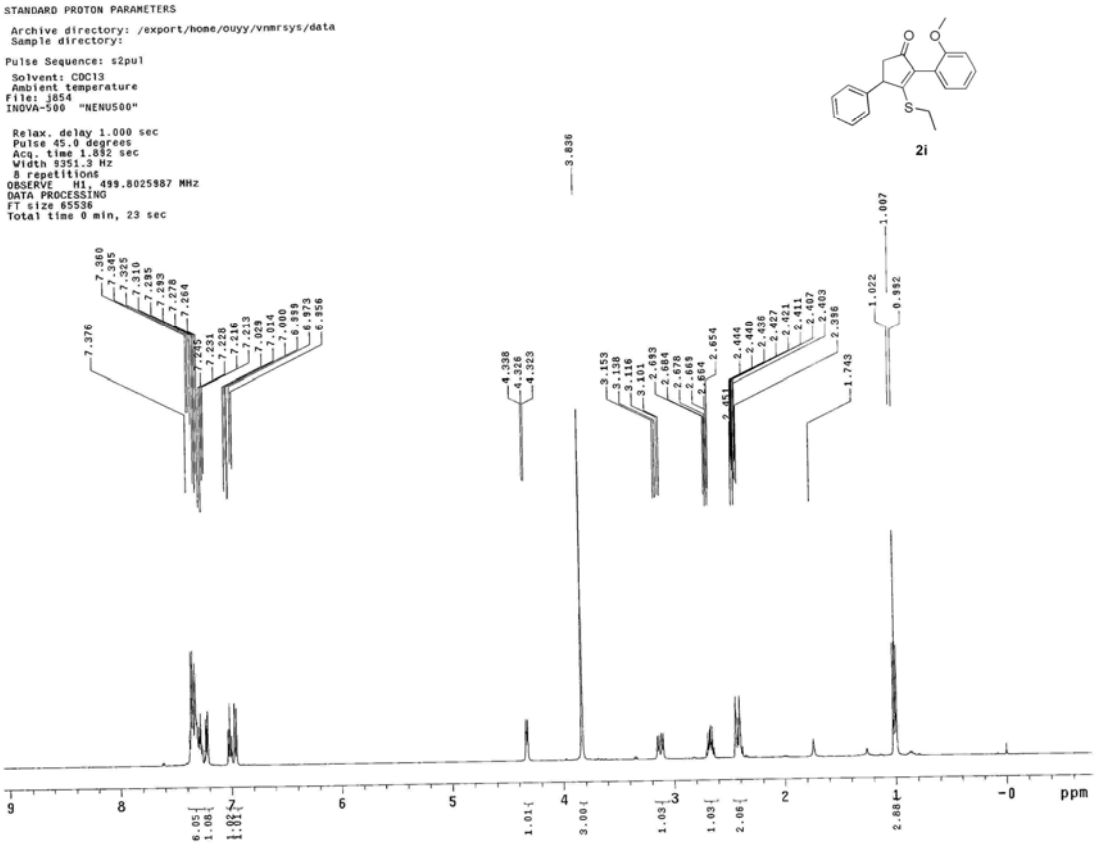

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: i926
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
128 repetitions
OBSERVE C13, 125.6754714 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
2f
ppm

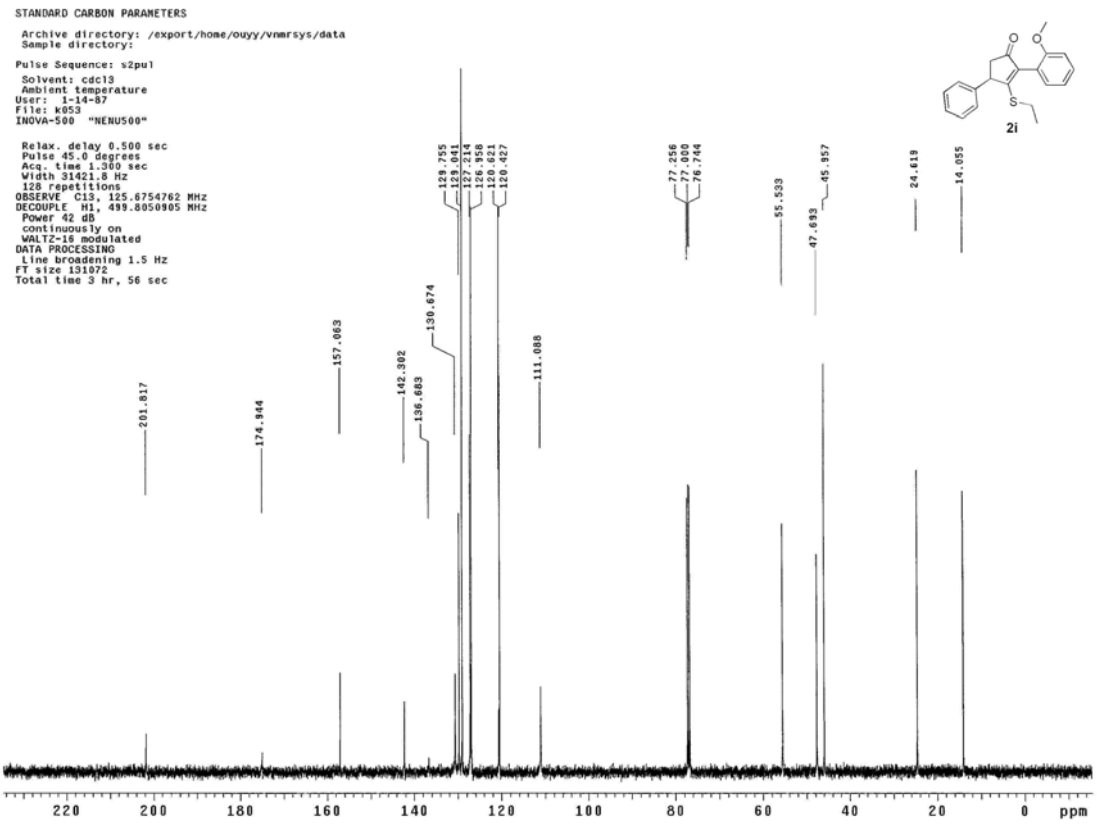

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: d188
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8578.2 Hz
8 repetitions
OBSERVE H1, 499.8025909 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
2g
ppm

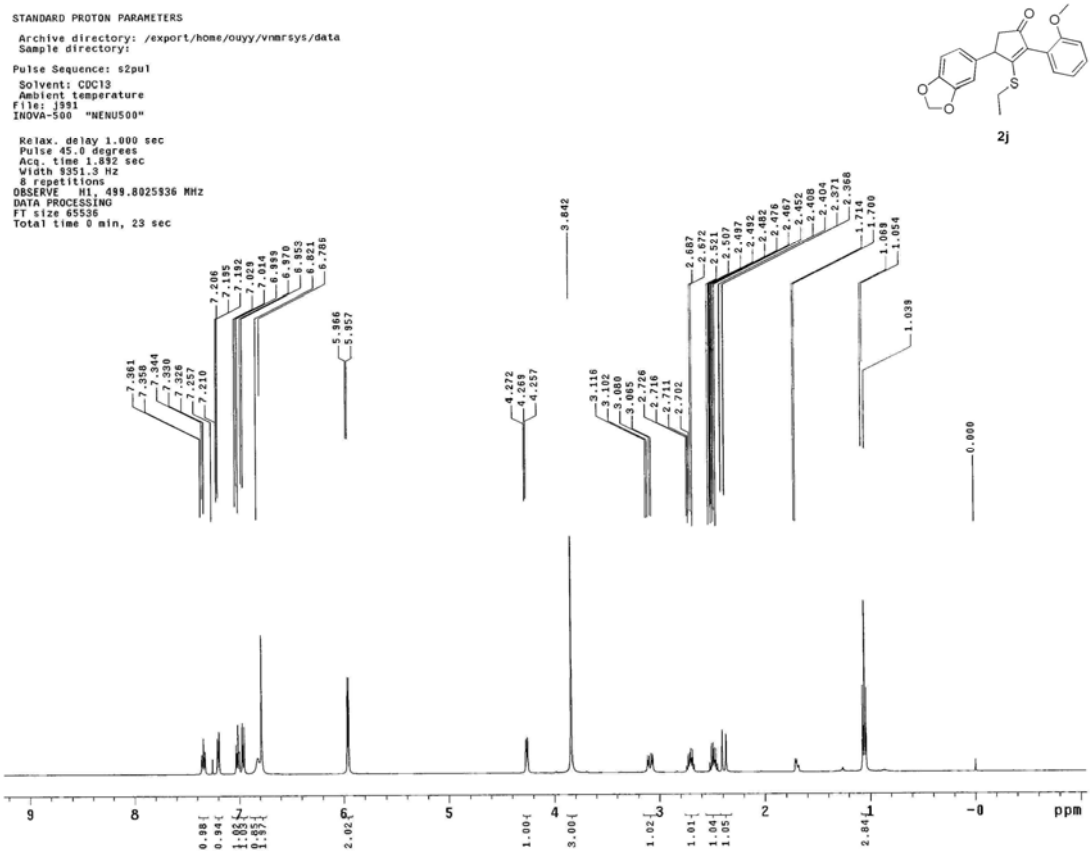

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: d200
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
192 repetitions
OBSERVE C13, 125.6754670 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec
2g
ppm

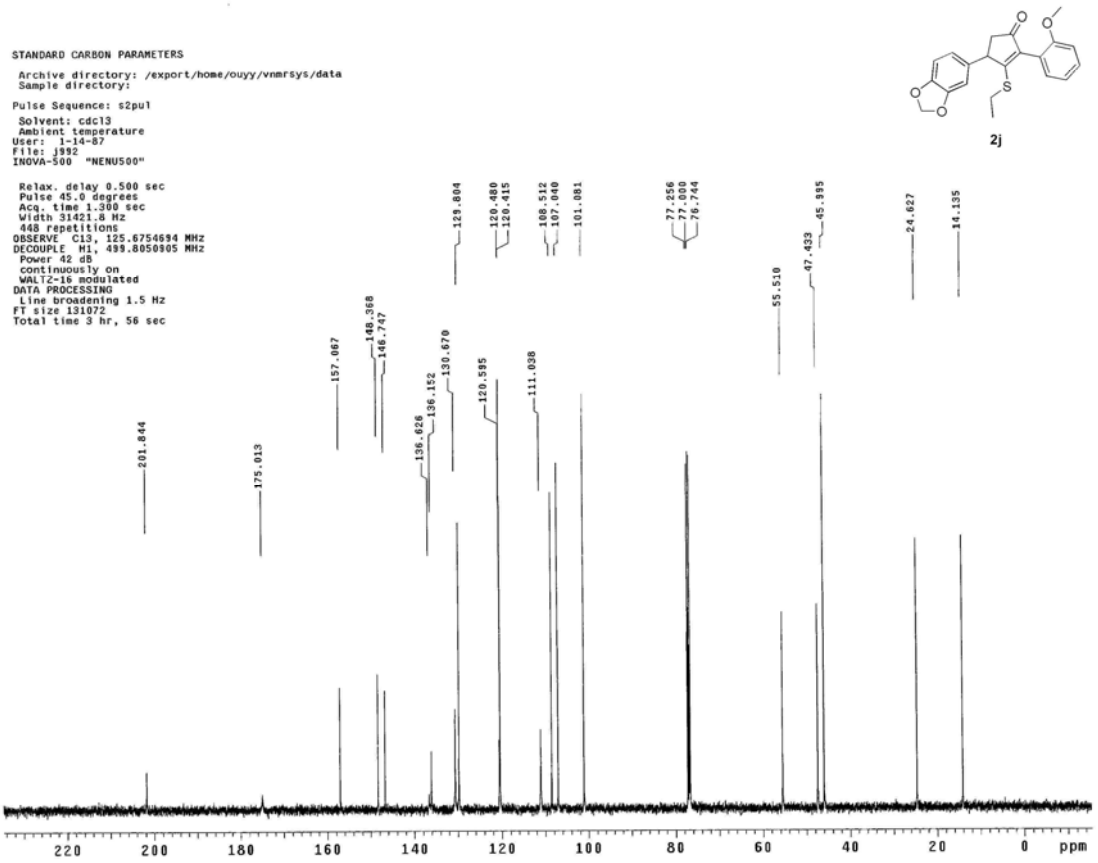

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: d364
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8578.2 Hz
8 repetitions
OBSERVE H1, 499.8025891 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
2h
7.356
7.339
7.286
6.935
6.918
3.824
2.931
2.917
2.647
2.634
2.611
2.597
2.583
2.569
2.553
2.517
2.492
2.476
2.466
2.451
1.680
1.071
-0.000
10
9
8
7
6
5
4
3
2
1
-0
ppm
1.82
1.88
3.00
0.97
2.66
1.34
11.63

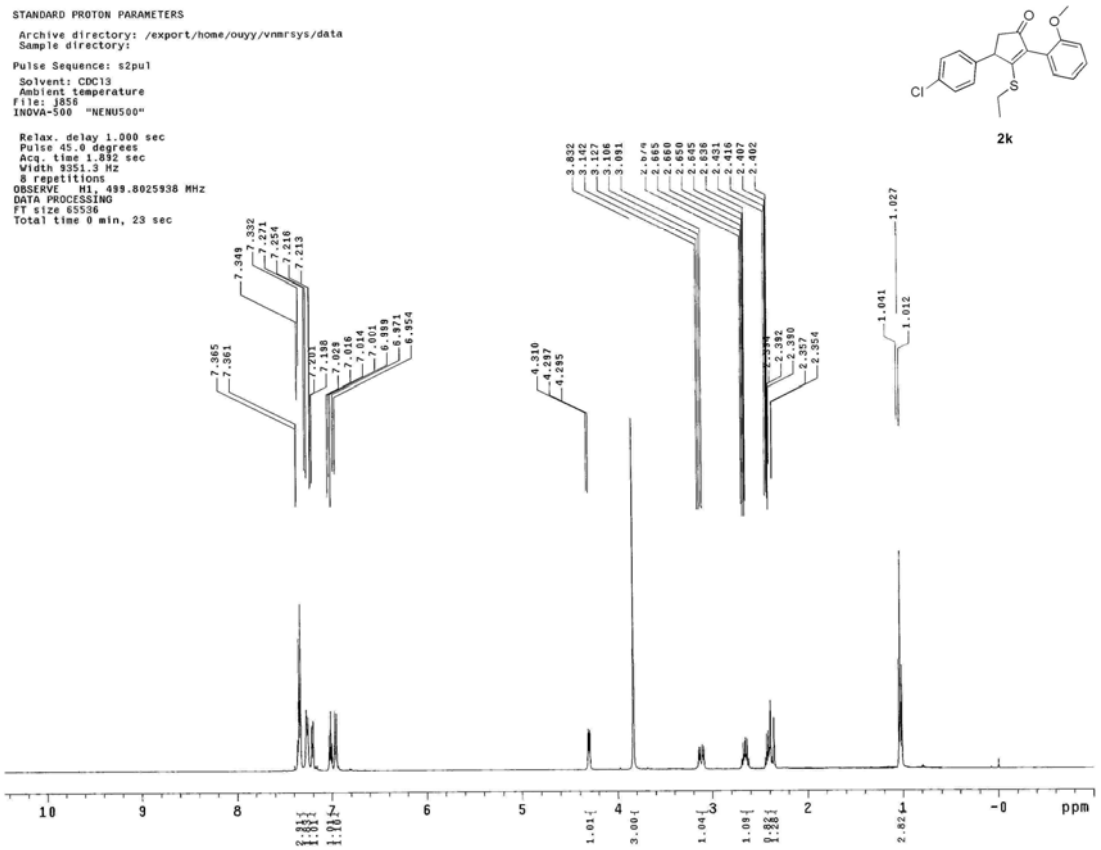

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: d373
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
64 repetitions
OBSERVE C13, 125.6754675 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec
2h
204.007
171.999
159.260
139.418
130.762
124.139
113.613
77.256
77.000
76.744
55.205
54.030
40.829
35.427
27.896
27.870
14.025
220
200
180
160
140
120
100
80
60
40
20
0
ppm

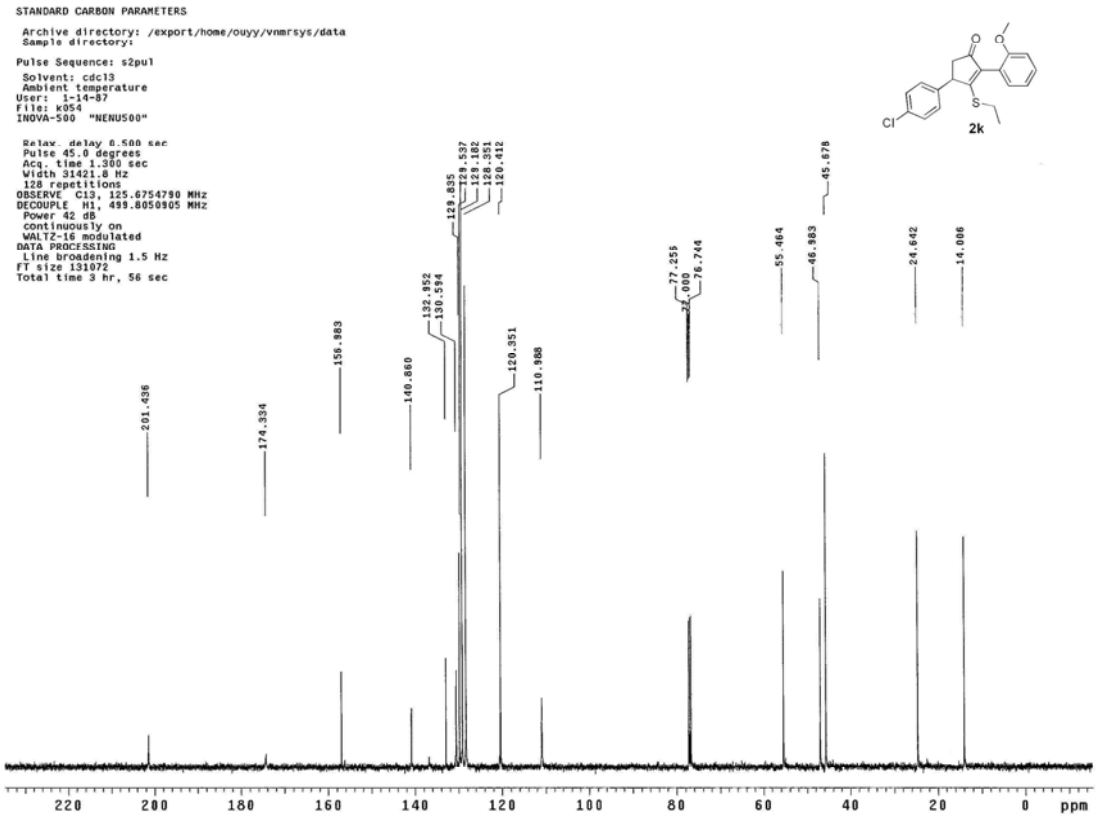

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: j854
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.882 sec
Width 8351.3 Hz
8 repetitions
OBSERVE H1, 499.8025987 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
2i
ppm

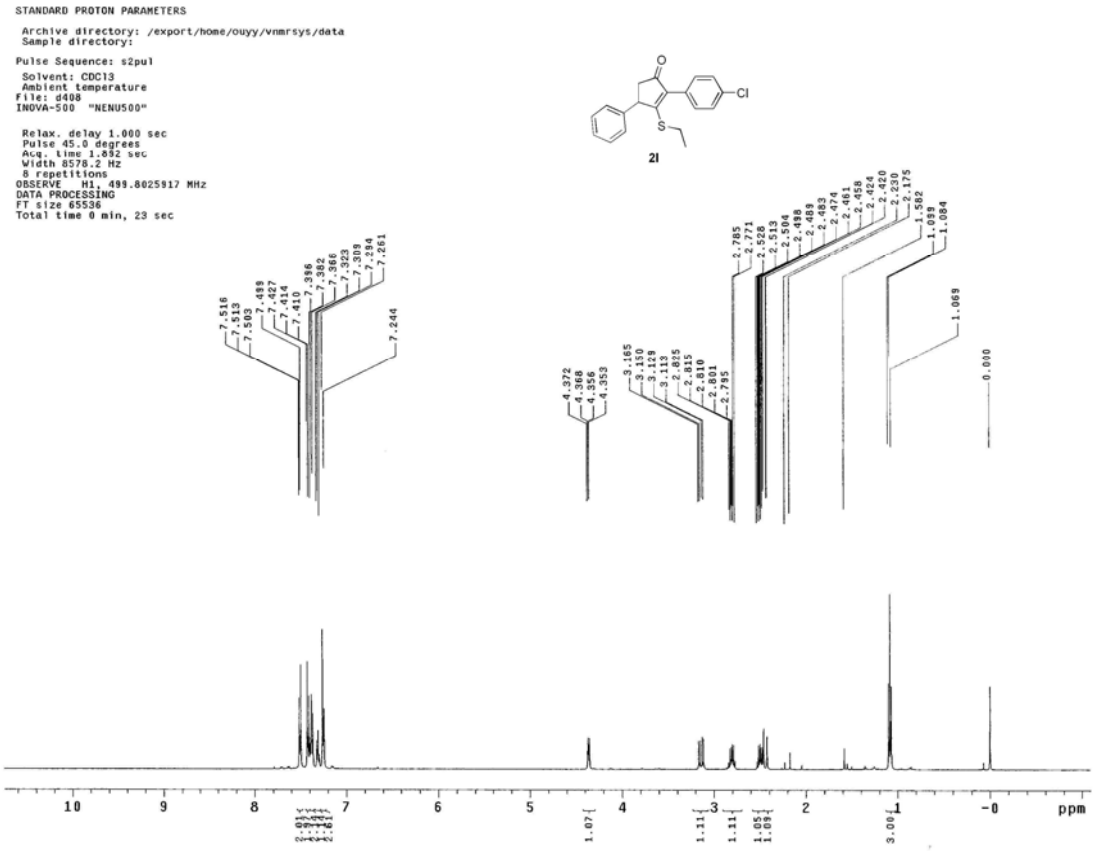

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: k053
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
128 repetitions
OBSERVE C13, 125.6754762 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
2i
ppm

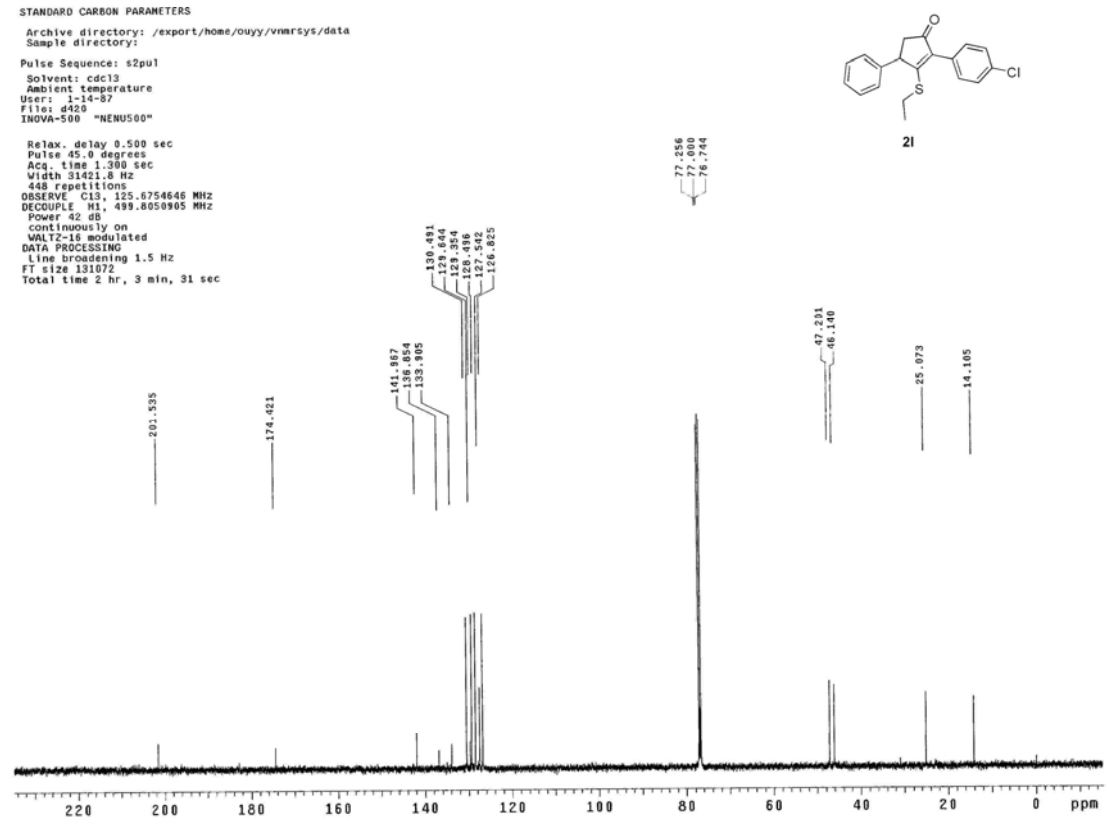

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: j991
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8351.3 Hz
8 repetitions
OBSERVE H1, 499.8025936 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
2j
ppm

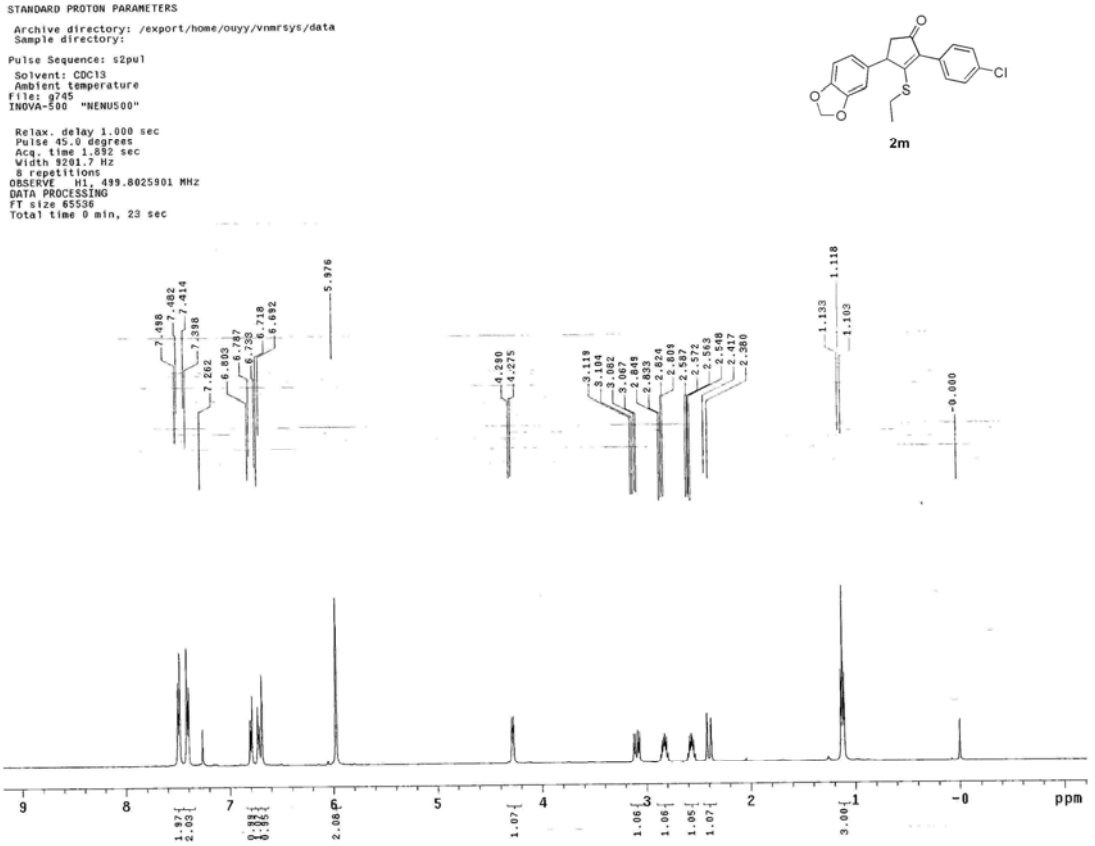

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: j992
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
448 repetitions
OBSERVE C13, 125.6754694 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
2j
ppm

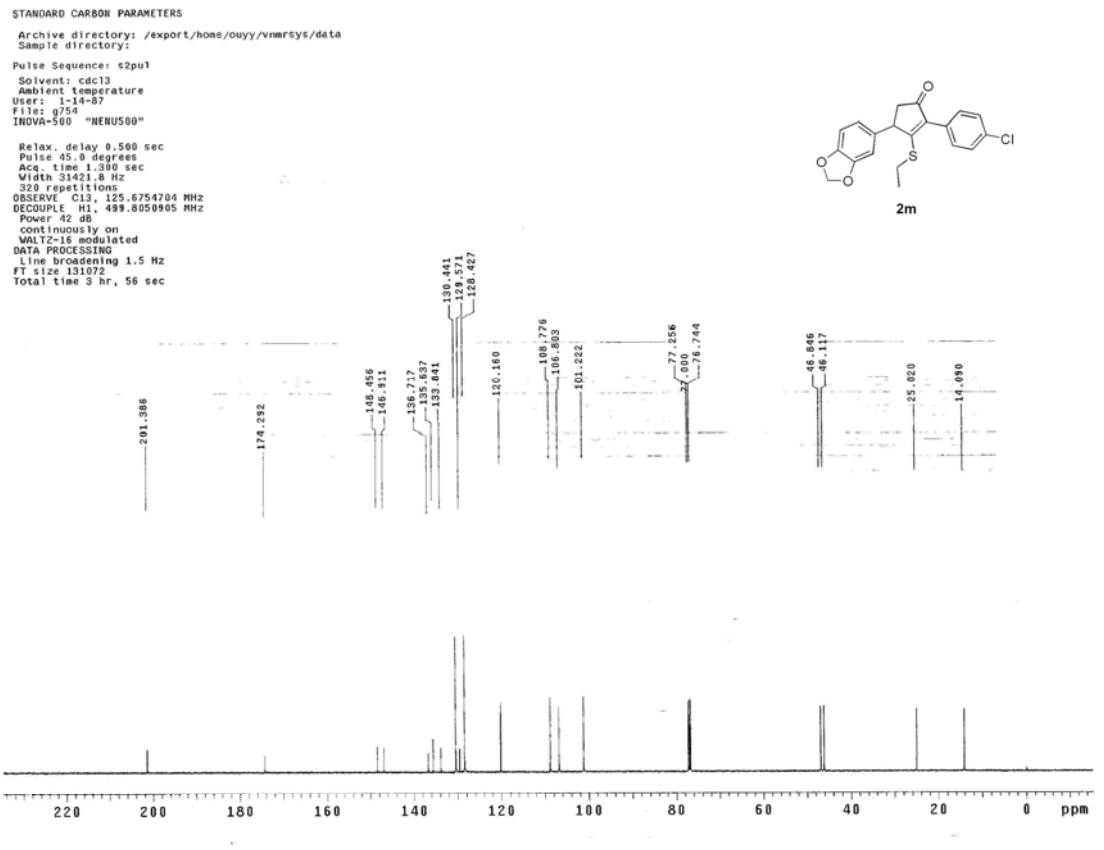

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: j856
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 9351.3 Hz
8 repetitions
OBSERVE H1, 499.8025938 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
2k
ppm

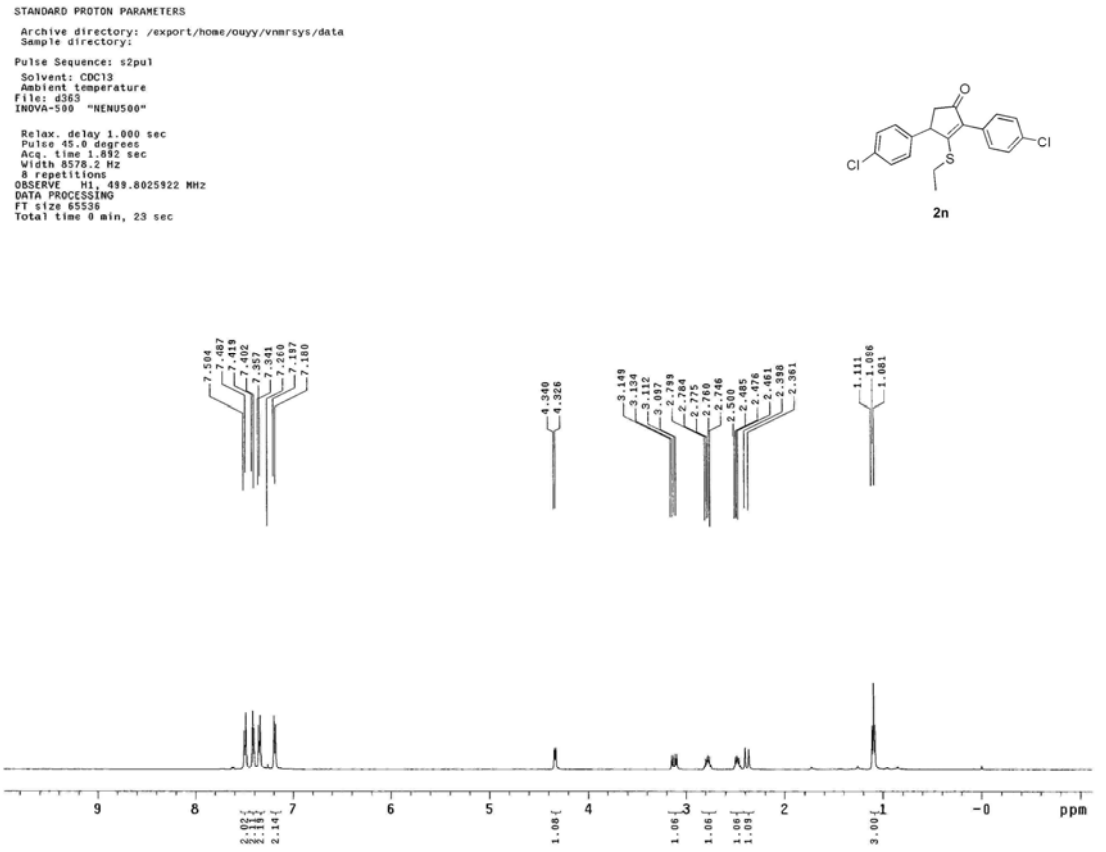

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: k054
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
128 repetitions
OBSERVE C13, 125.6754780 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
2k
ppm

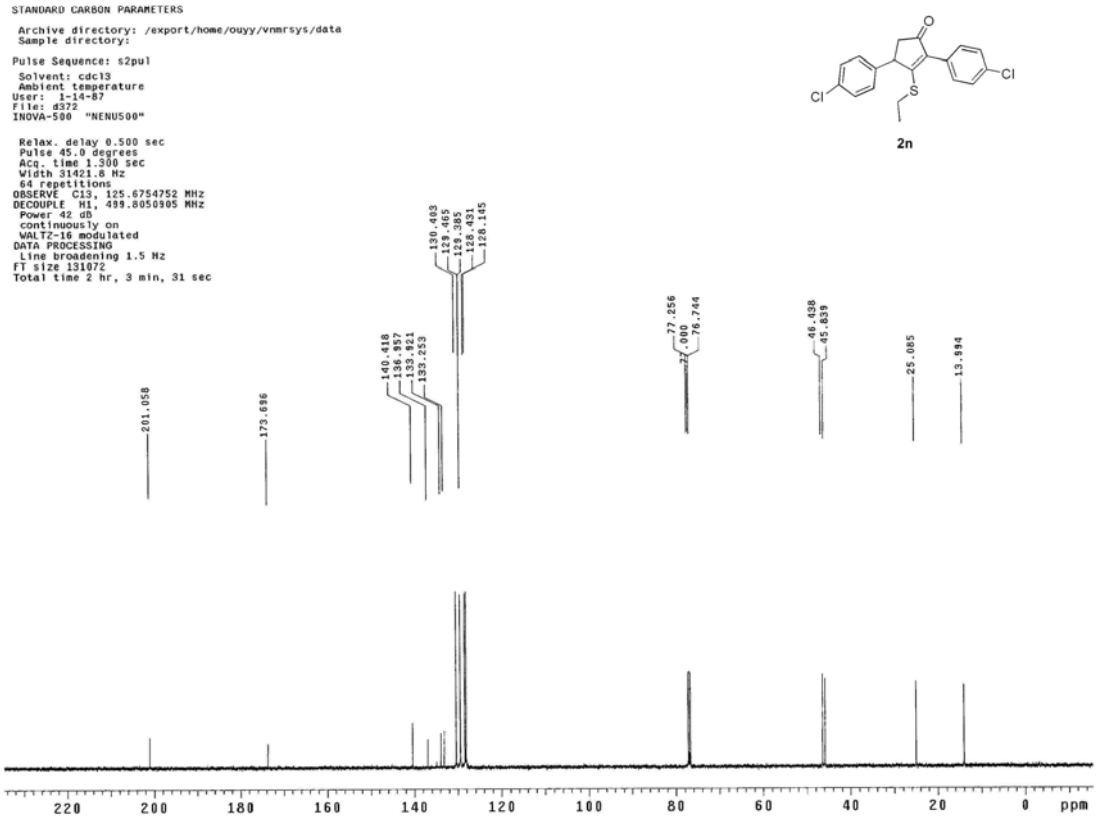

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: d408
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8578.2 Hz
8 repetitions
OBSERVE H1, 499.8025917 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
2l
ppm

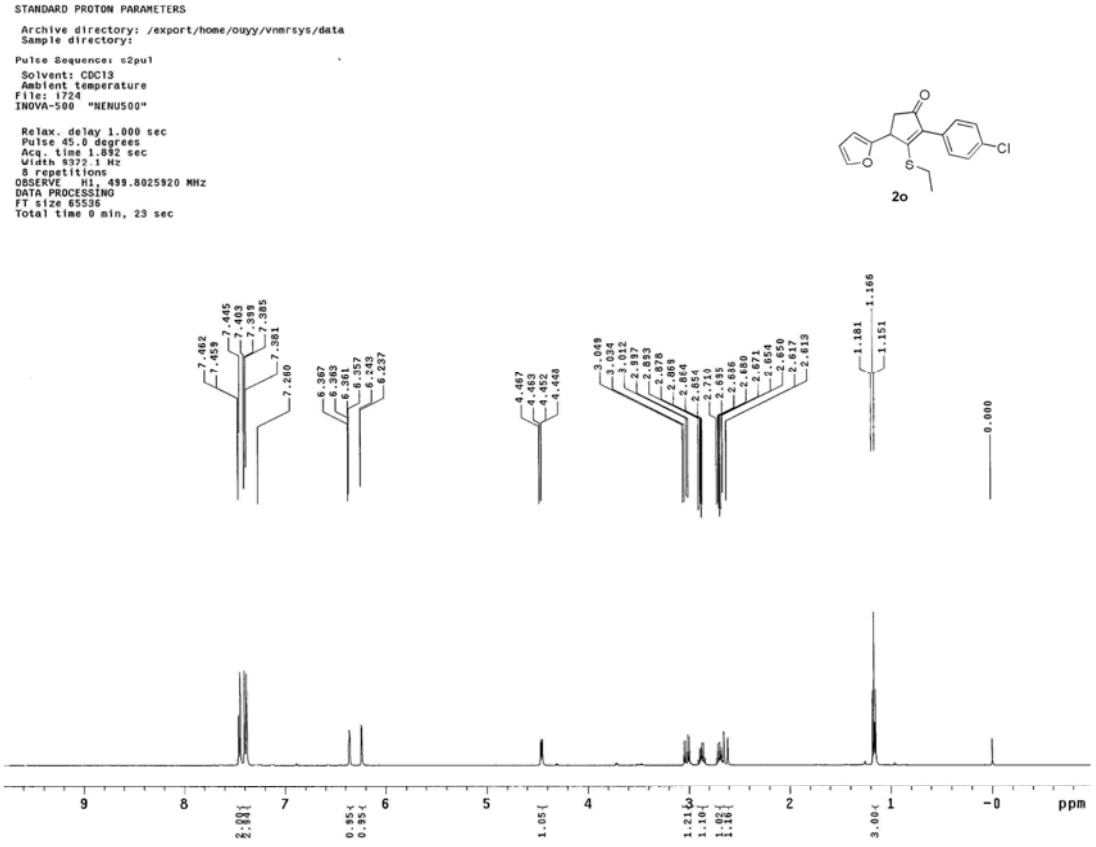

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: d420
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
448 repetitions
OBSERVE C13, 125.6754646 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec
2l
ppm

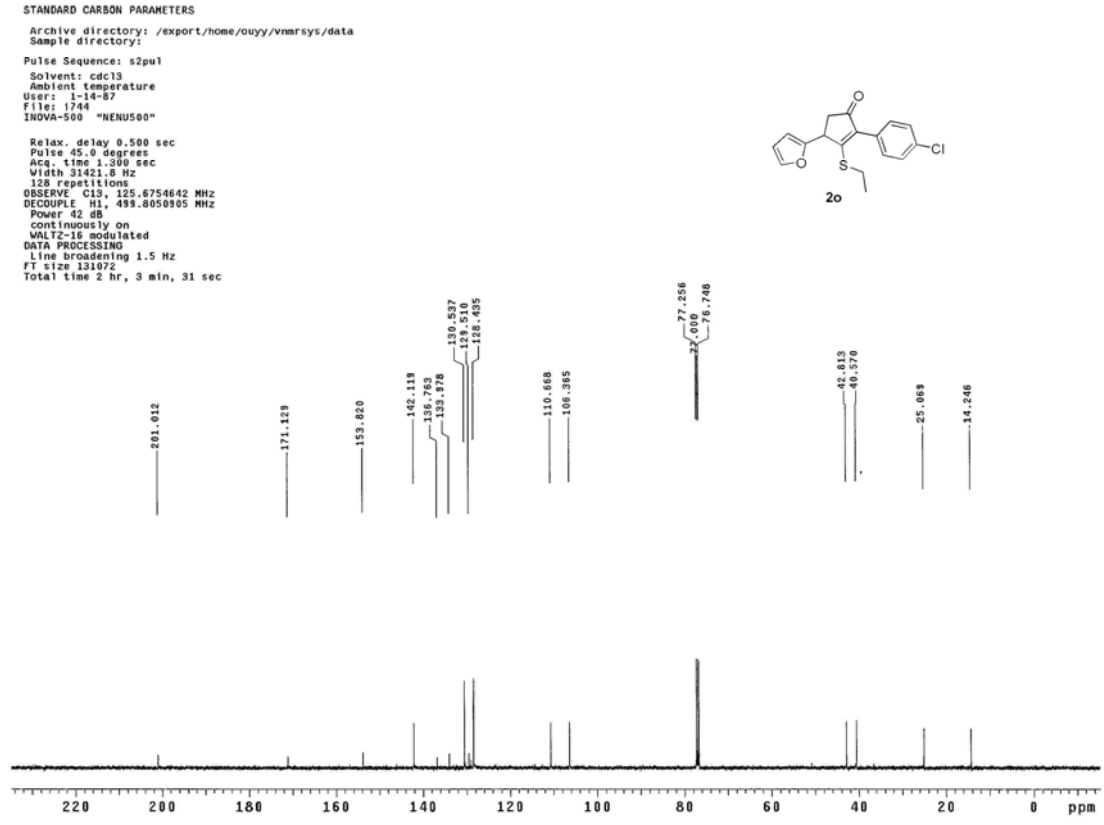

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: g745
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 9201.7 Hz
8 repetitions
OBSERVE H1, 499.8025901 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
2m
ppm

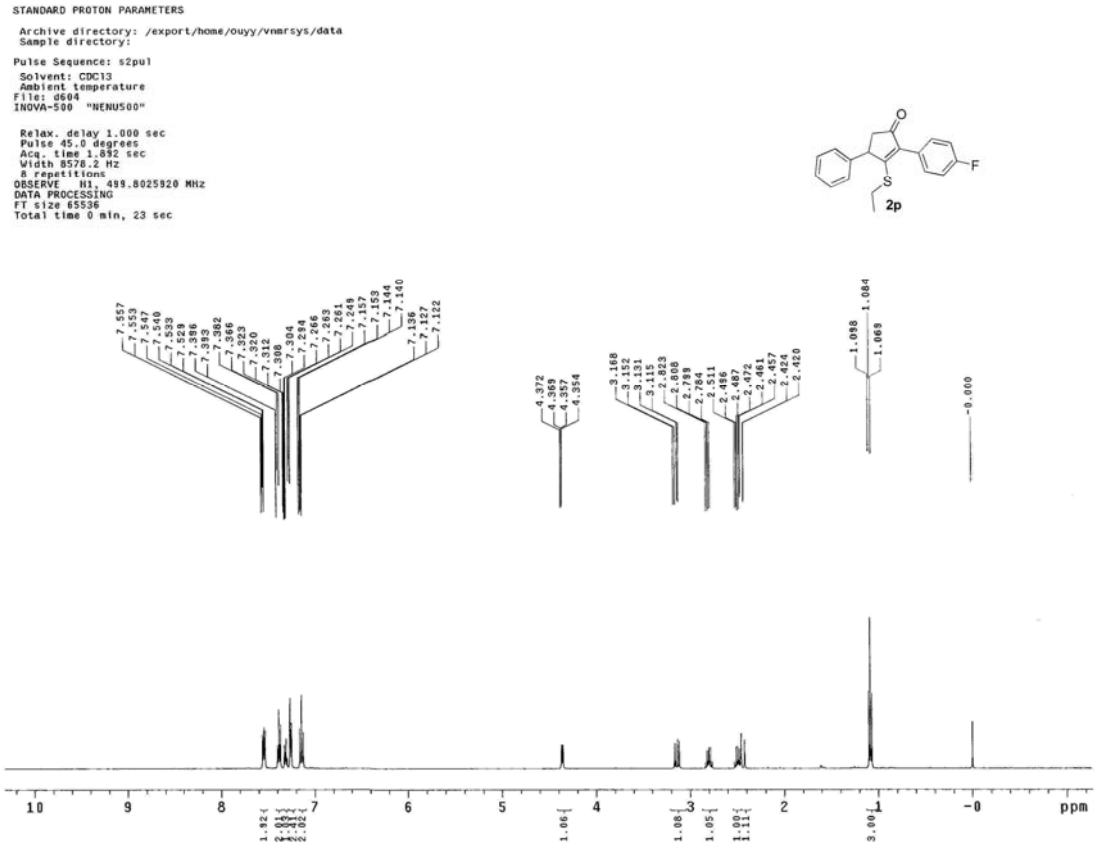

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: g754
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
320 repetitions
OBSERVE C13, 125.6754704 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
2m
ppm

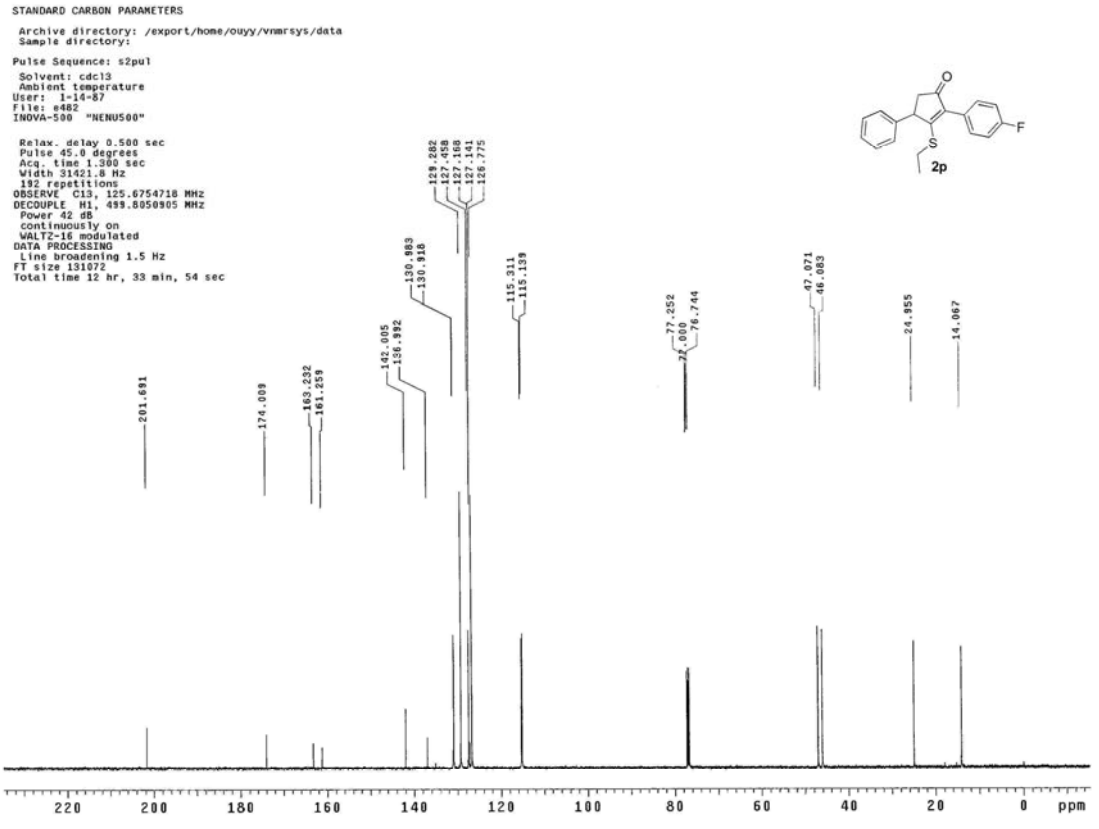

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: d363
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8578.2 Hz
8 repetitions
OBSERVE H1, 499.8025922 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
2n
7.504
7.487
7.419
7.402
7.357
7.341
7.260
7.197
7.180
4.340
4.326
3.149
3.134
3.112
3.097
2.799
2.784
2.775
2.760
2.746
2.500
2.485
2.476
2.461
2.398
2.381
1.111
1.006
1.081
ppm

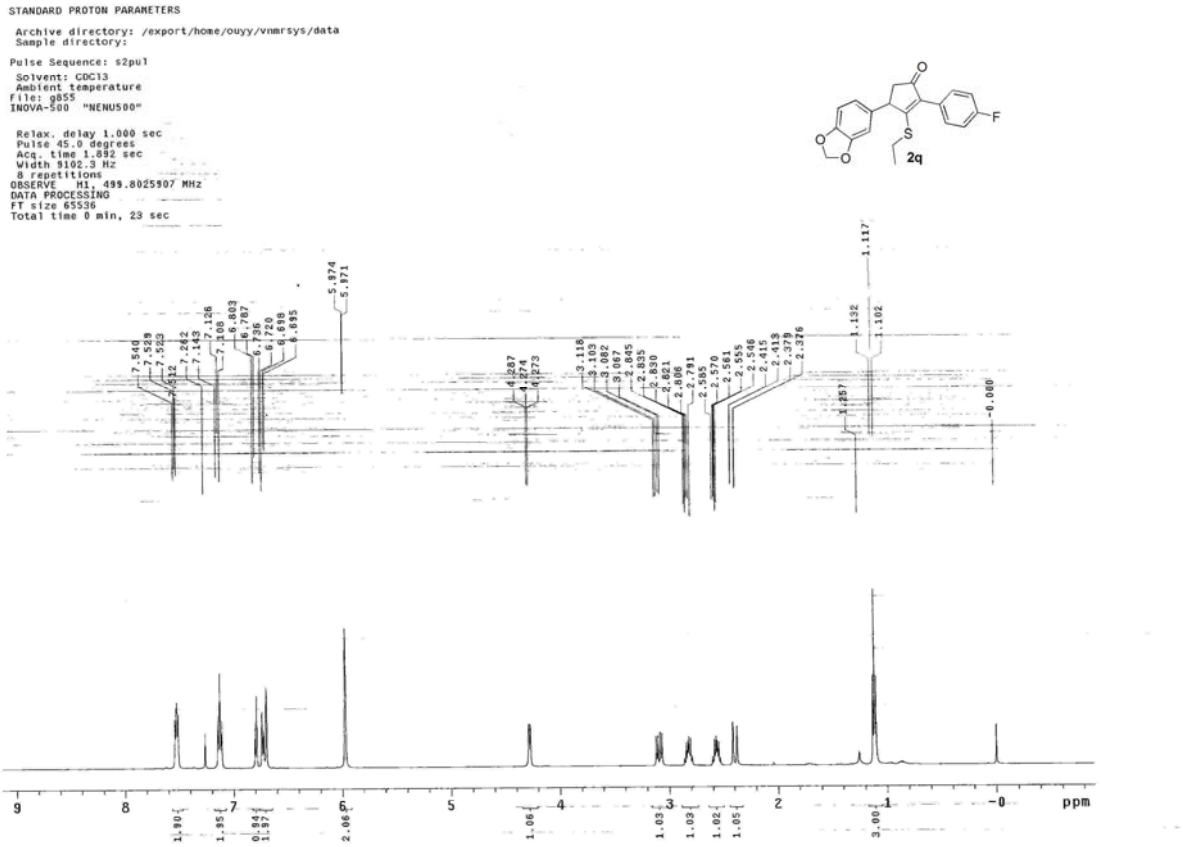

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: d372
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
64 repetitions
OBSERVE C13, 125.6754752 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec
2n
201.058
173.696
140.418
136.957
133.921
133.253
130.403
129.465
129.385
128.451
128.145
77.256
77.000
76.744
46.438
45.839
25.085
13.894
ppm

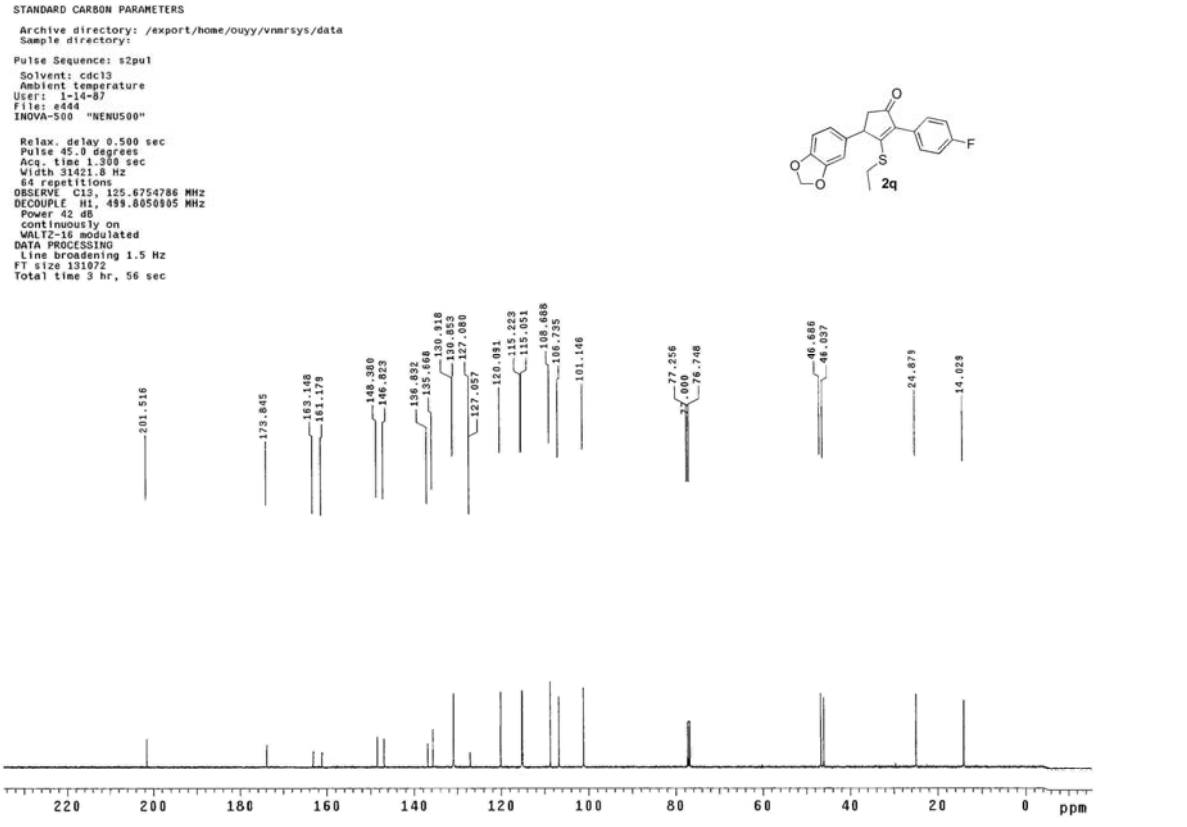

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: 1724
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.882 sec
Width 8372.1 Hz
8 repetitions
OBSERVE H1, 499.8025920 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
2o
ppm

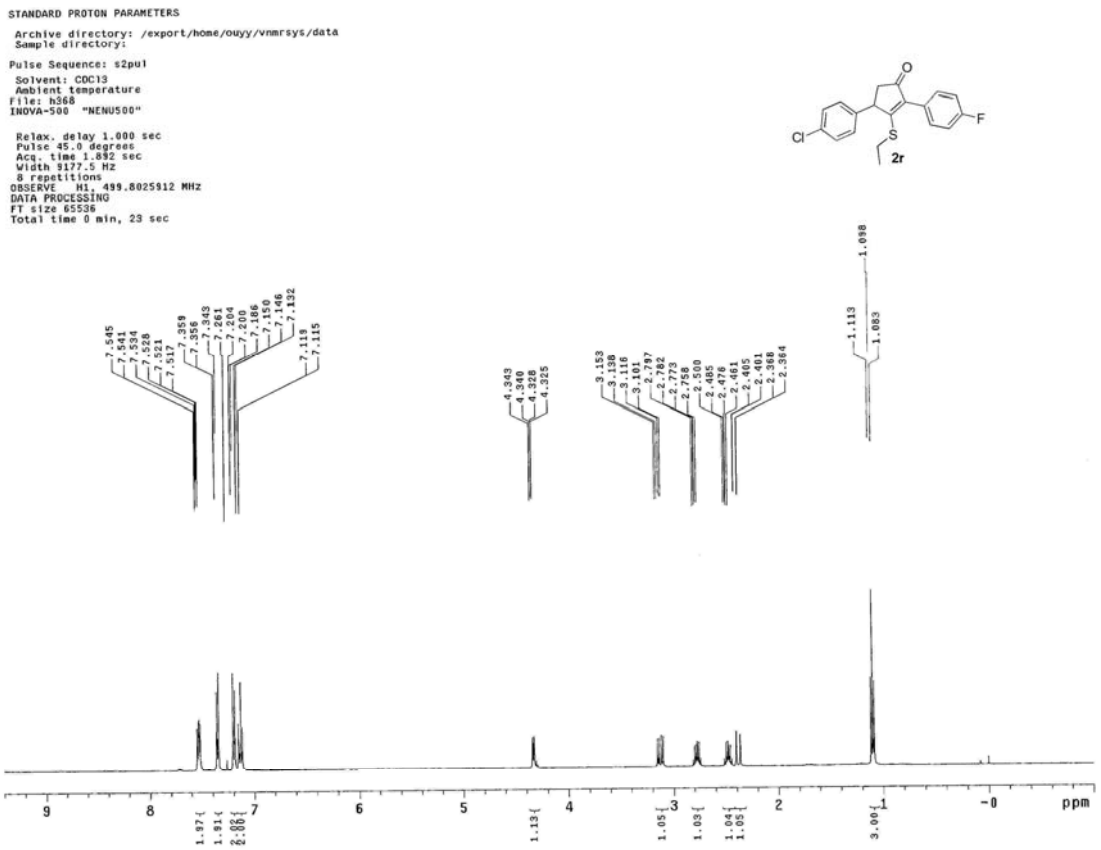

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: 1744
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
128 repetitions
OBSERVE C13, 125.6754642 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec
2o
ppm

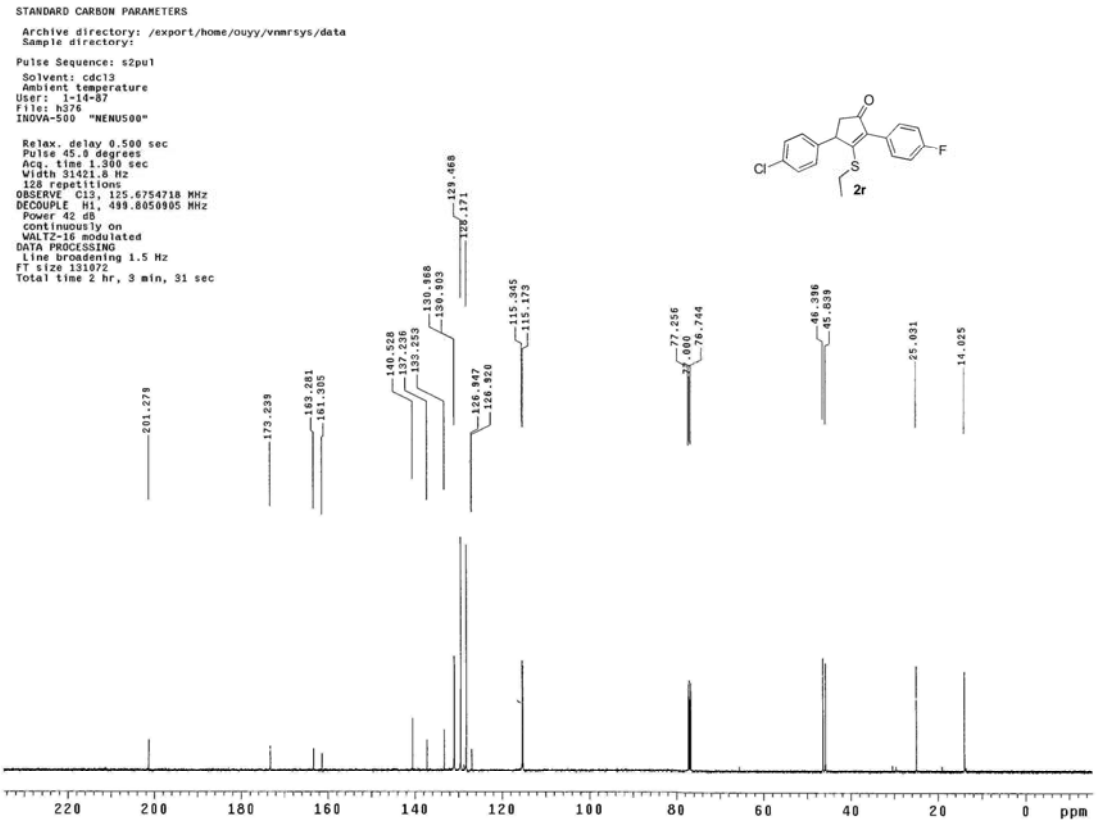

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: d604
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8578.2 Hz
8 repetitions
OBSERVE H1, 499.8025820 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
2p
ppm

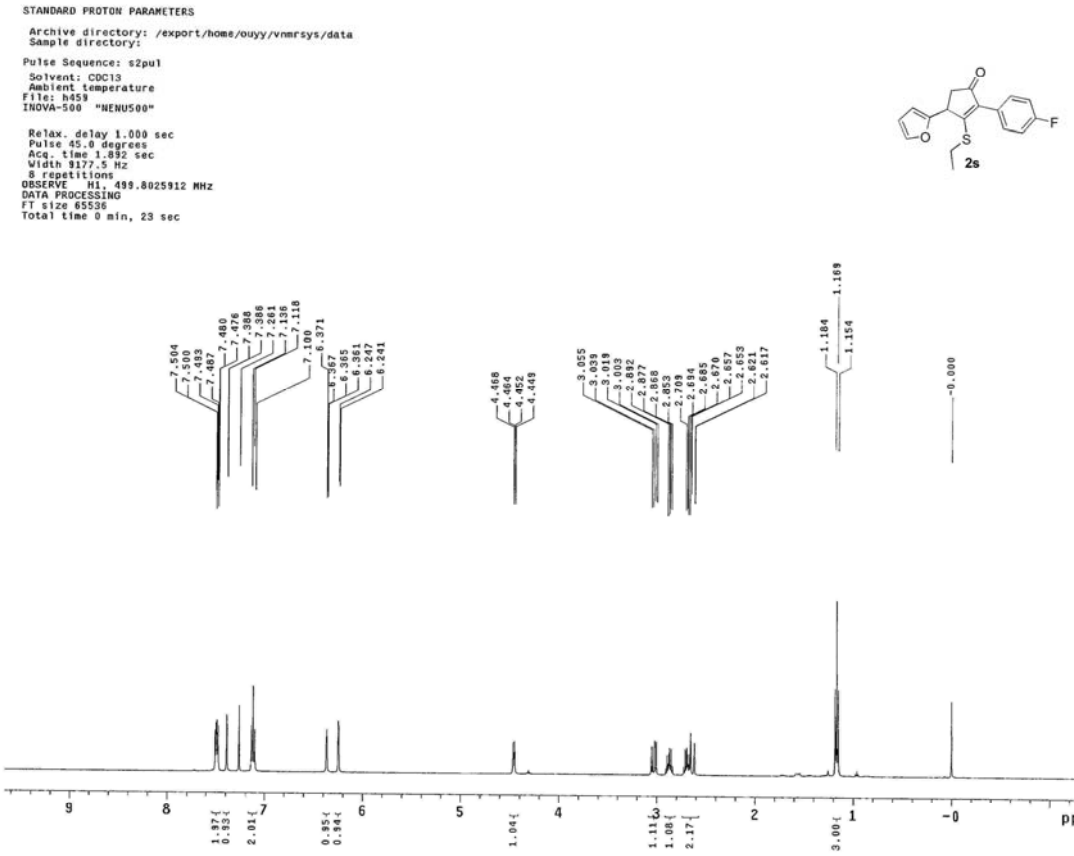

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: e482
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
192 repetitions
OBSERVE C13, 125.6754718 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 12 hr, 33 min, 54 sec
2p
ppm

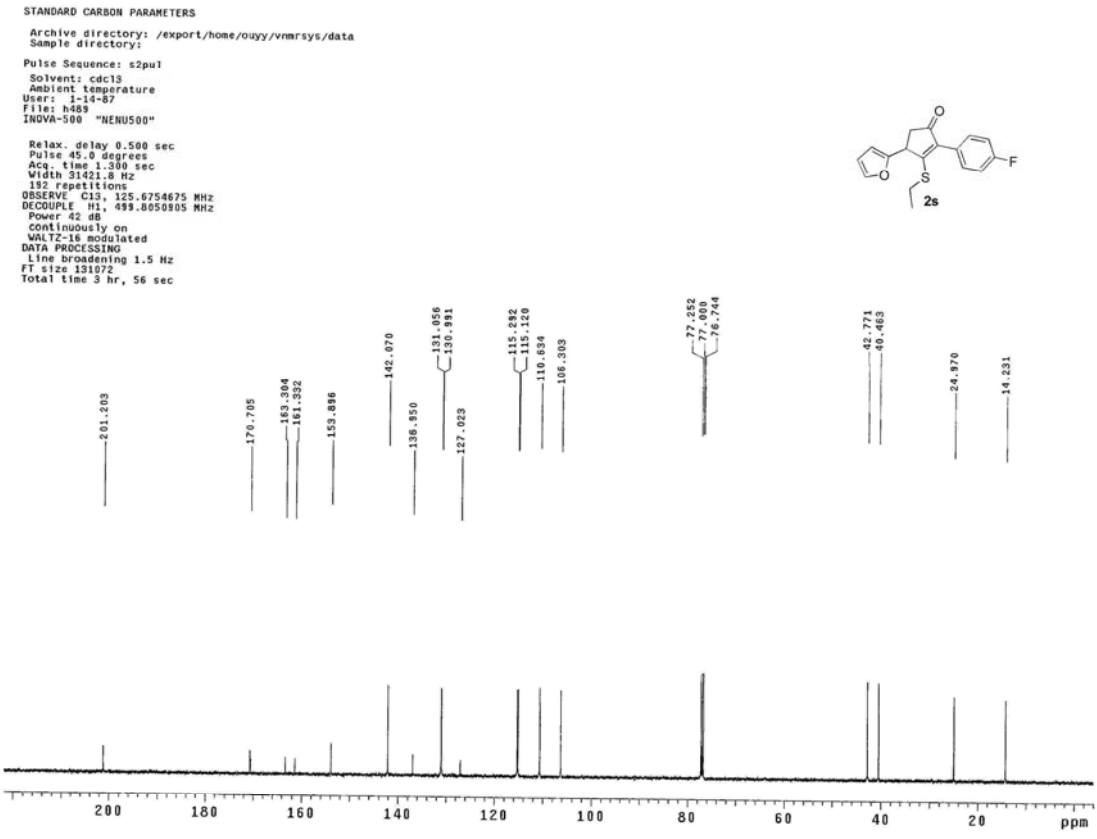

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: g855
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 9102.3 Hz
8 repetitions
OBSERVE H1, 499.8025907 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
2q
ppm

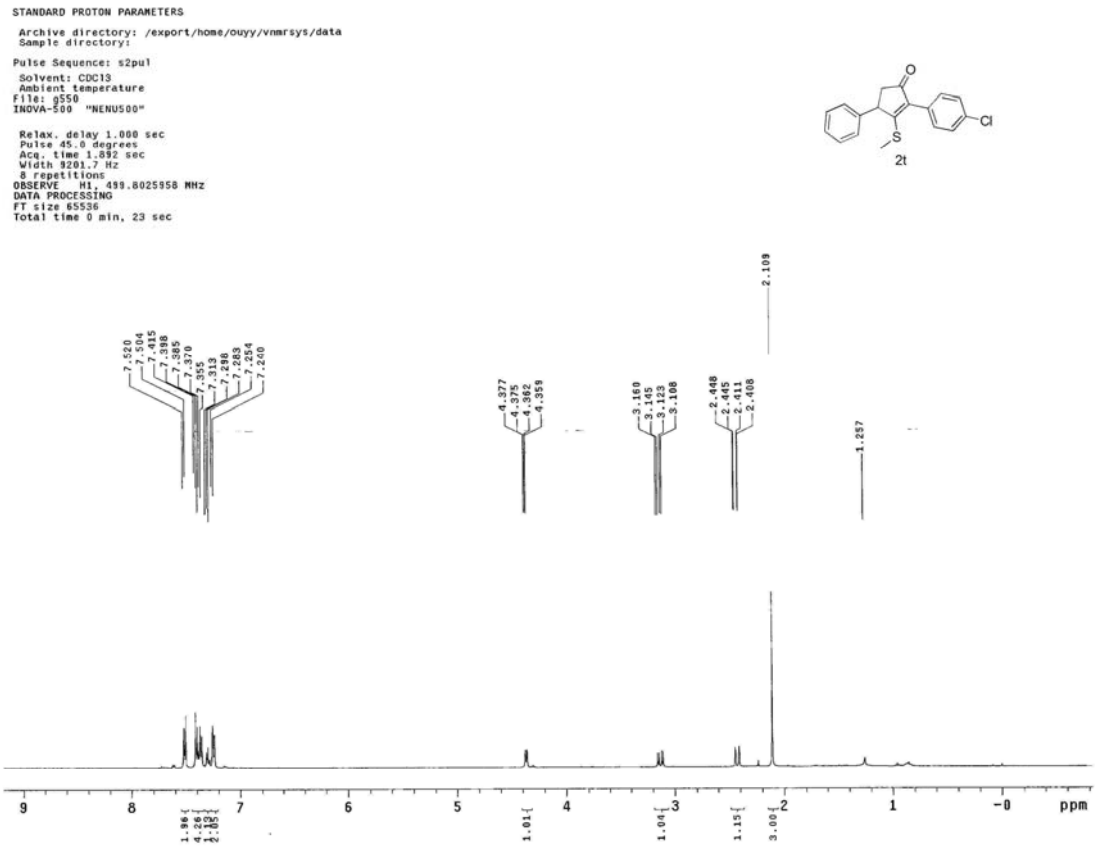

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-07
File: e444
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
64 repetitions
OBSERVE C13, 125.6754786 MHz
DECOUPLE H1, 499.8050805 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
2q
ppm

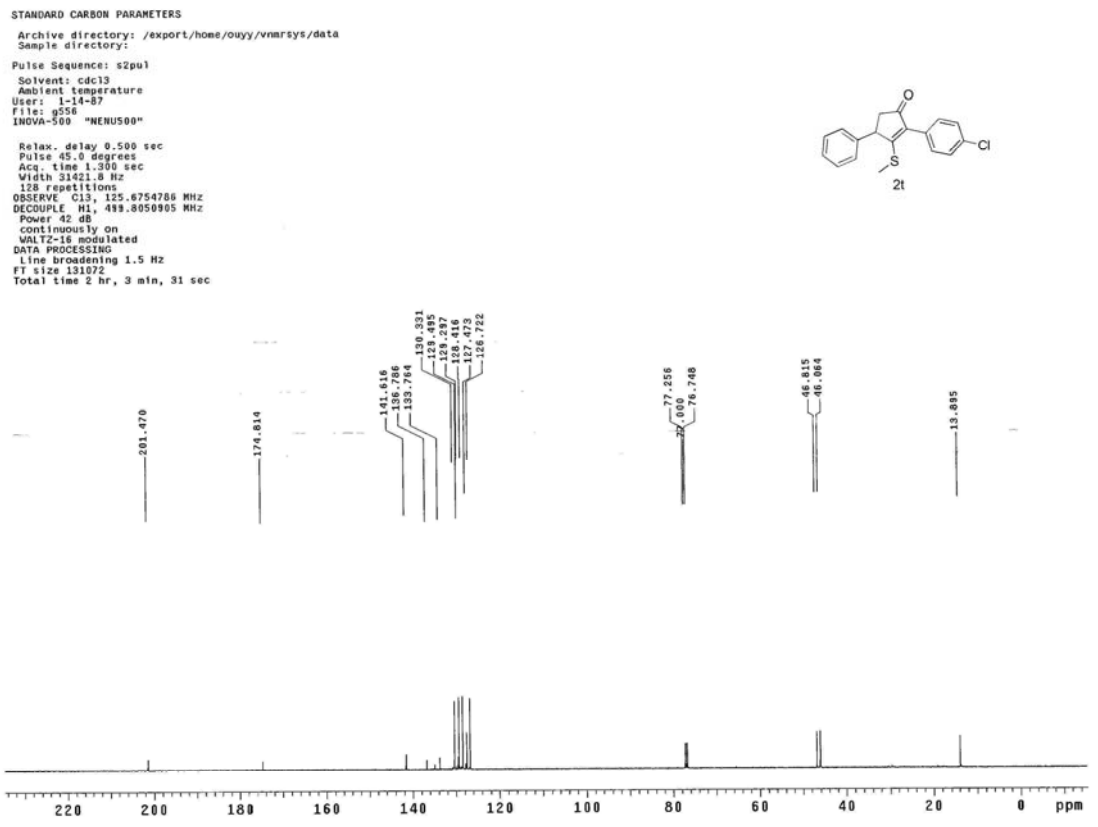

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: h368
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 9177.5 Hz
8 repetitions
OBSERVE H1, 499.8025912 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
2r
ppm

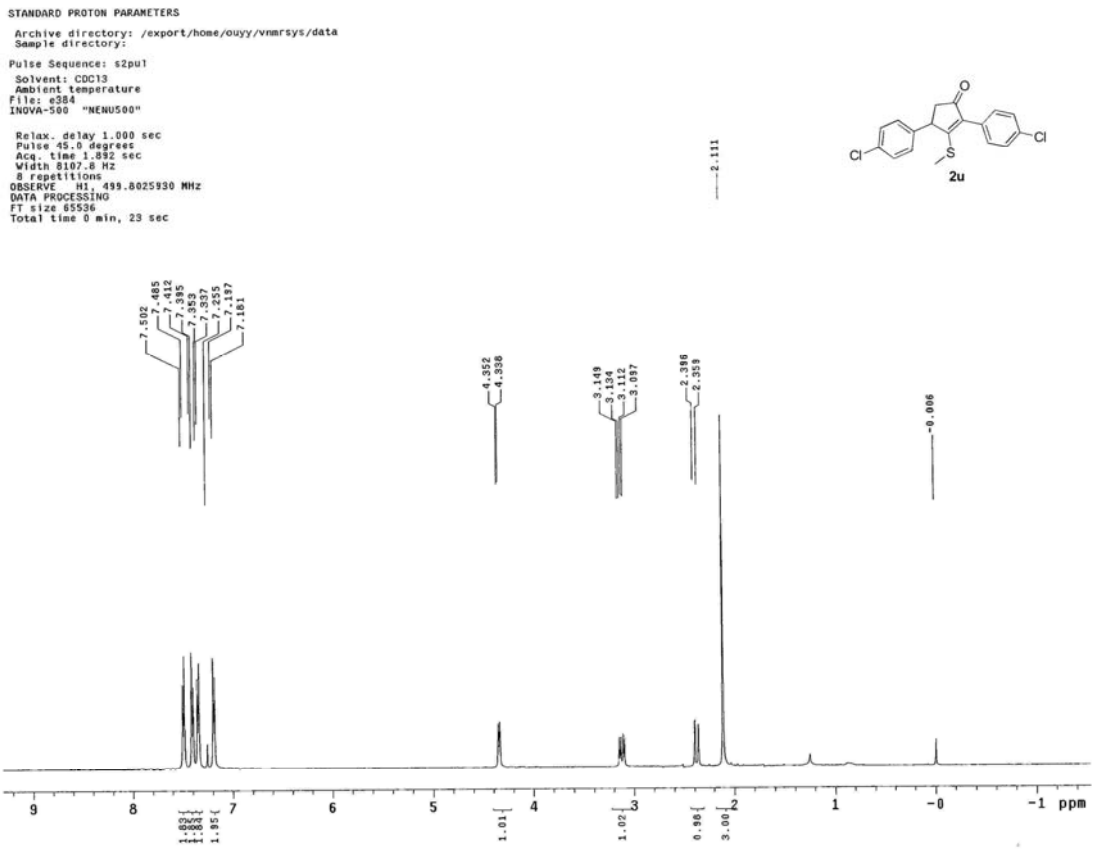

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: h376
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
128 repetitions
OBSERVE C13, 125.6754718 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously On
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec
2r
ppm

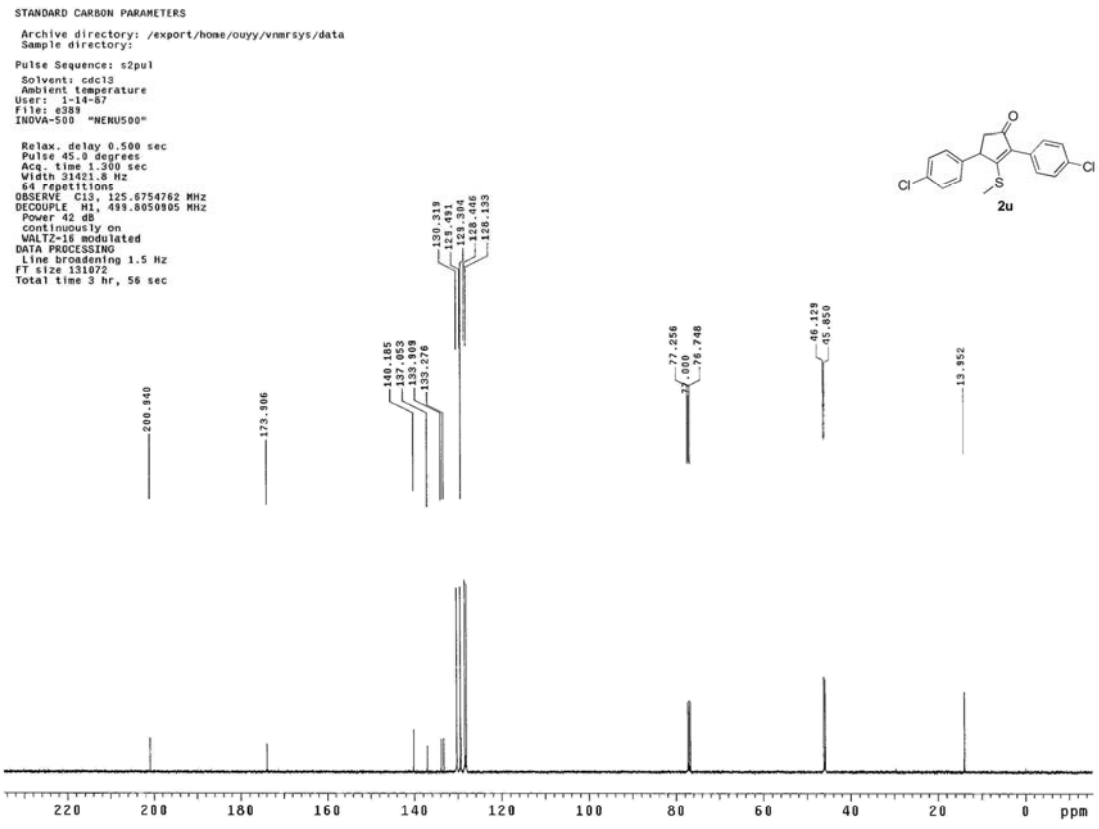

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: h459
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 9177.5 Hz
8 repetitions
OBSERVE H1, 499.8025912 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
2s
ppm

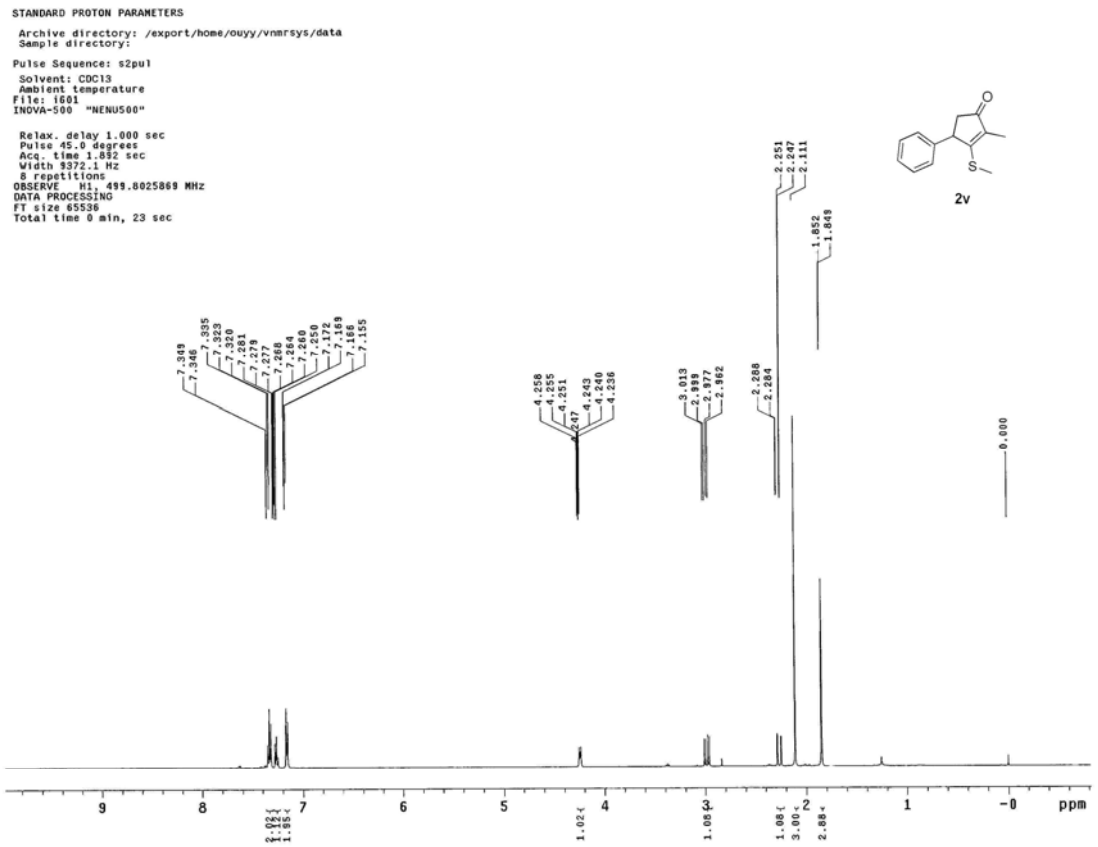

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: h489
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
192 repetitions
OBSERVE C13, 125.6754675 MHz
DECOUPLE H1, 499.8050805 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
2s
ppm

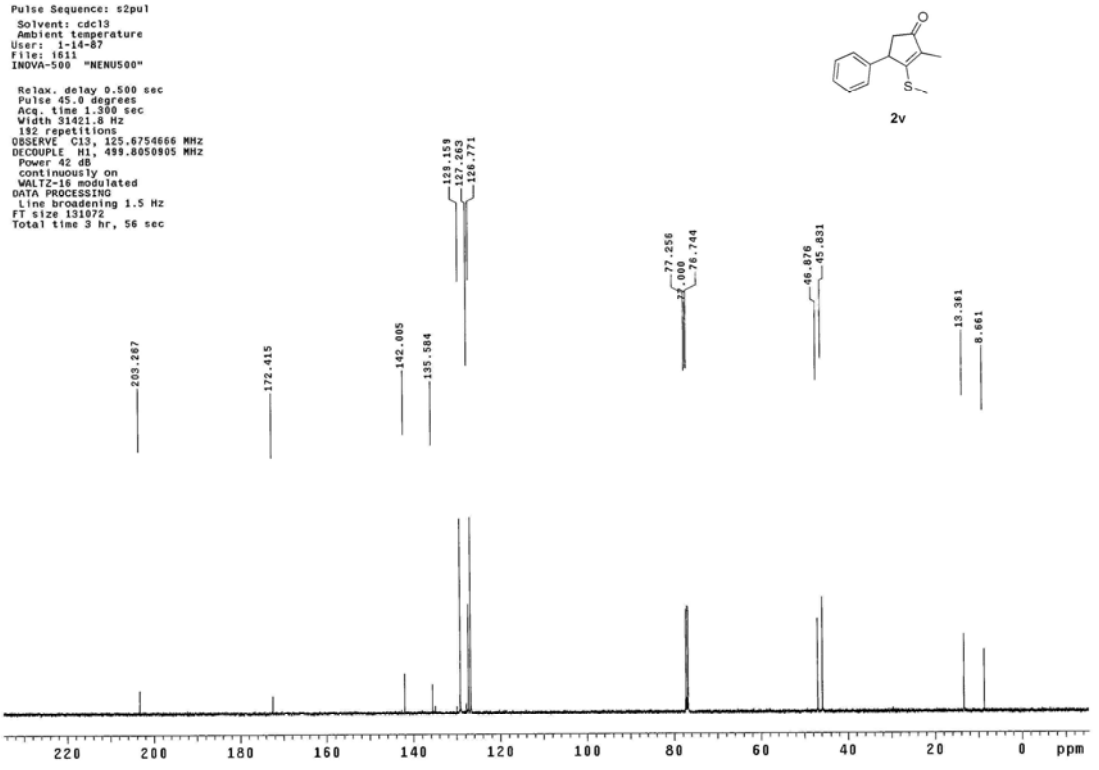

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: g550
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 9201.7 Hz
8 repetitions
OBSERVE H1, 499.8025958 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
2t
ppm

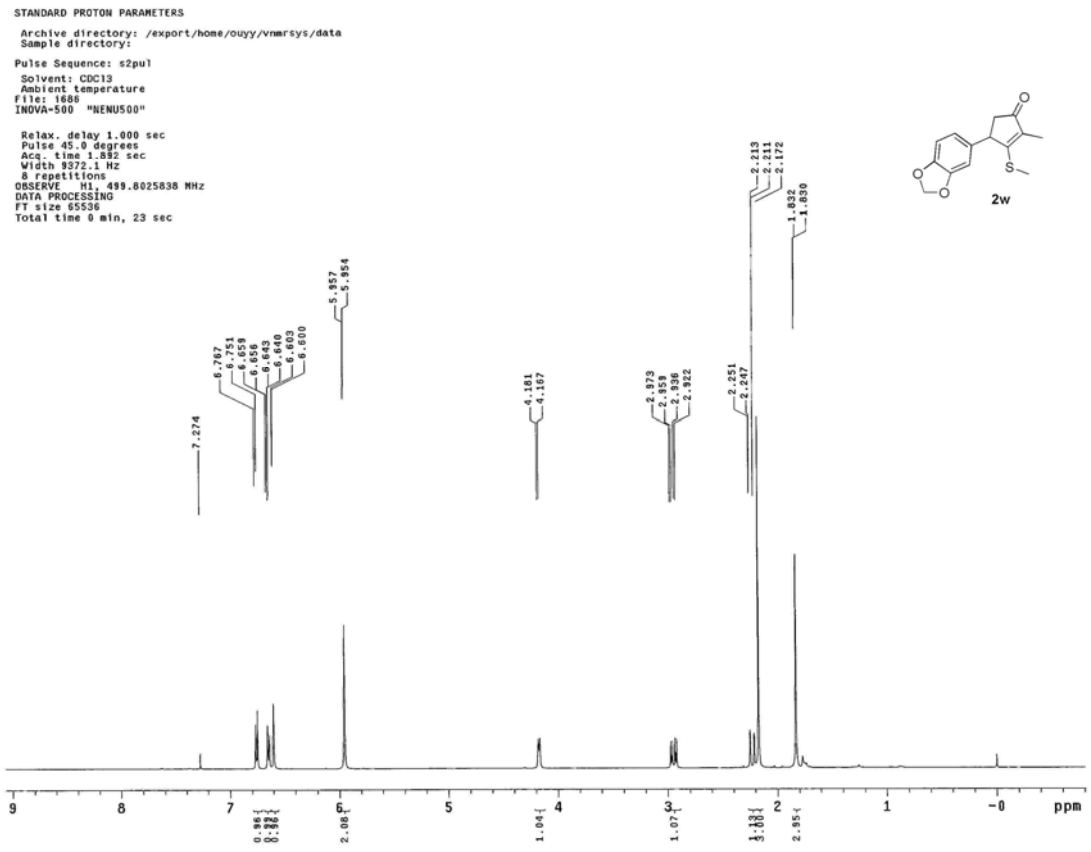

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: g556
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
128 repetitions
OBSERVE C13, 125.6754786 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec
2t
ppm

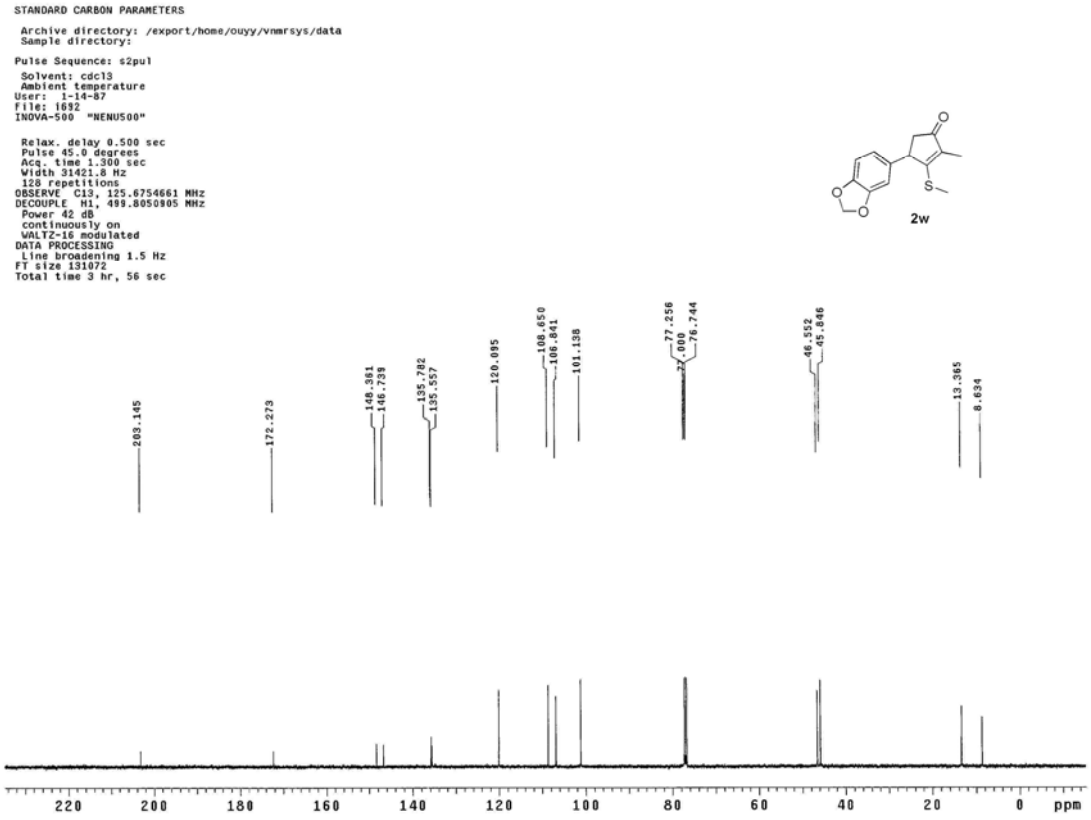

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: e384
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8107.8 Hz
8 repetitions
OBSERVE H1, 499.8025930 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
2u
7.502
7.485
7.412
7.395
7.359
7.337
7.255
7.237
7.161
4.352
4.338
3.149
3.134
3.112
3.097
2.386
2.359
2.111
0.006
1.03
1.00
1.00
1.95
1.01
1.02
0.98
3.00
9
8
7
6
5
4
3
2
1
-0
-1 ppm

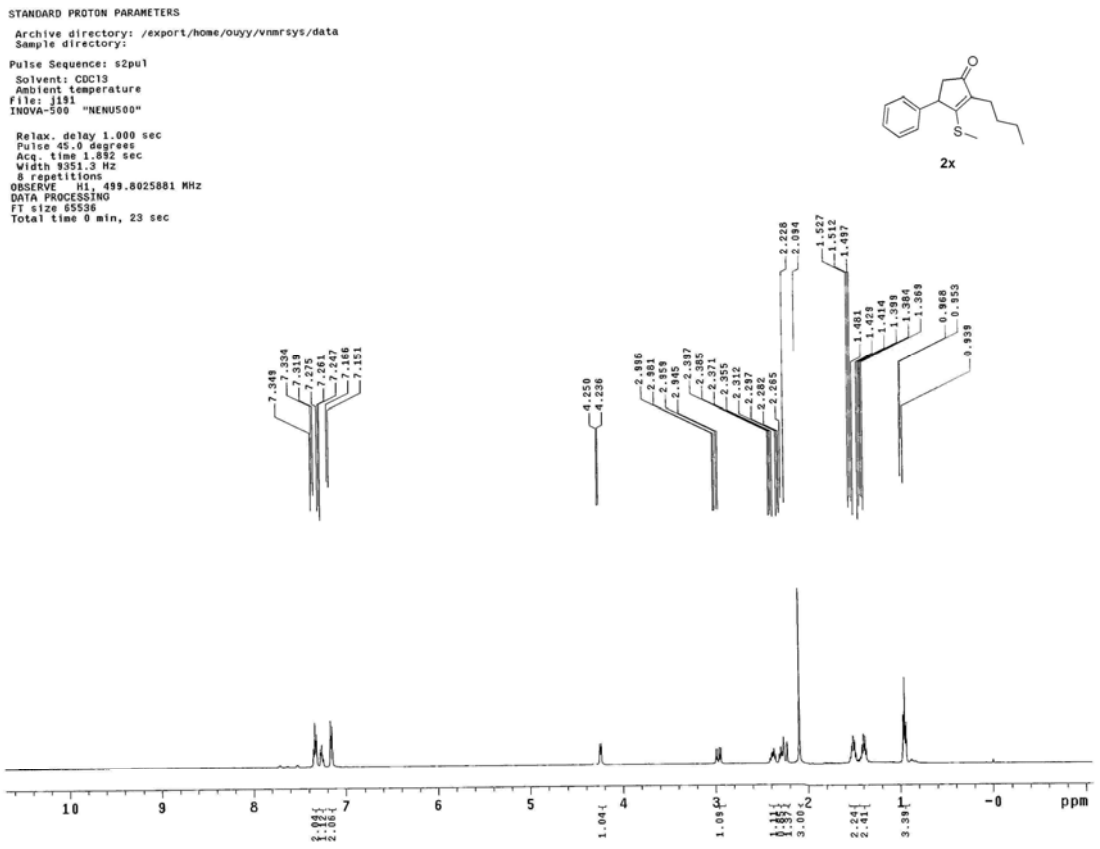

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: e389
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
64 repetitions
OBSERVE C13, 125.6754762 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
2u
200.340
173.906
140.185
137.053
133.908
133.276
130.319
129.491
129.304
128.446
128.133
77.256
77.000
76.748
46.129
45.850
13.952
220
200
180
160
140
120
100
80
60
40
20
0 ppm

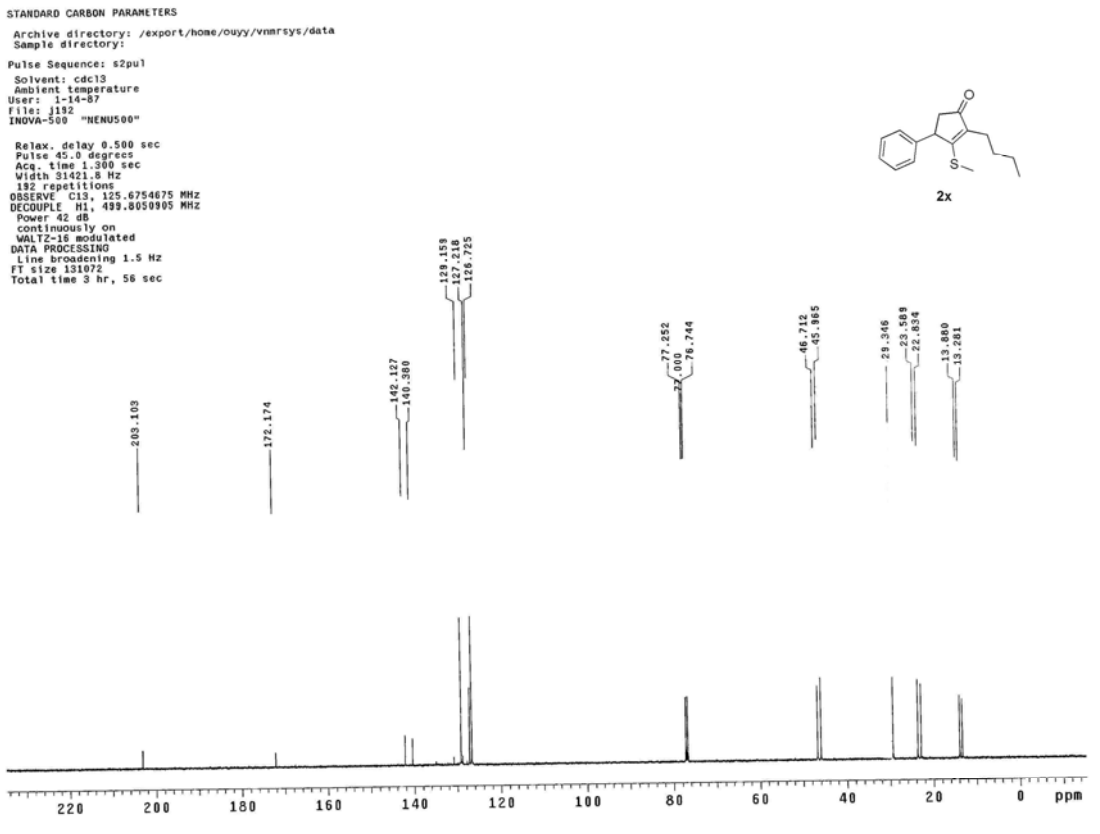

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: i601
INOVA-500 "NENUS00"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.852 sec
Width 9372.1 Hz
8 repetitions
OBSERVE H1, 499.8025869 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
2v
ppm

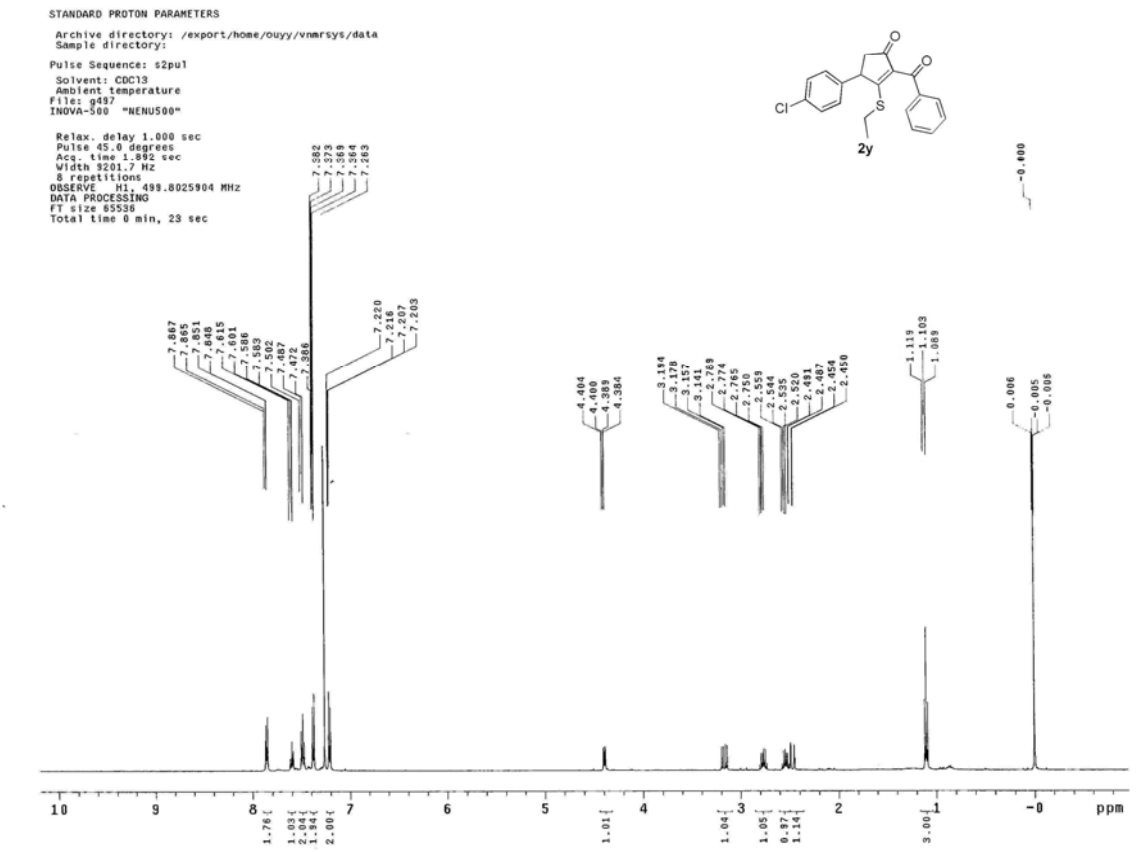

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: i611
INOVA-500 "NENUS00"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
192 repetitions
OBSERVE C13, 125.6754666 MHz
DECOUPLE H1, 499.8050805 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
2v
ppm

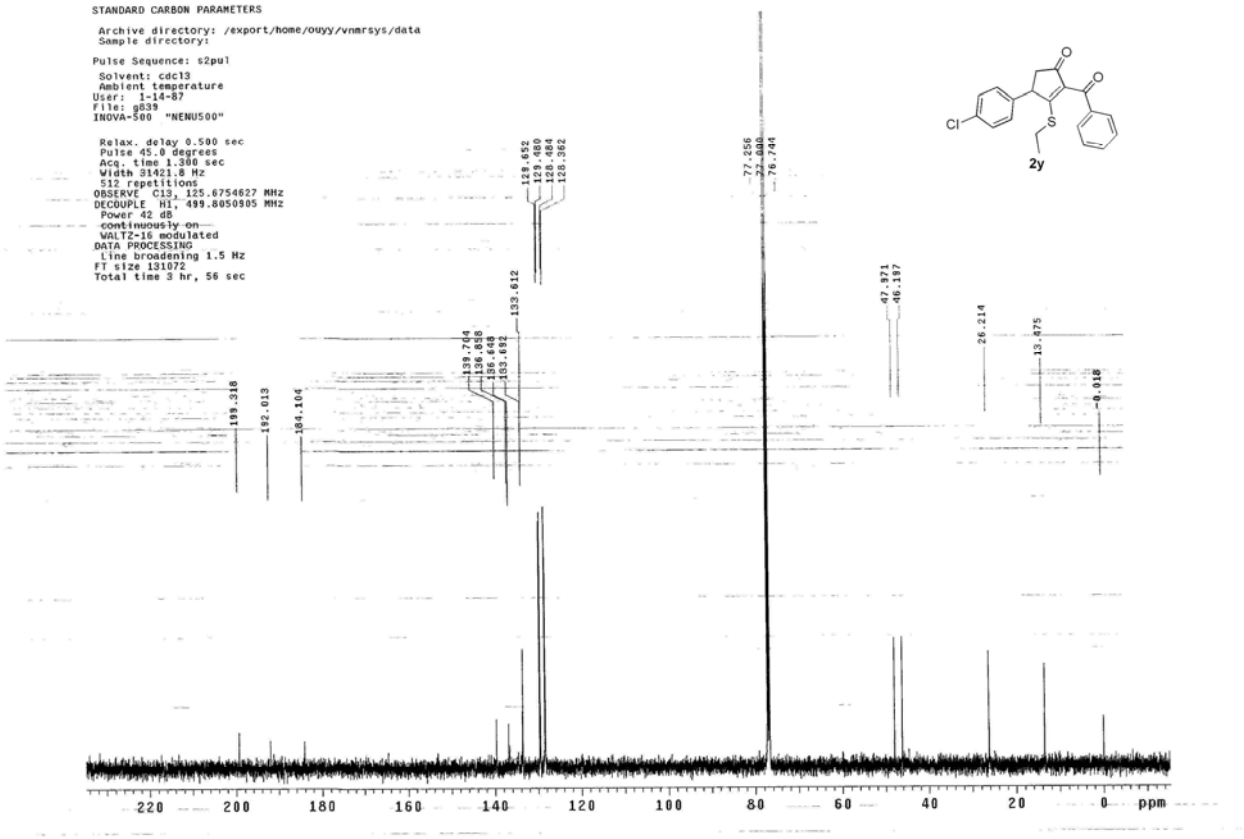

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: 1686
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.882 sec
Width 9372.1 Hz
8 repetitions
OBSERVE H1, 499.8025838 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
2w
7.274
6.787
6.751
6.659
6.656
6.643
6.640
6.603
6.600
5.957
5.954
4.181
4.167
2.973
2.959
2.936
2.922
2.251
2.247
2.213
2.211
2.172
1.832
1.830
ppm

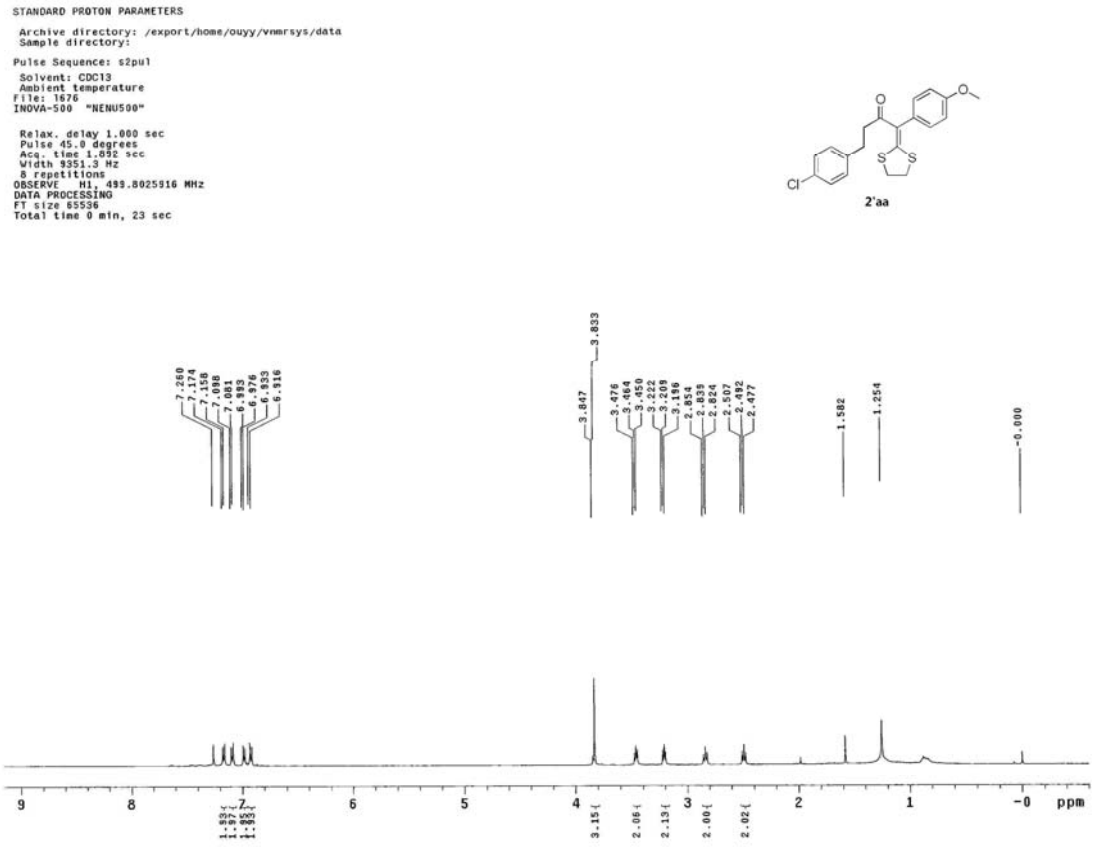

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: 1692
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
128 repetitions
OBSERVE C13, 125.6754661 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
2w
203.145
172.273
148.381
146.739
135.782
135.557
120.095
108.650
108.641
101.138
77.256
77.000
76.744
48.552
45.048
13.365
8.634
ppm

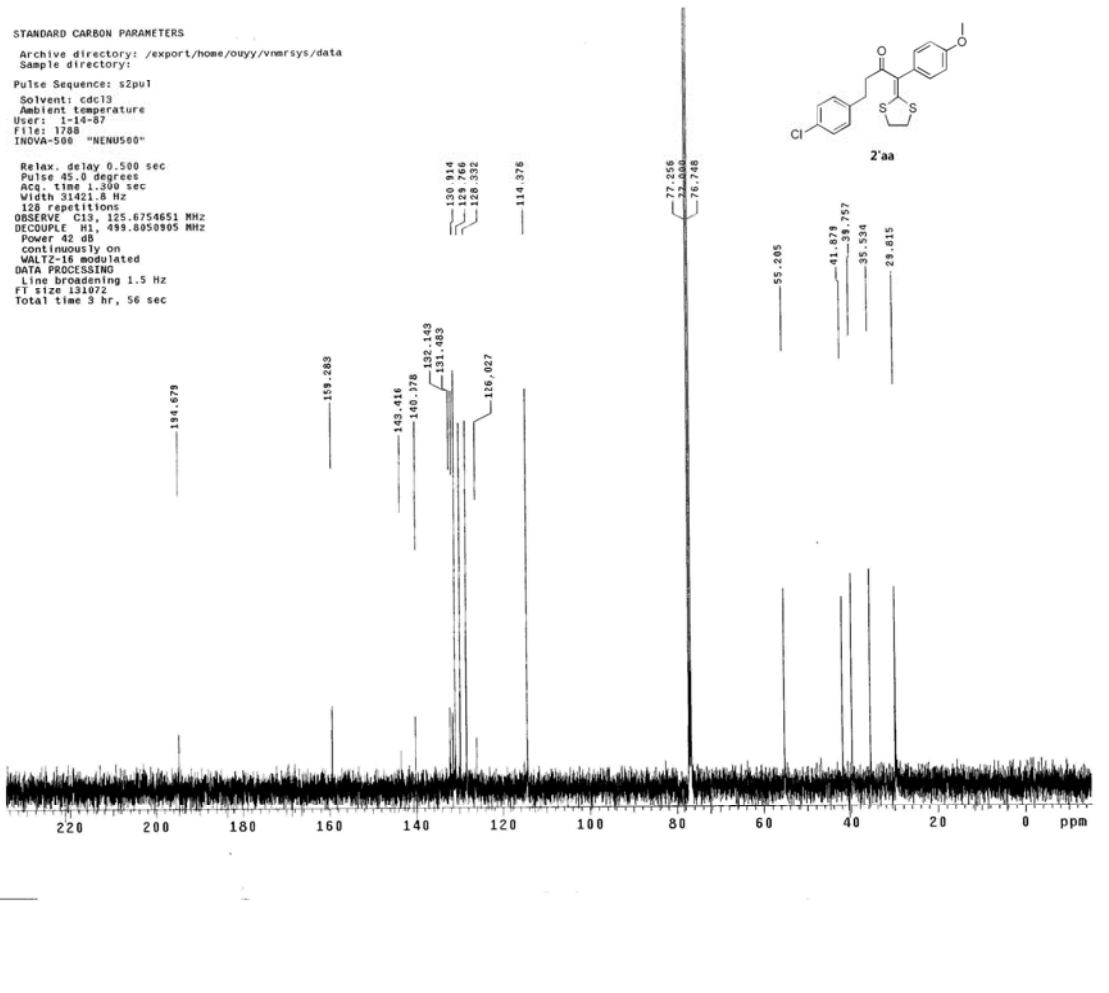

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: jl91
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 9351.3 Hz
8 repetitions
OBSERVE H1, 499.8025881 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
2x
ppm

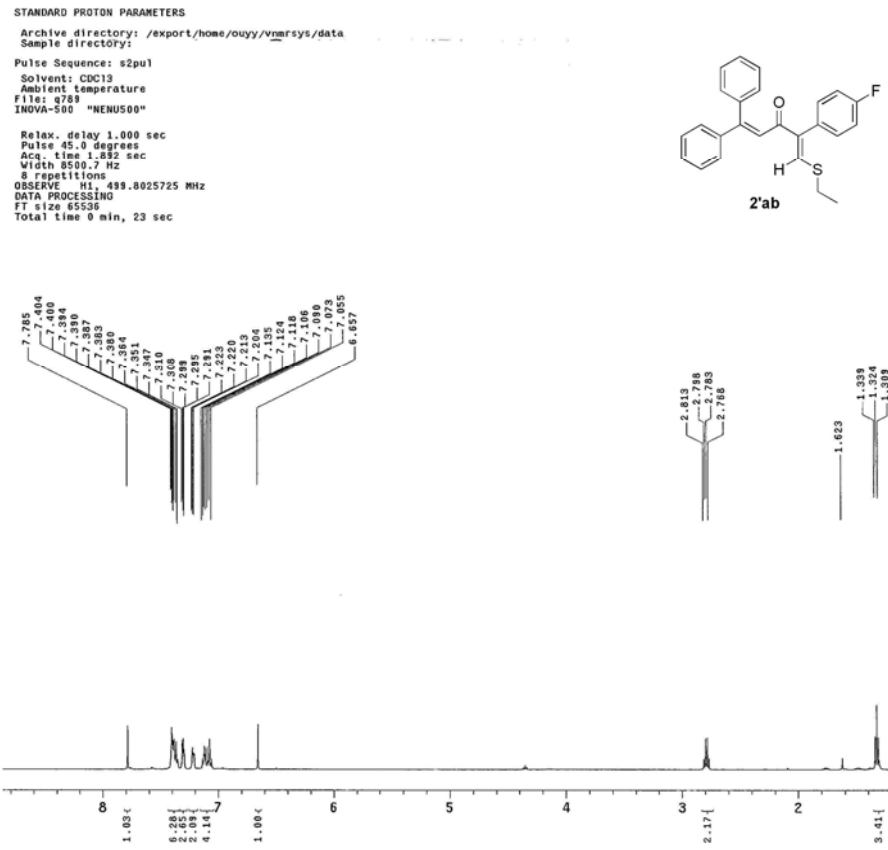

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: jl92
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
192 repetitions
OBSERVE C13, 125.6754675 MHz
DECOUPLE H1, 499.8059905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
2x
ppm

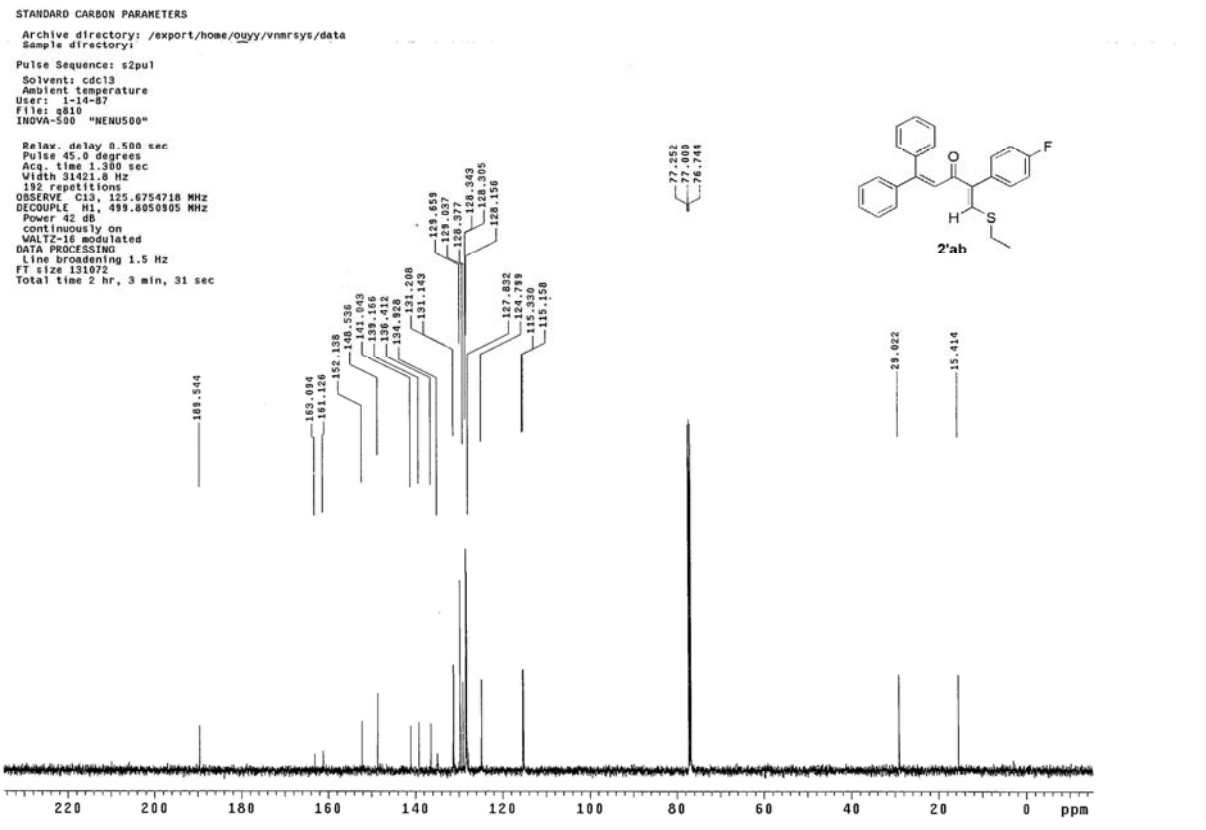

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: g497
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 9201.7 Hz
8 repetitions
OBSERVE H1, 499.8025904 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
2y
ppm

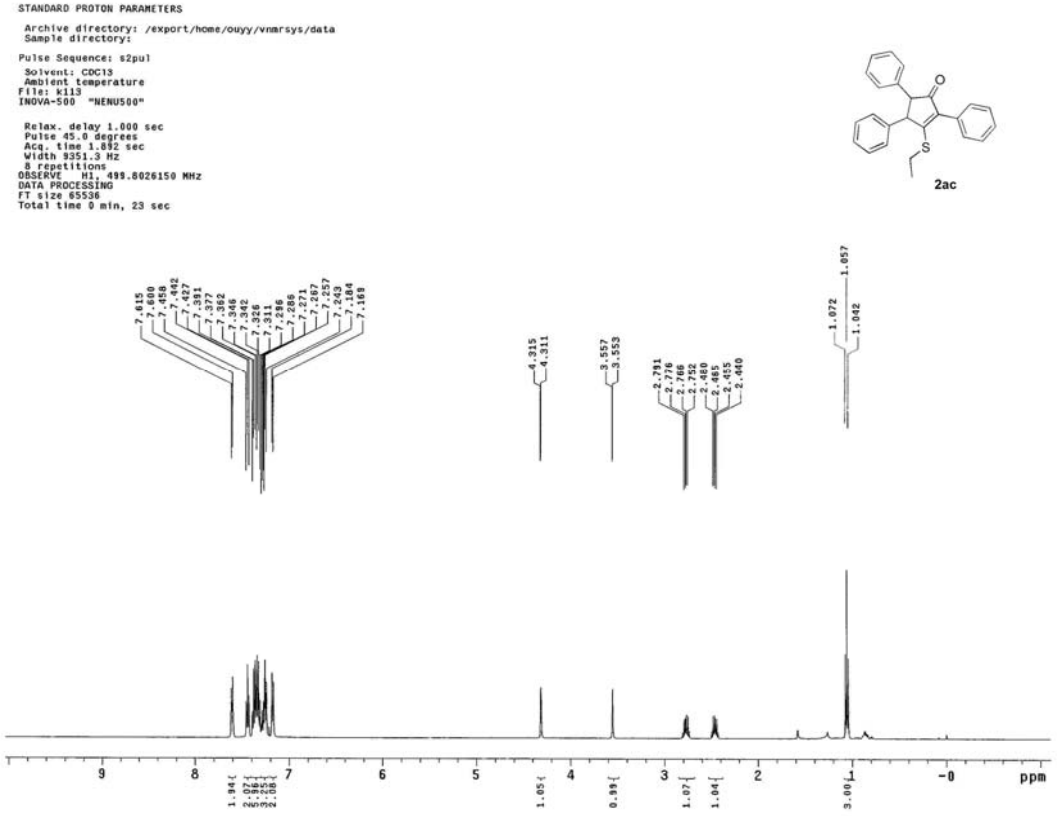

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: g839
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
512 repetitions
OBSERVE C13, 125.6754627 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
2y
ppm

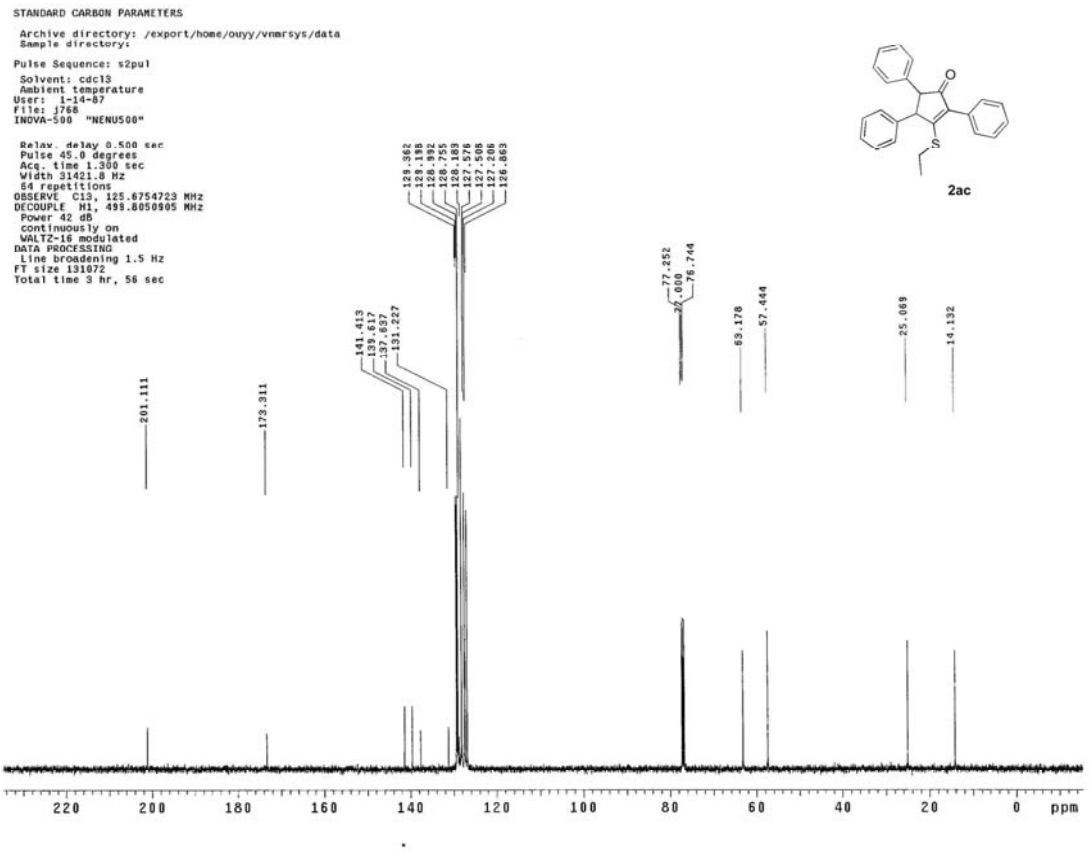

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: 1676
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.852 sec
Width 9351.3 Hz
8 repetitions
OBSERVE H1, 499.8025916 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
2'aa
7.260
7.174
7.158
7.098
7.081
6.993
6.976
6.953
6.916
3.833
3.847
3.476
3.464
3.450
3.222
3.209
3.196
2.854
2.839
2.824
2.807
2.492
2.477
1.582
1.254
-0.000
ppm

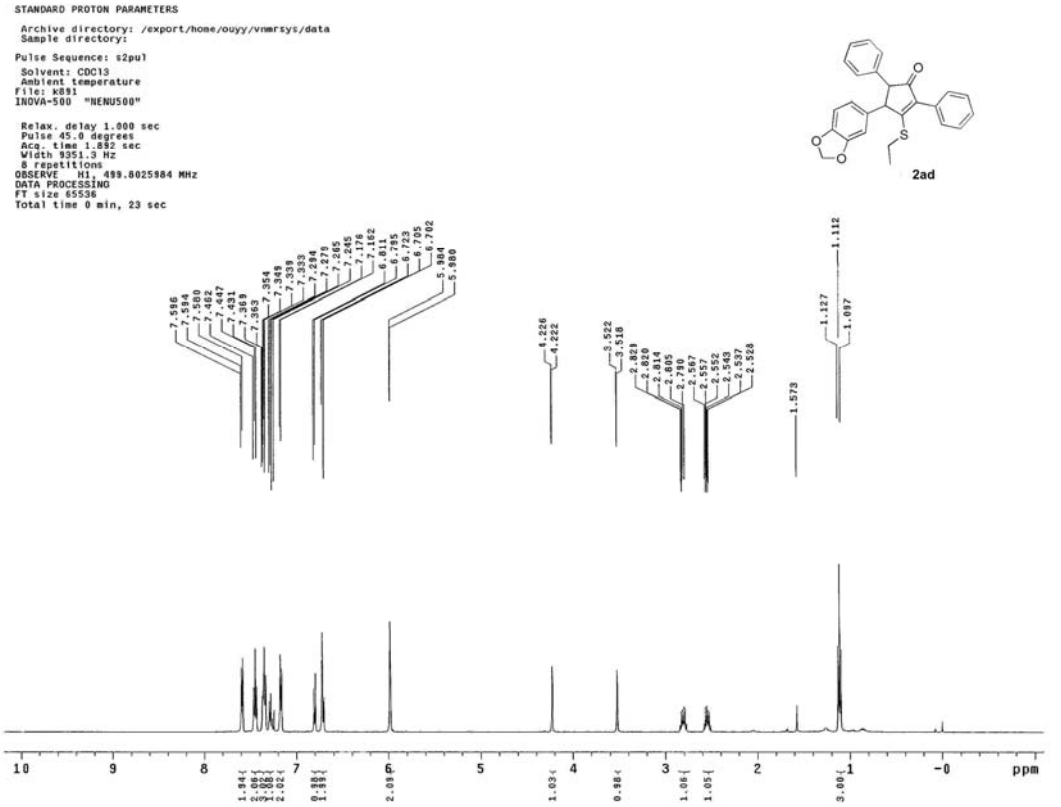

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: 1788
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
128 repetitions
OBSERVE C13, 125.6754651 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
2'aa
194.679
159.283
143.416
140.378
132.143
131.483
130.914
129.766
128.332
126.027
114.376
77.256
77.000
76.748
55.205
41.879
39.757
35.534
29.815
ppm

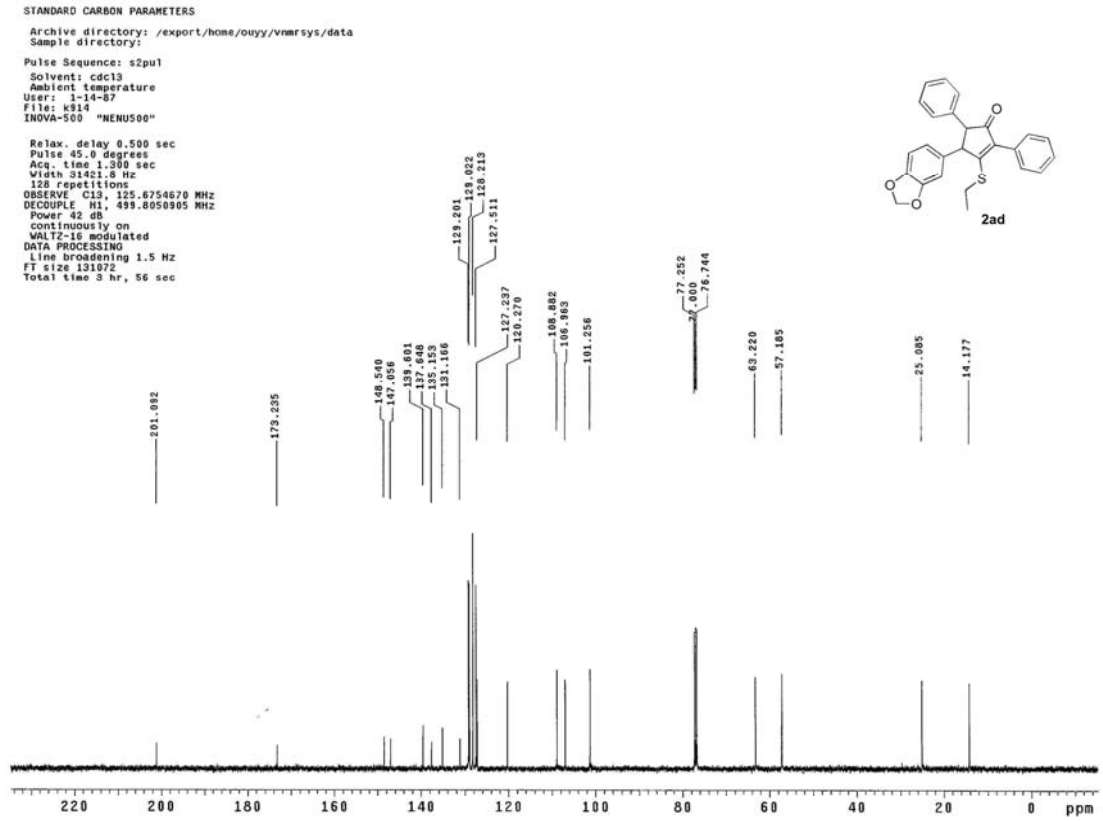

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: q789
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8500.7 Hz
8 repetitions
OBSERVE H1, 499.8025725 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
2'ab
ppm

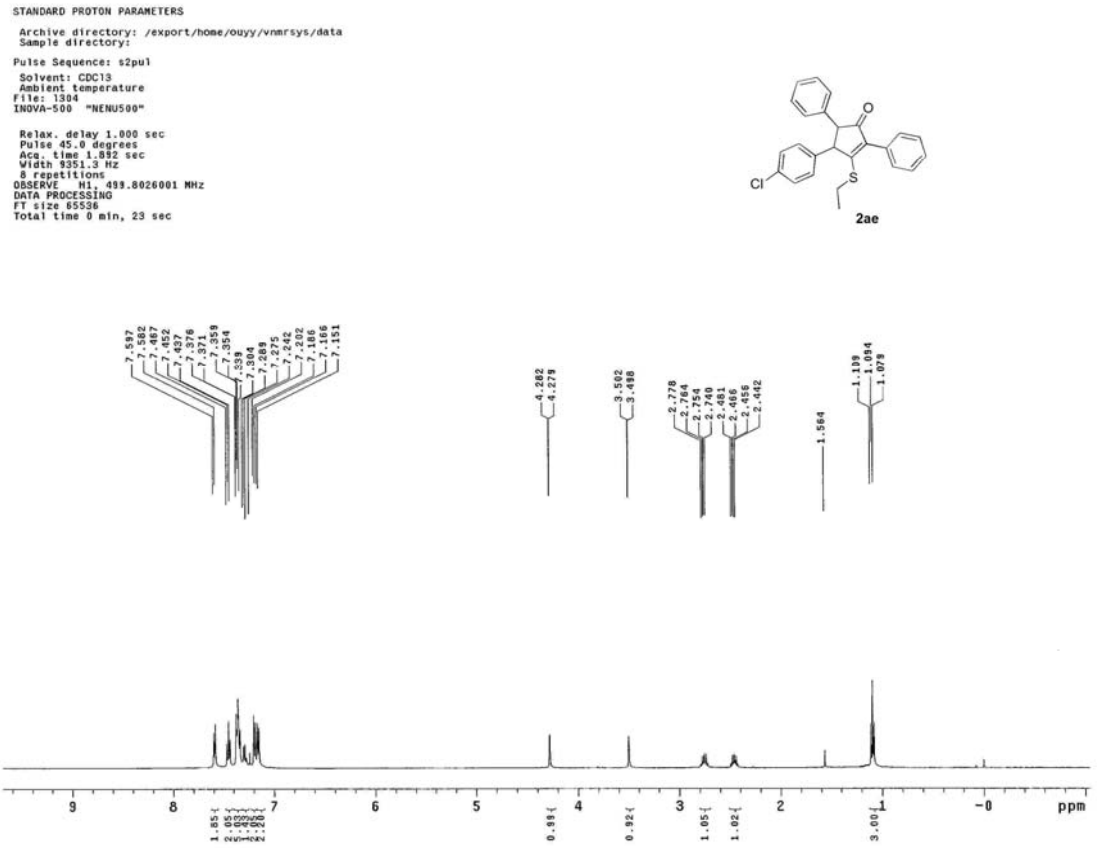

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: q810
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
192 repetitions
OBSERVE C13, 125.6754718 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec
2'ab
ppm

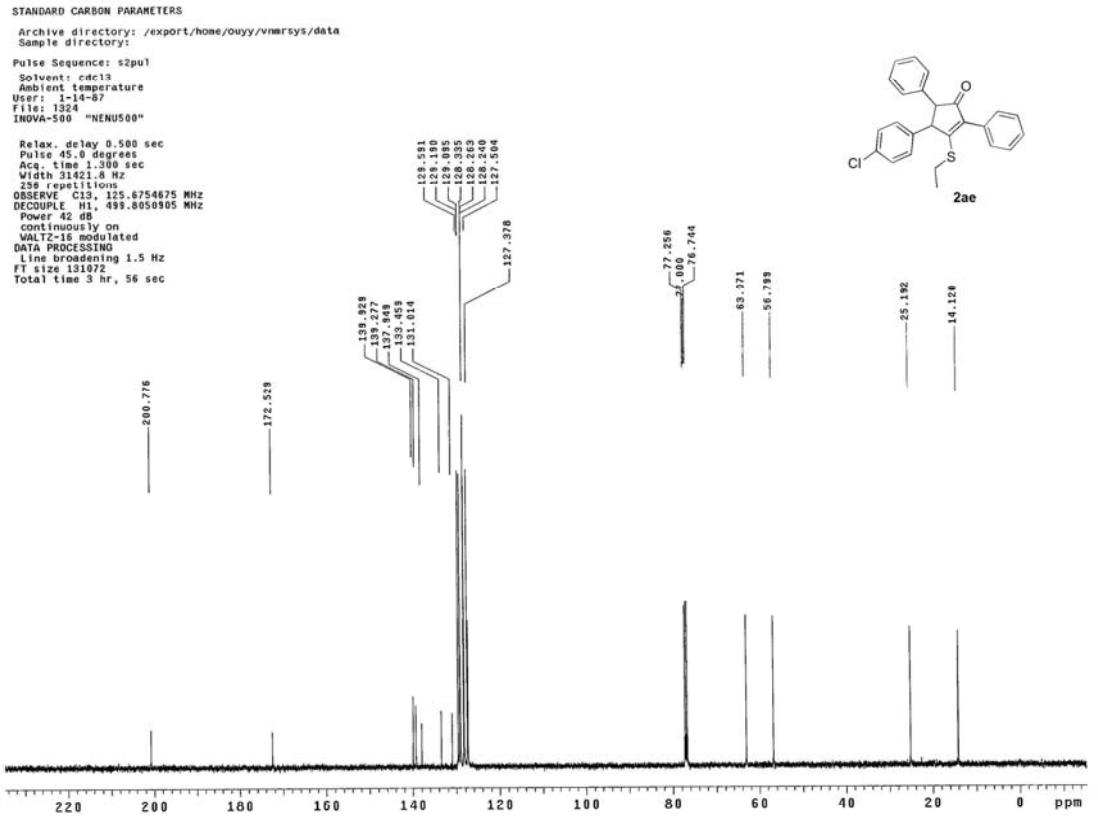

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: k113
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 9351.3 Hz
8 repetitions
OBSERVE H1, 499.8026150 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
2ac
ppm


STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: 1768
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
64 repetitions
OBSERVE C13, 125.6754723 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
2ac
ppm


STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: k881
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 9351.3 Hz
8 repetitions
OBSERVE H1, 499.8025984 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
2ad
ppm


STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: k914
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
128 repetitions
OBSERVE C13, 125.6754670 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
2ad
ppm


STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: 1304
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 9351.3 Hz
8 repetitions
OBSERVE H1, 499.8026001 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
2ae
7.597
7.582
7.467
7.452
7.437
7.376
7.371
7.359
7.354
7.339
7.304
7.269
7.275
7.242
7.202
7.166
7.151
4.282
4.279
3.502
3.498
2.778
2.764
2.754
2.740
2.481
2.466
2.455
2.442
1.564
1.109
1.094
1.079
9
8
7
6
5
4
3
2
1
0
ppm


STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: 1324
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
256 repetitions
OBSERVE C13, 125.6754675 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
2ae
129.591
129.180
129.095
128.335
128.263
128.240
127.504
127.378
77.256
77.000
76.744
63.071
56.789
25.182
14.124
200.776
172.529
139.928
139.277
137.849
133.459
131.614
220
200
180
160
140
120
100
80
60
40
20
0
ppm