Supporting Information

Gold-Catalyzed Nitrene Transfer to Activated Alkynes: Formation of α, β-Unsaturated Amidines

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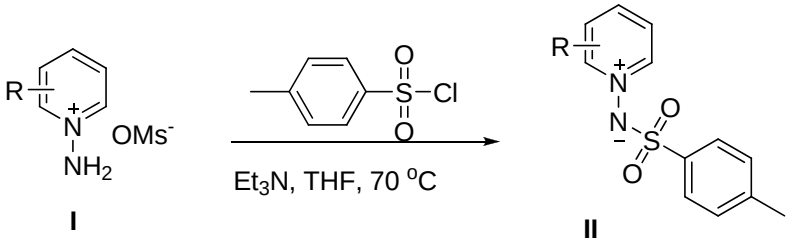
General Ethyl acetate (ACS grade), hexanes (ACS grade), diethyl ether (ACS grade) and anhydrous 1, 2-dichloroethane (HPLC grade) were purchased from Fisher Scientific and used without further purification. Methylene chloride and tetrahydrofuran were purified using MBraun Solvent Purifier. Commercially available reagents were used without further purification. Reactions were monitored by thin layer chromatography (TLC) using Sorbent Technologies' pre-coated silica gel plates. Flash column chromatography was performed over Sorbent Technologies' silica gel (230-400 mesh). ^{1}H NMR and ^{13}C NMR spectra were recorded on a Varian 500 MHz Unity plus spectrometer and a Varian 400 MHz spectrometer using residue solvent peaks as internal standards. Infrared spectra were recorded with a Perkin Elmer FT-IR spectrum 2000 spectrometer and are reported in reciprocal centimeter (cm^{-1}). Mass spectra were recorded with Micromass QTOF2 Quadrupole/Time-of-Flight Tandem mass spectrometer using electron spray ionization.

General procedure A : preparation of oxidants



Compound **I** were prepared according to the literature procedure.[1] Iminopyridinium ylide **II** were prepared from **I** according to the following procedure: to an ice-cold solution of **I** (2 mmol) and Et_3N (4 mmol) in anhydrous tetrahydrofuran (15 ml) was added 4-methylbenzenesulfonyl chloride (3 mmol). The reaction was allowed to reflux for 24 h at 70 °C. After cooling to room temperature, the reaction mixture was concentrated under *vacuum*. The residue was purified via silica gel flash chromatography to afford the desired product.

[1] Yoon, K.; Kode, B.; Bowen, L.; Redda, K. K. *J. Heterocyclic Chem.* **2001**, *38*, 69-76.

General procedure B: preparation of alkynes

The *N*-alkynyloxazolidinones were prepared according to the literature procedure[2] as follows: to a mixture of a 2-oxazolidinone (2.0 equiv), K_3PO_4 (2.0 equiv), $CuSO_4 \cdot 5H_2O$ (0.1 equiv), and 1,10-phenanthroline (0.2 equiv) in a round flask was added a solution of 1-bromoalkyne (1.0 equiv, 1 M) in DMF/toluene (1/10). The reaction mixture was heated to 100 °C for 24 h while being monitored with TLC analysis. Upon completion, the reaction mixture was cooled to room temperature, diluted with EtOAc, and filtered through Celite, and the filtrate was concentrated under *vacuum*. The crude products were purified by silica gel flash column chromatography to afford the desired alkyne products.

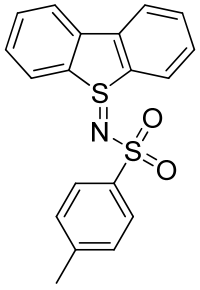
General procedure C: Gold-catalyzed synthesis α, β-unsaturated amidines

An oven-dried vial was charged with an alkyne (0.2 mmol) and (3,5-dichloropyridinium-1-yl)tosylamide (0.24 mmol, 1.2 equiv). DCE (4 ml) and $IPrAuNTf_2$ (8.6 mg, 5 mol %) were added. The reaction mixture was stirred at the indicated temperature until the substrate was completely consumed. The reaction mixture was concentrated under *vacuum*. The residue was purified via silica gel flash chromatography to give the amidine product.

Dibenzothiophene, 5,5-dihydro-5-[[(4-methylphenyl)sulfonyl]imino][3]

[2] Zhang, X.; Zhang, Y.; Huang, J.; Hsung, R. P.; Kurtz, K. C. M.; Oppenheimer, J.; Petersen, M.; E.; Sagamanova, I. K.; Shen, L.; Tracey, M. R. *J. Org. Chem.* **2006**, *71*, 4170.

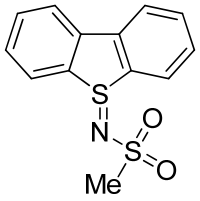
[3] Morita, H.; Tatami, A.; Maeda, T.; Kim, B. J.; Kawashima, W.; Yoshimura, T.; Abe, H.; Akasaka, T. *J. Org. Chem.* **2008**, *73*, 7159.



1

Compound **1** was prepared in 60 % yield according to the following procedure (eluents: ethyl acetate: hexanes = 10: 1): an oven-dried round flask was charged with a toluenesulfonamide (1.0 mmol), diacetoxyiodobenzene (1.3 mmol, 1.3 equiv), dibenzothiophene (1.3 mmol, 1.3 equiv), MgO (4.0 mmol, 4.0 equiv), DCM (10 ml) and $Rh_2(OAc)_4$ (8.82 mg, 2 mol %) was added. The reaction mixture was stirred at the room temperature while being monitored with TLC analysis. After 20 h, the reaction mixture was concentrated under *vacuum*. The residue was purified via silica gel flash chromatography to give desired the product. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (d, 2H, *J* = 8.0 Hz), 7.82 (d, 2H, *J* = 8.0 Hz), 7.61 -7.66 (m, 4H), 7.42 -7.47 (m, 2H), 7.25 (d, 2H, *J* = 8.0 Hz), 2.43 (s, 3H),); ^{13}C NMR (125 MHz, $CDCl_3$) δ 142.0, 141.3, 137.4, 137.2, 132.9, 130.0, 129.3, 127.5, 126.6, 122.4, 21.6; IR (neat): 3448, 1446, 1298, 1284, 1085, 939; MS (ES^+) Calculated for $[C_{19}H_{15}NO_2S_2Na]^+$: 376.04; Found: 376.04

Dibenzothiophene, 5,5-dihydro-5-[(methanesulfonyl)imino][4]



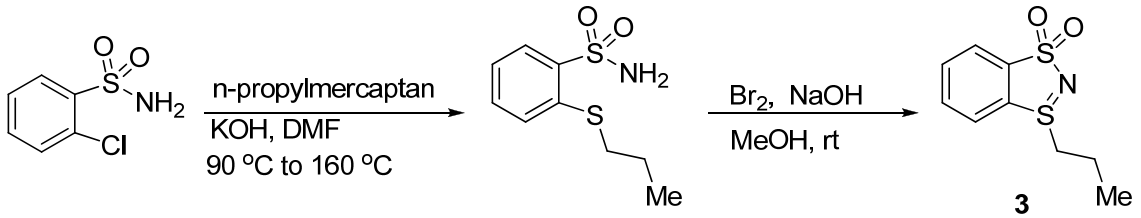
2

Compound **2** was prepared in 58 % yield according to the same procedure to compound **1.** (eluents: ethyl acetate: hexanes = 1: 1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, 2H, *J* =

[4] Desikan, V.; Liu, Y.; Toscano, J. P.; Jenks, W. S. *J. Org. Chem.* **2008**, *73*, 4398.

8.0 Hz), 7.92 (d, 2H, *J* = 8.0 Hz), 7.70 (td, 2H, *J* = 7.2, 1.2 Hz), 7.59 (td, 2H, *J* = 7.6, 1.2 Hz), 3.07 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 138.0, 137.2, 133.1, 130.1, 127.4, 122.6, 43.2; IR (neat): 3733, 3079, 1540, 1282, 1122, 968; MS (ES^+) Calculated for $[C_{13}H_{11}NO_2S_2Na]^+$: 300.01; Found: 300.04

1-Propyl-1λ^4-benzo[1,3,2]dithiazole 3,3-dioxide

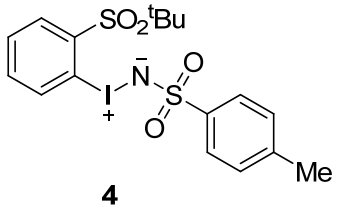


Compound **3** was prepared in 60 % yield from 2-chloro-benzenesulfonamide according to the following procedure: to a solution of potassium hydroxide (85%, 1.2 g, 20 mmol) and n-propylmercaptan (1.81 ml, 20 mmol) in 10 ml DMF at 90°C was added a solution of 2-chlorobenzenesulfonamide (1.91 g, 10 mmol) in 10 ml DMF. The reaction mixture was heated to reflux for 5 h, cooled, and the solvent was removed under *vacuum*. The residue was neutralized to pH = 7.0 by using 2 N hydrochloric acid and extracted with ether. The ether extracts were combined, washed with water and brine, dried with $MgSO_4$ and concentrated under *vacuum*. The resulting residue was purified via silica gel flash chromatography (eluents: ethyl acetate: hexane = 1: 1) to give 2-propylsulfanylbenzenesulfonamide (1.62 g, 70% yield).

To a solution of the above sulfide (2 mmol, 462 mg) in MeOH/H_2O (10 mL/2mL) was add Br_2 (3 mmol, 0.54 mL) and NaOH (4 mmol, 160 mg). The reaction mixture was stirred at room temperature for 30 min, and the solvent was removed under *vacuum*. The ether extracts were washed with water and brine, dried with $MgSO_4$ and concentrated. The resulting residue was purified via silica gel flash chromatography (eluents: ethyl acetate: hexane = 2: 1) to give the desired cyclic sulfilimine **3** (0.412 g, 90% yield). ^{1}H

NMR (500 MHz, $CDCl_3$) δ 8.04 (d, 1H, *J* = 8.0 Hz), 7.79 (dd, 1H, *J* = 7.5, 7.5 Hz), 7.73 (dd, 1H, *J* = 7.0, 7.0 Hz), 7.70 (dd, 1H, *J* = 7.0, 7.0 Hz), 3.29 (dt, 1H, *J* = 13.0, 8.0 Hz), 3.00 (dt, 1H, *J* = 13.0, 8.0 Hz), 1.88 – 1.96 (m, 2H), 1.13 (t, 1H, *J* = 7.5 Hz); ^{13}C NMR (125 MHz, $CDCl_3$) δ 137.4, 133.6, 133.3, 132.4, 124.3, 123.7, 55.0, 18.0, 12.9; IR (neat): 3459, 1650, 1635, 1444, 1284, 1151,; MS (ES^+) Calculated for $[C_9H_{11}NO_2S_2Na]^+$: 252.01; Found: 252.04

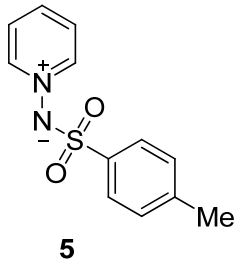
2-(*tert*-Butylsulfonyl)(*p*-toluenesulfonyliminoiodo)benzene



4

Compound **4** was prepared in 80 % yield according to the literature procedure.[5] ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35 (d, 1H, *J* = 8.4 Hz), 7.90 (dd, 1H, *J* = 7.6, 1.6 Hz), 7.86 (dd, 1H, *J* = 8.4, 1.6 Hz), 7.82 (d, 2H, *J* = 7.6 Hz), 7.71 (dd, 1H, *J* = 7.6, 7.6 Hz), 7.22 (d, 2H, *J* = 8.0 Hz), 2.39 (s, 3H), 1.45 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 142.0, 140.5, 136.1, 133.4, 131.9, 130.6, 129.3, 128.5, 126.7, 115.3, 63.5, 23.5, 21.5; IR (neat): 3367, 1648, 1299, 1162, 1137, 1089, 732; MS (ES^+) Calculated for $[C_{17}H_{20}NIO_4S_2Na]^+$: 516.98; Found: 516.02

1-(*p*-toluenesulfonylimino)pyridinium ylide[6]



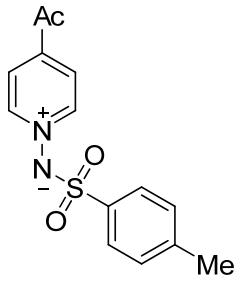
5

Compound **5** was prepared in 72 % yield according to the general procedure A (eluents: ethyl acetate: methanol = 20: 1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46 (d, 2H, *J* = 7.6 Hz),

[5] Macikenas, D.; Skrzypczak-Jankun, E.; Protasiewicz, J. D. *J. Am. Chem. Soc.* **1999**, *121*, 7164.
[6] Jiang, Y.; Zhou, G. C.; He, G. L.; He, L.; Li, J. L.; Zheng, S. L. Synthesis, **2007**, *10*, 1459.

7.97 (dd, 1H, *J* = 7.6, 7.6 Hz), 7.61 (d, 2H, *J* = 8.4 Hz), 7.57 (d, 2H, *J* = 7.6 Hz), 7.17 (d, 2H, *J* = 8.4 Hz), 2.36 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 145.2, 141.6, 138.6, 138.2, 129.2, 127.0, 126.6, 21.4; IR (neat): 3419, 1650, 1635, 1465, 1272, 1133; MS (ES^+) Calculated for $[C_{12}H_{12}N_2O_2SNa]^+$: 271.05; Found: 271.08

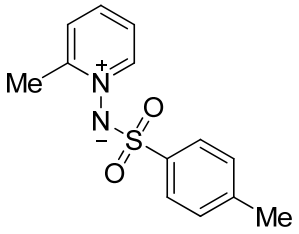
1-(*p*-toluenesulfonylimino)-4-acetylpyridinium ylide



6

Compound **6** was prepared in 75 % yield according to the general procedure A (eluents: ethyl acetate: methanol = 10: 1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.66 (d, 2H, *J* = 6.8 Hz), 7.95 (d, 2H, *J* = 6.8 Hz), 7.71 (d, 2H, *J* = 7.6 Hz), 7.21 (d, 2H, *J* = 7.6 Hz), 2.65 (s, 3H), 2.37 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 193.3, 142.6, 140.5, 138.3, 129.7, 127.4, 125.2, 121.7, 26.9, 21.7; IR (neat): 3120, 1697, 1436, 1157, 1128; MS (ES^+) Calculated for $[C_{14}H_{14}N_2O_3SNa]^+$: 313.06; Found: 313.09

1-(*p*-toluenesulfonylimino)-2-methylopyridinium ylide[6]

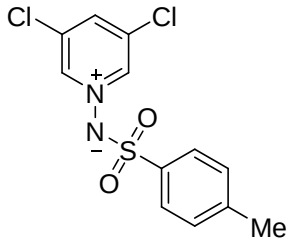


7

Compound **7** was prepared in 58 % yield according to the general procedure A (eluents: ethyl acetate: methanol = 10: 1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.62 (d, 1H, *J* = 6.0 Hz), 7.82 (td, 1H, *J* = 8.0, 1.2 Hz), 7.58 (d, 2H, *J* = 8.0 Hz), 7.48 (d, 1H, *J* = 8.0 Hz), 7.43 (dd, 1H, *J* = 7.6, 7.6 Hz), 7.17 (d, 2H, *J* = 8.0 Hz), 2.46 (s, 3H), 2.37 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 156.3, 146.6, 141.3, 140.7, 137.8, 129.3, 127.9, 126.5, 123.8, 21.4, 20.1;

IR (neat): 3419, 1492, 1459, 1276, 1137, 1087; MS (ES^+) Calculated for $[C_{13}H_{14}N_2O_2SNa]^+$: 285.07; Found: 285.06

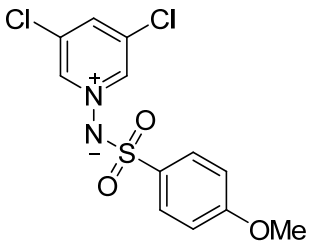
1-(*p*-toluenesulfonylimino)-3,5-dichloropyridinium ylide



8

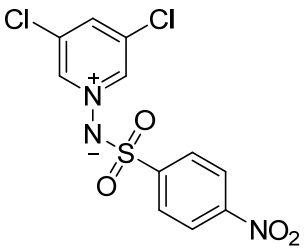
Compound **8** was prepared in 80 % yield according to the general procedure A (eluents: ethyl acetate: methanol = 20: 1). ^1H NMR (500 MHz, $CDCl_3$) δ 8.51 (s, 2H), 7.77 (s, 1H), 7.71 (d, 2H, *J* = 8.5 Hz), 7.24 (d, 2H, *J* = 8.5 Hz), 2.39 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 142.8, 139.6, 137.9, 135.7, 134.5, 129.8, 127.4, 21.8; IR (neat): 3419, 1650, 1635, 1556, 1294, 1132; MS (ES^+) Calculated for $[C_{12}H_{10}N_2O_2Cl_2SNa]^+$: 338.97; Found: 338.98

1-(4-methoxybenzenesulfonylimino)-3,5-dichloropyridinium ylide



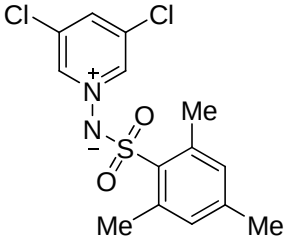
Compound was prepared in 75 % yield according to the general procedure A (eluents: ethyl acetate: methanole = 10: 1). ^1H NMR (500 MHz, $CDCl_3$) δ 8.51 (s, 2H), 7.78 (s, 1H), 7.76 (d, 2H, *J* = 8.0 Hz), 6.92 (d, 2H, *J* = 8.0 Hz), 3.84 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.6, 139.2, 135.4, 134.5, 132.5, 129.5, 114.3, 55.8; IR (neat): 3095, 1593, 1495, 1255; MS (ES^+) Calculated for $[C_{12}H_{10}N_2O_3Cl_2SNa]^+$: 354.97; Found: 354.96

1-(4-nitrobenzenesulfonylimino)-3,5-dichloropyridinium ylide



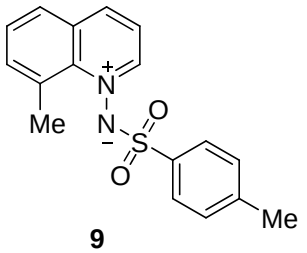
Compound was prepared in 78 % yield according to the general procedure A (eluents: ethyl acetate: methanol = 10: 1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.49 (s, 2H), 8.29 (d, 2H, *J* = 9.0 Hz), 7.97 (d, 2H, *J* = 9.0 Hz), 7.95 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 147.3, 144.2, 140.8, 137.6, 134.8, 128.1, 128.0, 124.2; IR (neat): 3099, 2981, 1920, 1556, 1527, 1348, 1139; MS (ES^+) Calculated for $[C_{11}H_7N_3O_4Cl_2SNa]^+$: 369.94; Found: 369.95

1-(2,4,6-trimethylbenzenesulfonylimino)-3,5-dichloropyridinium ylide



Compound was prepared in 60 % yield according to the general procedure A (eluents: ethyl acetate). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.37 (s, 2H), 7.68 (s, 1H), 6.92 (s, 2H), 2.64 (s, 6H), 2.27 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 144.2, 139.0, 137.8, 134.2, 133.8, 133.7, 131.4, 22.7, 20.6; IR (neat): 2958, 1720, 1560, 1382, 1313, 1148; MS (ES^+) Calculated for $[C_{14}H_{14}N_2O_2Cl_2SNa]^+$: 367.01; Found: 366.95

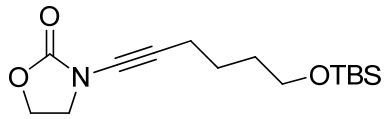
1-(*p*-toluenesulfonylimino)-8-methylquinolinium ylide



9

Compound **9** was prepared in 20 % yield according to the general procedure A (eluents: ethyl acetate: methanol = 10: 1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.77 (dd, 1H, *J* = 6.0, 1.6 Hz), 8.41 (dd, 1H, *J* = 8.0, 1.6 Hz), 7.79 – 7.82 (m, 1H), 7.56 – 7.61 (m, 2H), 7.48 (dd, 1H, *J* = 8.4, 6.0 Hz), 7.40 (d, *J* = 8.4 Hz), 7.05 (d, *J* = 8.4 Hz), 3.08 (s, 3H), 2.31 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 148.7, 141.5, 141.0, 140.8, 139.4, 137.9, 133.7, 131.8, 129.0, 128.9, 127.3, 126.6, 119.8, 26.0, 21.4; IR (neat): 3419, 3066, 2933, 2244, 1519, 1276, 1135, 1085, 881; MS (ES^+) Calculated for $[C_{17}H_{16}N_2O_2SNa]^+$: 335.08; Found: 335.11

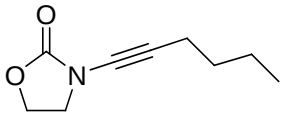
3-(6-(*tert*-Butyldimethylsilyloxy)hex-1-ynyl)oxazolidin-2-one[7]



10

Compound **10** was prepared in 70 % yield according to the general procedure B (eluents: ethyl acetate: hexanes = 1: 2). ^{1}H NMR (500 MHz, $CDCl_3$) δ 4.41 (t, 2H, *J* = 7.5 Hz), 3.87 (t, 2H, *J* = 7.5 Hz), 3.62 (t, 2H, *J* = 6.0 Hz), 2.32 – 2.35 (m, 2H), 1.55 – 1.62 (m, 4H), 0.89 (s, 9H), 0.05 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 156.5, 71.0, 70.1, 62.8, 62.6, 47.0, 32.0, 26.0, 25.3, 18.4, -5.2; IR (neat): 2929, 2857, 2271, 1770, 1415, 1112, 836; MS (ES^+) Calculated for $[C_{15}H_{27}NO_3SiNa]^+$: 320.17; Found: 320.18

3-(Hex-1-ynyl)oxazolidin-2-one[8]



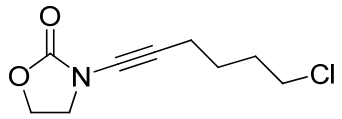
13a

Compound **13a** was prepared in 75 % yield according to the general procedure B (eluents: ethyl acetate: hexanes = 1: 2). ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.41 (t, 2H, *J* = 8.0 Hz), 3.87 (t, 2H, *J* = 8.0 Hz), 2.30 (t, 2H, *J* = 7.2 Hz), 1.47 – 1.55 (m, 2H), 1.36 – 1.45 (m, 2H), 0.90 (t, 3H, *J* = 7.2 Hz); ^{13}C NMR (125 MHz, $CDCl_3$) δ 156.5, 71.2, 70.0, 62.8, 47.1, 30.9, 22.0, 18.1, 13.6; IR (neat): 2933, 2873, 2273, 1770,

[7] Lu, B.; Li, C.; Zhang, L. *J. Am. Chem. Soc.* **2010**, *132*, 14070-14072.
[8] Davies, P. W.; Cremonesi, A.; Martin, N. *Chem. Commun.* **2011**, 379.

1415, 1207, 1116, 1033; MS (ES^+) Calculated for $[C_9H_{13}NO_2Na]^+$: 190.08; Found: 190.10

3-(6-Chlorohex-1-ynyl)oxazolidin-2-one[8]



13b

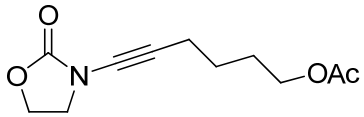
Compound **13b** was prepared in 50 % yield according to the literature procedure (eluents: ethyl acetate: hexanes = 1: 2). ^1H NMR (500 MHz, $CDCl_3$) δ 4.38 – 4.42 (m, 2H), 3.84 – 3.88 (m, 2H), 3.54 – 3.57 (m, 2H), 2.33 – 2.36 (m, 2H), 1.84 – 1.89 (m, 2H), 1.65 – 1.69 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 156.5, 70.6, 70.2, 62.8, 46.9, 44.5, 31.5, 25.9, 17.8; IR (neat): 2946, 2267, 1770, 1417, 1207, 1114, 1035; MS (ES^+) Calculated for $[C_9H_{12}NClO_2Na]^+$: 224.05; Found: 224.05

3-(5-Phenylpent-1-ynyl)oxazolidin-2-one

13c

Compound **13c** was prepared in 80 % yield according to the general procedure B (eluents: ethyl acetate: hexanes = 1: 2). ^1H NMR (400 MHz, $CDCl_3$) δ 7.26 – 7.31 (m, 2H), 7.17 – 7.21 (m, 3H), 4.42 (t, 2H, *J* = 8.0 Hz), 3.87 (t, 2H, *J* = 8.0 Hz), 2.72 (t, 2H, *J* = 7.6 Hz), 2.33 (t, 2H, *J* = 7.2 Hz), 1.82 – 1.89 (m, 2H),; ^{13}C NMR (125 MHz, $CDCl_3$) δ 156.6, 141.4, 128.4, 128.3, 125.8, 70.7, 70.5, 62.8, 47.0, 34.8, 30.3, 17.9; IR (neat): 2923, 2269, 1770, 1415, 1112, 1207; MS (ES^+) Calculated for $[C_{14}H_{15}NO_2Na]^+$: 252.10; Found: 252.13

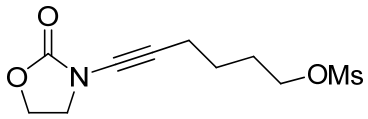
6-(2-Oxooxazolidin-3-yl)hex-5-ynyl acetate



13d

Compound **13d** was prepared in 76 % yield according to the general procedure B (eluents: ethyl acetate: hexanes = 1: 2). ^{1}H NMR (500 MHz, $CDCl_3$) δ 4.41 (t, 2H, *J* = 8.0 Hz), 4.07 (t, 2H, *J* = 7.0 Hz), 3.87 (t, 2H, *J* = 8.0 Hz), 2.35 (t, 2H, *J* = 7.0 Hz), 2.04 (s, 3H), 1.70 – 1.76 (m, 2H), 1.56 – 1.62 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 171.0, 156.5, 70.5, 63.9, 62.8, 47.0, 27.8, 25.2, 21.0, 18.1; IR (neat): 2954, 2269, 1770, 1729, 1417, 1245, 1035; MS (ES^+) Calculated for $[C_{11}H_{15}NO_4Na]^+$: 248.09; Found: 248.09

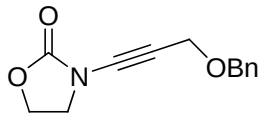
6-(2-Oxooxazolidin-3-yl)hex-5-ynyl methanesulfonate



13e

Compound **13e** was prepared in 65 % yield according to the general procedure B (eluents: ethyl acetate: hexanes = 1: 1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 4.41 (t, 2H, *J* = 8.0 Hz), 4.26 (t, 2H, *J* = 6.5 Hz), 3.87 (t, 2H, *J* = 8.0 Hz), 3.01(s, 3H), 2.38 (t, 2H, *J* = 7.0 Hz), 1.85 – 1.91 (m, 2H), 1.61 – 1.69 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 156.5, 70.9, 70.0, 69.5, 62.8, 46.9, 37.4, 28.2, 24.6, 17.9 ; IR (neat): 2938, 1768, 1419, 1349, 1170; MS (ES^+) Calculated for $[C_{10}H_{15}NO_5SNa]^+$: 284.06; Found: 284.09

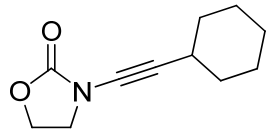
3-(3-(Benzyloxy)prop-1-ynyl)oxazolidin-2-one



13f

Compound **13f** was prepared in 70 % yield according to the general procedure B (eluents: ethyl acetate: hexanes = 1: 1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.27 – 7.37 (m, 5H), 4.60 (s, 2H), 4.46 (t, 2H, *J* = 8.0 Hz), 4.34 (s, 2H), 3.92 (t, 2H, *J* = 8.0 Hz); ^{13}C NMR (125 MHz, $CDCl_3$) δ 156.0, 137.3, 128.3, 128.0, 127.7, 71.5, 67.8, 64.8, 63.0, 57.5, 46.7; IR (neat): 2861, 2260, 1770, 1419, 1205; MS (ES^+) Calculated for $[C_{13}H_{13}NO_3Na]^+$: 254.08; Found: 254.08

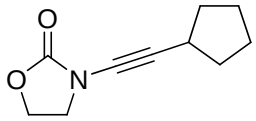
3-(Cyclohexylethynyl)oxazolidin-2-one[8]



13g

Compound **13g** was prepared in 80 % yield according to the general procedure B (eluents: ethyl acetate: hexanes = 1: 2). ^{1}H NMR (500 MHz, $CDCl_3$) δ 4.38 (t, 2H, *J* = 8.5 Hz), 3.85 (t, 2H, *J* = 8.5 Hz), 2.44 – 2.48 (m, 1H), 1.75 – 1.83 (m, 2H), 1.63 – 1.71 (m, 2H), 1.46 – 1.52 (m, 1H), 1.36 – 1.46 (m, 2H), 1.22 – 1.32 (m, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 156.7, 75.2, 70.4, 63.0, 47.4, 33.0, 29.0, 26.0, 25.1; IR (neat): 2929, 2854, 2269, 1770, 1415, 1209; MS (ES^+) Calculated for $[C_{11}H_{15}NO_2Na]^+$: 216.10; Found: 216.10

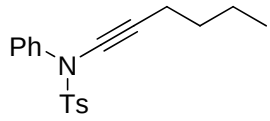
3-(Cyclopentylethynyl)oxazolidin-2-one



13h

Compound **13h** was prepared in 77 % yield according to the general procedure B (eluents: ethyl acetate: hexanes = 1: 2). ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.38 (t, 2H, *J* = 8.0 Hz), 3.84 (t, 2H, *J* = 8.0 Hz), 2.65 – 2.73 (m, 1H), 1.84 – 1.94 (m, 2H), 1.64 – 1.71 (m, 2H), 1.48 – 1.61 (m, 4H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 156.7, 75.2, 70.0, 63.0, 47.3, 34.1, 30.0, 25.1; IR (neat): 2960, 2869, 1770, 1421, 1209, 1114; MS (ES^+) Calculated for $[C_{10}H_{13}NO_2Na]^+$: 202.08; Found: 202.09

***N*-1-Hexyn-1-yl-4-methyl-N-phenylbenzenesulfonamide**[8]

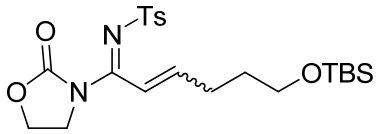


13l

Compound **13l** was prepared in 55 % yield according to the general procedure B (eluents: ethyl acetate: hexanes = 1: 2). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.55 (d, 2H, *J* = 8.5 Hz), 7.24 – 7.33 (m, 7H), 2.43 (s, 3H), 2.29 (t, 2H, *J* = 7.0 Hz), 1.40 – 1.52 (m, 2H), 1.35 –

1.39 (m, 2H), 0.90 (t, 3H, J = 7.5 Hz); ^{13}C NMR (125 MHz, $CDCl_3$) δ 144.5, 139.3, 132.9, 129.2, 128.8, 128.2, 127.2, 126.0, 73.8, 70.3, 30.9, 21.9, 21.7, 18.2, 13.6; IR (neat): 2931, 2254, 1594, 1488, 1373, 1176; MS (ES^+) Calculated for $[C_{19}H_{21}NO_2SNa]^+$: 350.11; Found: 350.12

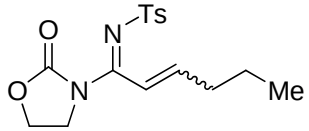
_N_-(6-(_tert_-Butyldimethylsilyloxy)-1-(2-oxooxazolidin-3-yl)hex-2-enylidene)-4-methylbenzenesulfonamide



11

Compound **11** (E/Z = 4/1) was prepared in 92 % yield according to the general procedure C (eluents: ethyl acetate: hexanes = 1: 1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.80 (d, 2H, J = 8.0 Hz), 7.28 (d, 2H, J = 8.0 Hz), 6.86 (dt, 1H, J = 16.0, 7.0 Hz), 6.73 (d, 2H, J = 16.0 Hz), 6.29 (minor, d, 2H, J = 12.5 Hz), 6.86 (minor, dt, 1H, J = 12.0, 7.5 Hz), 4.37 (t, 2H, J = 8.0 Hz), 3.95 (t, 2H, J = 8.0 Hz), 3.68 (t, 2H, J = 6.5 Hz), 2.41 (s, 3H), 2.36 – 2.42 (m, 2H), 1.71 – 1.77 (m, 2H), 0.89 (s, 9H), 0.05 (s, 6H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.0, 153.0, 150.2, 143.1, 139.4, 129.3, 126.6, 118.8, 62.2, 61.9, 44.6, 30.8, 29.9, 25.9, 21.5, 18.3, -5.4; IR (neat): 3419, 2952, 2929, 1650, 1573, 1394, 1089; MS (ES^+) Calculated for $[C_{22}H_{34}N_2O_5SSiNa]^+$: 489.19; Found: 489.19

4-Methyl-_N_-(1-(2-oxooxazolidin-3-yl)hex-2-enylidene)benzenesulfonamide

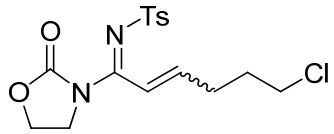


14a

Compound **14a** (E/Z = 4/1) was prepared in 93 % yield according to the general procedure C (eluents: ethyl acetate: hexanes = 1: 1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.75 (d, 2H, J = 8.0 Hz), 7.23 (d, 2H, J = 8.0 Hz), 6.82 (dt, 1H, J = 16.0, 7.0 Hz), 6.68 (d, 2H, J = 16.0 Hz), 4.32 (t, 2H, J = 8.0 Hz), 3.88 (t, 2H, J = 8.0 Hz), 2.37 (s, 3H), 2.24 – 2.29 (m, 2H), 1.48 – 1.56 (m, 2H), 0.93 (t, 3H, J = 8.0 Hz); ^{13}C NMR (125 MHz, $CDCl_3$)

δ 162.0, 152.9, 150.4, 143.0, 139.3, 129.2, 126.5, 118.7, 61.9, 44.7, 35.4, 21.5, 21.0, 13.7; IR (neat): 3419, 1783, 1648, 1540, 1394, 1349, 1153, 1089 ; MS (ES^+) Calculated for $[C_{16}H_{20}N_2O_4SNa]^+$: 359.10; Found: 359.10

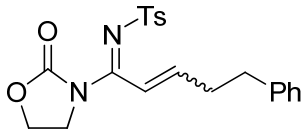
_N_-(6-Chloro-1-(2-oxooxazolidin-3-yl)hex-2-enylidene)-4-methylbenzenesulfonamide



14b

Compound **14b** (E/Z = 2/1) was prepared in 81 % yield according to the general procedure C (eluents: ethyl acetate: hexanes = 1: 1). ^1H NMR (500 MHz, $CDCl_3$) δ 7.79 (d, 2H, *J* = 8.0 Hz), 7.28 (d, 2H, *J* = 8.0 Hz), 6.72 – 6.81 (m, 2H), 6.37 (minor, d, 1H, *J* = 12.0 Hz), 5.91 (minor, dt, 1H, *J* = 12.0, 8.0 Hz), 4.38 – 4.42 (minor, m, 2H), 4.35 – 4.40 (m, 2H), 4.00 (minor, t, 2H, *J* = 8.0 Hz), 3.94 (t, 2H, *J* = 8.0 Hz), 3.64 (t, 2H, *J* = 7.0 Hz), 3.54 (minor, t, 2H, *J* = 6.0 Hz), 2.46 – 2.52 (m, 2H), 2.37 (s, 3H), 2.22 – 2.28 (minor, m, 2H), 1.97 – 2.04 (m, 2H), 1.84 – 1.90 (minor, m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.4, 161.9, 153.3, 152.7, 147.8, 147.7, 143.7, 143.5, 139.5, 138.9, 137.4, 129.6, 127.3, 126.9, 121.0, 120.4, 64.5, 62.4, 62.2, 44.9, 44.8, 44.3, 44.2, 30.9, 30.7, 30.5, 27.5, 21.8; IR (neat): 3312, 2936, 2763, 2739, 2119, 1443, 1352; MS (ES^+) Calculated for $[C_{16}H_{19}ClN_2O_4SNa]^+$: 393.07; Found: 393.07

4-Methyl-_N_-(1-(2-oxooxazolidin-3-yl)-5-phenylpent-2-enylidene)benzenesulfonamide

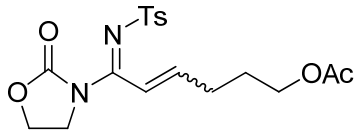


14c

Compound **14c** (E/Z = 3/1) was prepared in 88 % yield according to the general procedure C (eluents: ethyl acetate: hexanes = 1: 1). ^1H NMR (500 MHz, $CDCl_3$) δ 7.81 (d, 2H, *J* = 8.5 Hz), 7.16 – 7.32 (m, 7H), 6.88 (dt, *J* = 16.0, 6.0 Hz, 1H), 6.79 (d, 1H, *J* = 16.0 Hz), 6.30 (minor, d, 1H, *J* = 12.0 Hz), 6.02 (minor, dt, 1H, *J* = 12.0, 7.5 Hz), 4.37 (t,

1H, *J* = 8.0 Hz), 3.95 (t, 1H, *J* = 8.0 Hz), 2.86 (t, 1H, *J* = 8.0 Hz), 2.63 – 2.67 (m, 2H), 2.43 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 161.8, 152.9, 148.8, 143.0, 140.8, 139.3, 129.3, 128.4, 128.3, 127.0, 126.3, 119.0, 62.0, 44.6, 35.1, 33.9, 21.6; IR (neat): 2923, 2854, 1781, 1648, 1552, 1382, 1313, 1149, 1091; MS (ES^+) Calculated for $[C_{21}H_{22}N_2O_4SNa]^+$: 421.12; Found: 421.16

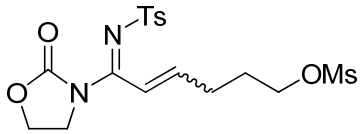
(6*E*)-6-(2-Oxooxazolidin-3-yl)-6-(tosylimino)hex-4-enyl acetate



14d

Compound **14d** (E/Z = 2/1) was prepared in 79 % yield according to the general procedure C (eluents: ethyl acetate: hexanes = 1: 1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.78 (d, 2H, *J* = 8.0 Hz), 7.27 (d, 2H, *J* = 8.0 Hz), 6.84 (dt, 1H, *J* = 16.0, 6.5 Hz), 6.74 (d, 1H, *J* = 16.0 Hz), 6.31 (minor, d, 1H, *J* = 12.5 Hz), 5.99 (dt, 1H, *J* = 12.5, 7.5 Hz), 4.41 (minor, t, 2H, *J* = 8.0 Hz), 4.36 (t, 2H, *J* = 8.0 Hz), 4.14 (t, 2H, *J* = 8.0 Hz), 3.97 – 4.06 (m, 2H), 3.93 (t, 2H, *J* = 8.0 Hz), 2.41 (s, 3H), 2.28 – 2.42 (m, 2H), 2.09 – 2.13 (minor, m, 2H), 2.07 (s, 3H), 2.02 (minor, s, 3H), 1.84 – 1.90 (m, 2H), 1.70 – 1.74 (minor, m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 171.3, 171.2, 162.4, 162.0, 153.3, 152.6, 148.5, 143.7, 143.4, 139.6, 138.9, 138.6, 129.6, 127.3, 126.8, 119.8, 119.6, 101.9, 63.9, 63.7, 62.2, 44.8, 44.3, 30.0, 29.8, 27.6, 27.2, 27.0, 21.8, 21.7, 21.2, 19.3; IR (neat): 3747, 3733, 2954, 1783, 1731, 1558, 1540, 1394, 1243, 1153, 1089; MS (ES^+) Calculated for $[C_{18}H_{22}N_2O_6SNa]^+$: 417.11; Found: 417.10

(6Z)-6-(2-Oxooxazolidin-3-yl)-6-(tosylimino)hex-4-enyl methanesulfonate

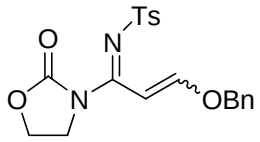


14e

Compound **14e** (E/Z = 3/2) was prepared in 72 % yield according to the general procedure C (eluents: ethyl acetate: hexanes = 1: 1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.77

(d, 2H, *J* = 8.0 Hz), 7.28 (d, 2H, *J* = 8.0 Hz), 6.71 – 6.78 (m, 2H), 6.39 (minor, d, 1H, *J* = 12.5 Hz), 5.94 (minor, dt, 1H, *J* = 12.5, 7.5 Hz), 4.43 (minor, t, 2H, *J* = 8.0 Hz), 4.38 (t, 2H, *J* = 8.0 Hz), 4.33 (t, 2H, *J* = 6.0 Hz), 4.20 (minor, t, 2H, *J* = 6.0 Hz), 4.00 (minor, t, 2H, *J* = 8.0 Hz), 3.93 (t, 2H, *J* = 8.0 Hz), 3.03 (s, 3H), 2.99 (minor, s, 3H), 2.43 – 2.49 (m, 2H), 2.42 (s, 3H), 2.22 – 2.27 (minor, m, 2H), 1.99 – 2.03 (m, 2H), 1.86 – 1.90 (minor, m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.2, 161.8, 153.3, 152.9, 146.8, 143.7, 143.5, 139.5, 138.9, 137.2, 129.6, 129.1, 127.2, 126.8, 121.2, 120.8, 69.9, 69.3, 62.4, 62.3, 44.7, 44.2, 37.6, 37.3, 29.1, 28.1, 27.5, 26.5, 21.8, 21.7; IR (neat): 2925, 1781, 1648, 1552, 1402, 1351, 1172, 1153; MS (ES^+) Calculated for $[C_{17}H_{22}N_2O_7S_2Na]^+$: 453.08; Found: 453.07

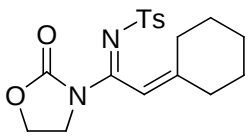
_N_-(3-(Benzyloxy)-1-(2-oxooxazolidin-3-yl)allylidene)-4-methylbenzenesulfonamide



14f

Compound **14f** (E/Z = 5/1) was prepared in 75 % yield according to the general procedure C (eluents: ethyl acetate: hexanes = 1: 1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.00 (d, 2H, *J* = 12.0 Hz), 7.80 (d, 2H, *J* = 8.0 Hz), 7.35 – 7.41 (m, 5H), 7.27 (d, 2H, *J* = 8.0 Hz), 6.61 (d, 2H, *J* = 12.0 Hz), 5.09 (s, 2H), 4.33 (t, 2H, *J* = 8.0 Hz), 3.95 (t, 2H, *J* = 8.0 Hz), 2.42 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 165.4, 160.5, 153.6, 142.9, 139.6, 134.6, 129.3, 128.7, 128.6, 127.9, 126.4, 96.2, 73.8, 61.7, 45.2, 21.6; IR (neat): 3747, 3733, 3033, 2321, 1772, 1633, 1540, 1384, 1145, 1089; MS (ES^+) Calculated for $[C_{20}H_{20}N_2O_5SNa]^+$: 423.09; Found: 423.14

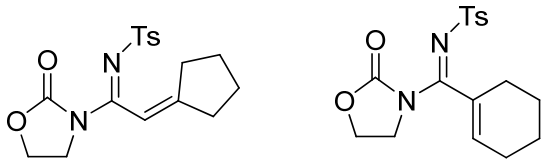
(*E*)-*N*-(2-Cyclohexylidene-1-(2-oxooxazolidin-3-yl)ethylidene)-4-methylbenzenesulfonamide



14g

Compound **14g** was prepared in 90 % yield according to the general procedure C (eluents: ethyl acetate: hexanes = 1: 1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.85 (d, 2H, *J* = 8.0 Hz), 7.35 (d, 2H, *J* = 8.0 Hz), 5.98 (s, 1H), 4.46 (t, 2H, *J* = 8.0 Hz), 4.12 (t, 2H, *J* = 8.0 Hz), 2.50 (s, 3H), 2.29 – 2.32 (m, 2H), 2.02 – 2.07 (m, 2H), 1.69 – 1.73 (m, 2H), 1.52 – 1.60 (m, 4H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 163.4, 152.3, 152.0, 143.1, 138.7, 129.1, 127.1, 110.9, 61.7, 44.3, 36.3, 31.6, 27.1, 26.6, 25.8, 21.5; IR (neat): 3419, 2933, 2857, 1791, 1650, 1540, 1384, 1375, 1155, 1089; MS (ES^+) Calculated for $[C_{18}H_{22}N_2O_4SNa]^+$: 385.12; Found: 385.12

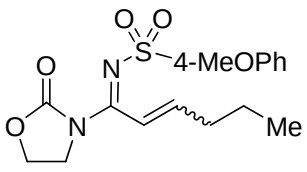
***N*-(2-Cyclopentylidene-1-(2-oxooxazolidin-3-yl)ethylidene)-4-methylbenzenesulfonamide (14h)**



14h (major) (minor)

Compound **14h** was prepared in 76% yield along with the cyclohexene side product in 15% yield according to the general procedure C (eluents: ethyl acetate: hexanes = 1: 1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.84 (d, 2H, *J* = 8.0 Hz), 7.36 (d, 2H, *J* = 8.0 Hz), 6.34 (brs, 1H), 5.98 (minor, brs, 1H), 4.47 (t, 2H, *J* = 8.0 Hz), 4.12 (t, 2H, *J* = 8.0 Hz), 2.50 – 2.53 (m, 2H), 2.50 (s, 3H), 2.13 – 2.19 (m, 2H), 1.73 – 1.76 (m, 4H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 163.6, 159.4, 152.4, 143.4, 138.9, 129.4, 127.2, 110.5, 62.2, 44.8, 34.8, 31.6, 26.4, 25.6, 21.8; IR (neat): 3448, 2956, 2356, 1791, 1540, 1384, 1155, 1087; MS (ES^+) Calculated for $[C_{17}H_{20}N_2O_4SNa]^+$: 371.10; Found: 371.11

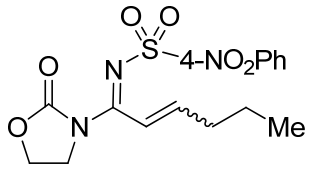
4-Methoxy-*N*-(1-(2-oxooxazolidin-3-yl)hex-2-enylidene)benzenesulfonamide



14i

Compound **14i** (E/Z = 5/1) was prepared in 85 % yield according to the general procedure C (eluents: ethyl acetate: hexanes = 1: 1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (d, 2H, *J* = 8.8 Hz), 6.94 (d, 2H, *J* = 8.8 Hz), 6.78 – 6.86 (m, 1H), 6.70 (d, 1H, *J* = 16.0 Hz), 4.36 (t, 2H, *J* = 8.0 Hz), 3.96 (t, 2H, *J* = 8.0 Hz), 3.85 (s, 3H), 2.27 – 2.32 (m, 2H), 1.50 – 1.60 (m, 2H), 0.97 (t, 3H, *J* = 7.2 Hz); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.9, 162.1, 153.3, 150.6, 134.4, 129.0, 119.0, 114.1, 62.2, 55.8, 44.9, 35.7, 21.3, 13.9; IR (neat): 3312, 2936, 2763, 2739, 2119, 1443, 1352; MS (ES^+) Calculated for $[C_{16}H_{20}N_2O_5SNa]^+$: 375.10; Found: 375.10

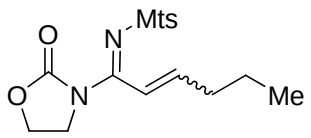
4-Nitro-*N*-(1-(2-oxooxazolidin-3-yl)hex-2-enylidene)benzenesulfonamide



14j

Compound **14j** (E/Z = 4/1) was prepared in 88 % yield according to the general procedure C (eluents: ethyl acetate: hexanes = 1: 1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.34 (d, 2H, *J* = 8.5 Hz), 8.12 (d, 2H, *J* = 8.5 Hz), 7.02 (td, 1H, *J* = 16.0, 7.0 Hz), 6.82 (d, 1H, *J* = 16.0 Hz), 4.40 (t, 2H, *J* = 8.0 Hz), 3.93 (t, 2H, *J* = 8.0 Hz), 2.33 – 2.38 (m, 2H), 1.56 – 1.64 (m, 2H), 1.01 (t, 3H, *J* = 7.5 Hz); ^{13}C NMR (125 MHz, $CDCl_3$) δ 163.3, 152.8, 152.3, 150.0, 148.2, 128.1, 124.3, 119.3, 62.2, 44.8, 35.9, 21.4, 13.9; IR (neat): 3733, 2960, 1783, 1648, 1558, 1384, 1313, 1153, 1089; MS (ES^+) Calculated for $[C_{15}H_{17}N_3O_6SNa]^+$: 390.07; Found: 390.10

2,4,6-Trimethyl-*N*-(1-(2-oxooxazolidin-3-yl)hex-2-enylidene)benzenesulfonamide

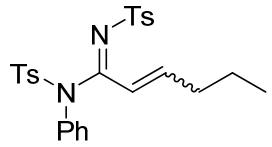


14k

Compound **14k** (E/Z = 5/1) was prepared in 80 % yield according to the general procedure C (eluents: ethyl acetate: hexanes = 1: 2). ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.92 (s, 2H), 6.69 (dt, 1H, *J* = 16.8, 6.8 Hz), 6.60 (d, 1H, *J* = 16.8 Hz), 4.37 (t, 2H, *J* = 8.0 Hz),

3.96 (t, 2H, J = 8.0 Hz), 2.61 (s, 6H), 2.19 (s, 3H), 2.19 - 2.25 (m, 2H), 1.47 – 1.53 (m, 2H), 0.94 (t, 3H, J = 7.2 Hz); ^{13}C NMR (125 MHz, $CDCl_3$) δ 161.9, 153.2, 149.4, 141.9, 139.4, 138.7, 131.5, 118.6, 61.9, 44.8, 35.3, 22.8, 21.0, 20.8, 13.6; IR (neat): 3744, 3032, 1558, 1440, 1297, 1139; MS (ES^+) Calculated for $[C_{18}H_{24}N_2O_4SNa]^+$: 387.14; Found: 387.08

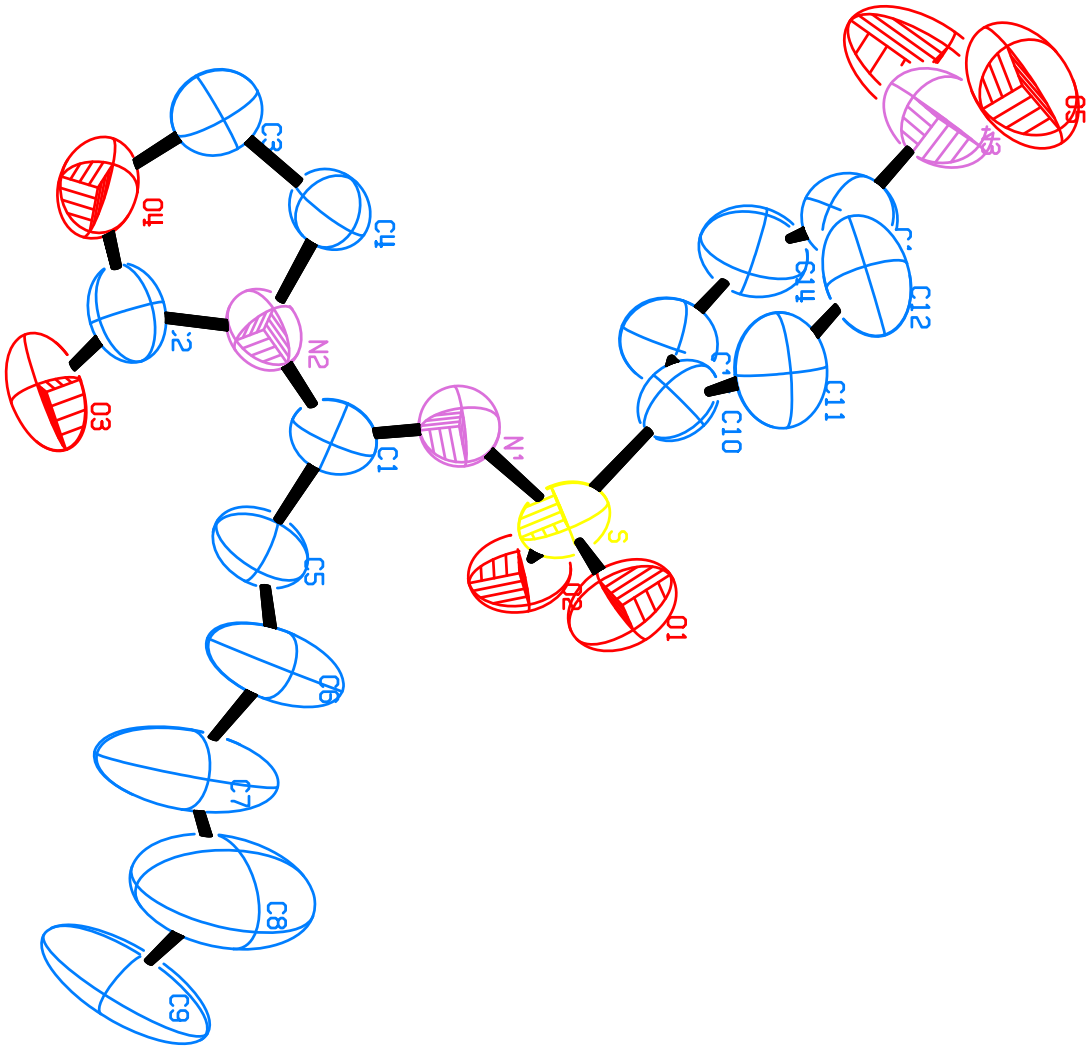
(1*E*)-*N*-Phenyl-*N,N'*-ditosylhex-2-enimidamide

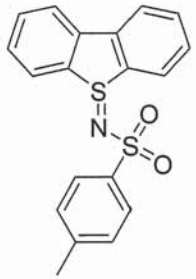


14l

Compound **14l** (E/Z = 3/2) was prepared in 62 % yield according to the general procedure C (eluents: ethyl acetate: hexanes = 1: 1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, 2H, J = 8.4 Hz), 7.35 – 7.40 (m, 5H), 7.16 – 7.25 (m, 4H), 6.98 (d, 2H, J = 8.4 Hz), 6.55 (dt, 1H, J = 16.0, 7.2 Hz), 6.11 (d, 1H, J = 16.0 Hz), 2.50 (s, 3H), 2.37 (s, 3H), 1.94 - 1.99 (m, 2H), 1.12 – 1.21 (m, 2H), 0.63 (t, 3H, J = 7.2 Hz); ^{13}C NMR (125 MHz, $CDCl_3$) δ 163.0, 151.7, 144.7, 143.5, 138.8, 138.3, 135.1, 130.3, 129.6, 129.5, 129.4, 129.0, 127.4, 121.8, 101.8, 35.2, 21.9, 21.3, 13.6; IR (neat): 3735, 2960, 1648, 1596, 1560, 1540, 1371, 1155, 1087; MS (ES^+) Calculated for $[C_{26}H_{28}N_2O_4S_2Na]^+$: 519.14; Found: 519.13

ORTEP description of E-14j





1

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lcq2-36

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solvent      cdcl3    dof         -1425.0
file /home/Zhang/c~   dm              nnn
 qli/lcq2-36-3.fid    dmm               c
   ACQUISITION        dmf             200
sfrq        399.951       PROCESSING
tn               H1    lb            0.10
at            2.502    fn           65536
np            36008    math             f
sw           7196.8
fb        not used     werr
bs               2     wexp
pw             8.0     wbs
pw             8.0     wnt
tpwr            57          DISPLAY
d1            3.000    sp           -185.7
tof            -6.9    wp           3539.3
nt               10    vs               28
ct               10    sc                0
alock             n    wc              250
gain      not used     hzmm          14.16
      FLAGS            is           261.78
il                n    rfl          4501.8
in                n    rfp          2903.6
dp                y    th                3
hs               nn    ins           3.000
                       ai     ph
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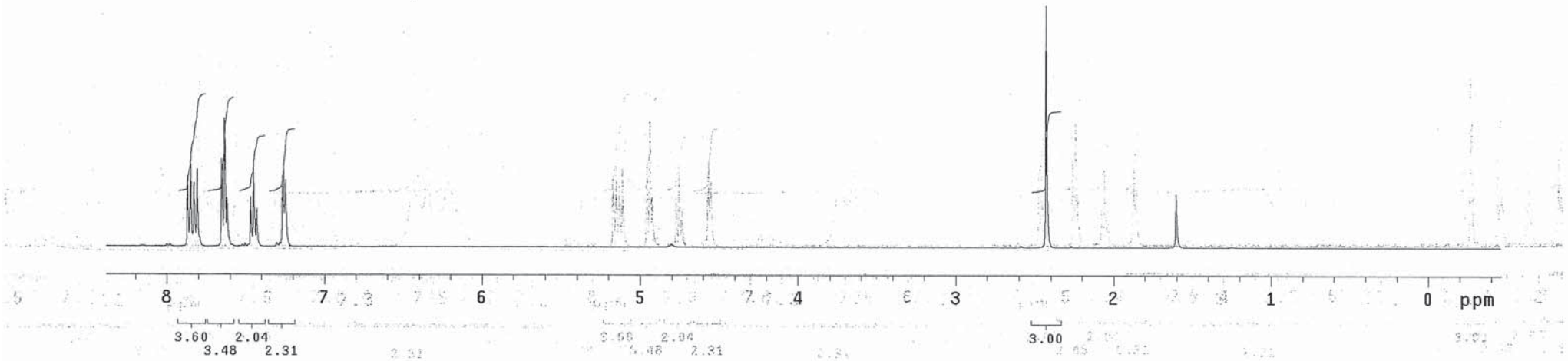

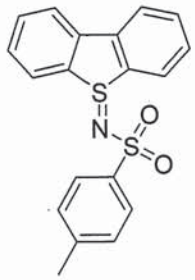

1

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lcq3-36-13C

exp25  CARBON

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solvent       cdcl3   gain              54
file            exp   spin        not used
   ACQUISITION         hst           0.008
sw           28258.6   pw90          9.200
at             1.300   alfa         10.000
np             73498         FLAGS
fb             16000   il                n
bs                 2   in                n
d1             3.000   dp                y
nt             10000   hs               nn
ct               160        PROCESSING
   TRANSMITTER         lb             0.50
tn                C13   lsfid             2
sfrq         125.702   fn          not used
tof            865.4        DISPLAY
tpwr              56   sp            -861.6
pw             13.500   wp           20075.4
    DECOUPLER          rfl          11036.8
dn                H1   rfp           9678.0
dof                0   rp              65.8
dm               nny   lp           -1038.9
decwave                      PLOT
dpwr              36   wc               250
dmf            11101   sc                 0
                       vs              2141
                       th                 4
                       ai  cdc  ph
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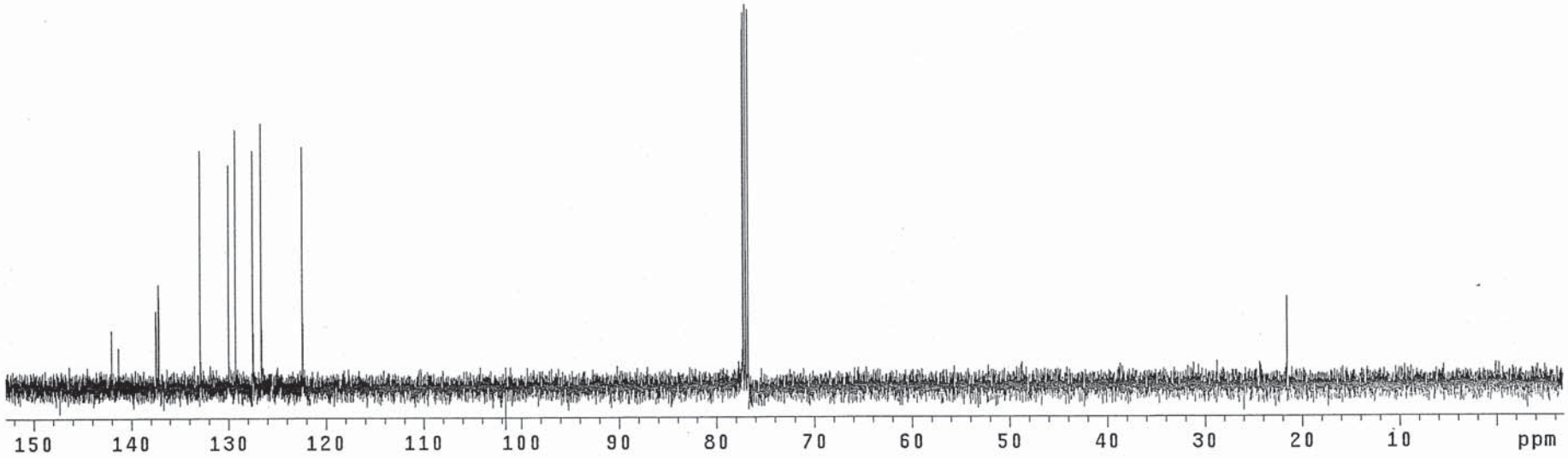

lcq2-76

exp25 s2pul

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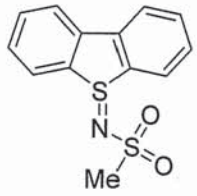
file	/home/Zhang/c~ qli/lcq2-76.fid	dm	nnn
		dmm	c
ACQUISITION		dmf	200
sfrq	399.951	PROCESSING	
tn	H1	lb	0.10
at	2.502	fn	65536
np	36008	math	f
sw	7196.8		
fb	not used	werr	
bs	2	wexp	
pw	8.0	wbs	
pw	8.0	wnt	
tpwr	57	DISPLAY	
d1	3.000	sp	-94.5
tof	-6.9	wp	3572.9
nt	8	vs	25
ct	8	sc	0
alock	n	wc	250
gain	not used	hzmm	14.29
FLAGS		is	500.00
il	n	rfl	4503.1
in	n	rfp	2903.6
dp	y	th	3
hs	nn	ins	3.000
		ai ph	



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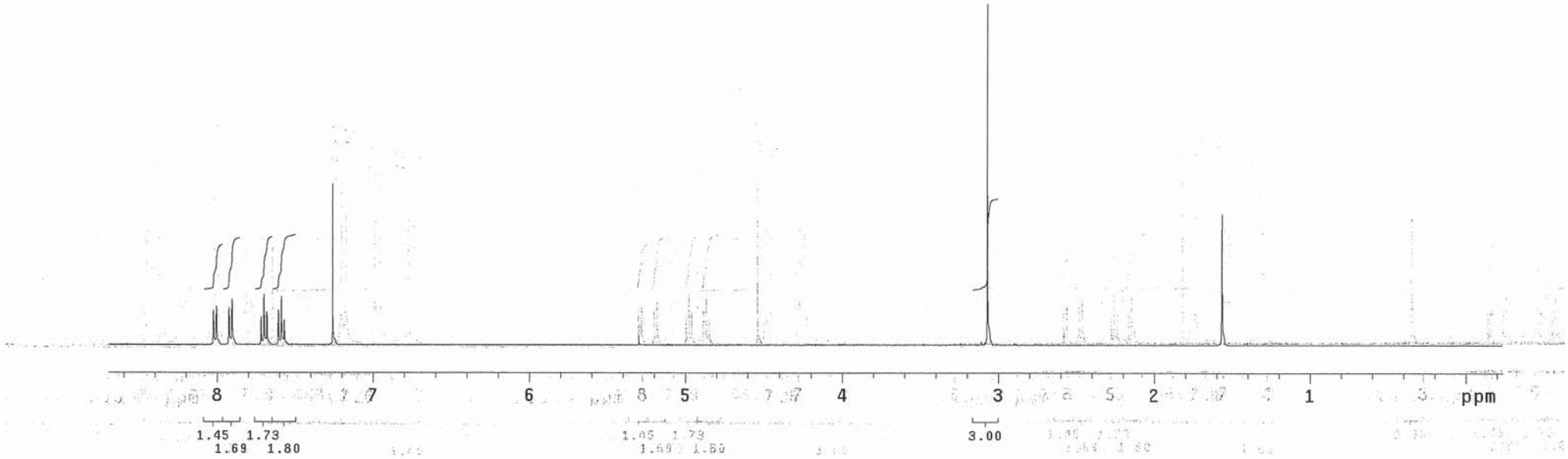

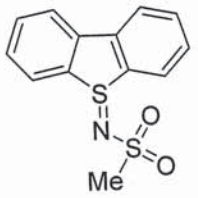

2

lcq2-76-13C

exp25 CARBON

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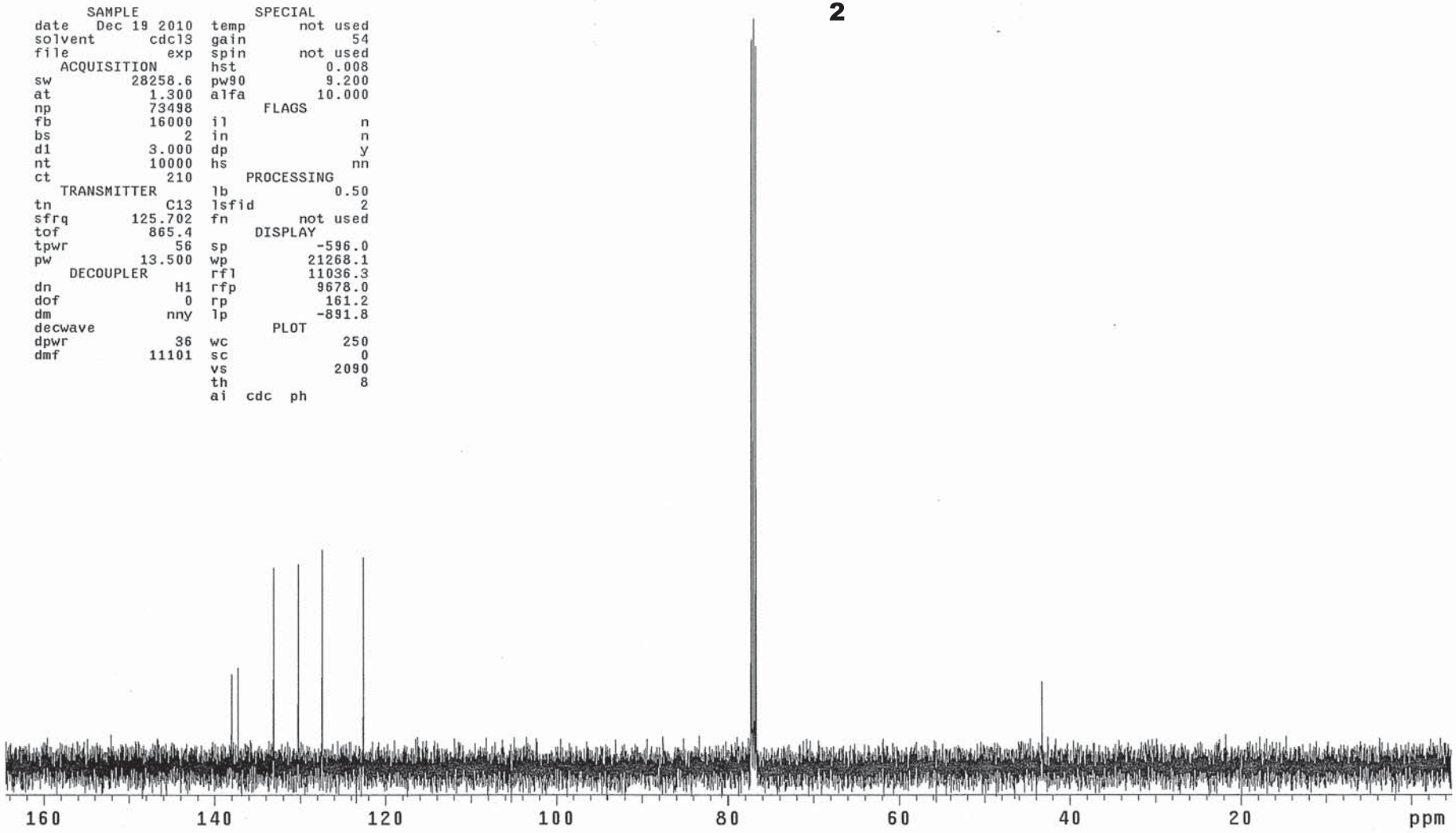
file	exp	spin	not used
ACQUISITION		hst	0.008
sw	28258.6	pw90	9.200
at	1.300	alfa	10.000
np	73498	FLAGS	
fb	16000	il	n
bs	2	in	n
d1	3.000	dp	y
nt	10000	hs	nn
ct	210	PROCESSING	
TRANSMITTER		lb	0.50
tn	C13	lsfid	2
sfrq	125.702	fn	not used
tof	865.4	DISPLAY	
tpwr	56	sp	-596.0
pw	13.500	wp	21268.1
DECOUPLER		rfl	11036.3
dn	H1	rfp	9678.0
dof	0	rp	161.2
dm	nny	lp	-891.8
decwave		PLOT	
dpwr	36	wc	250
dmf	11101	sc	0
		vs	2090
		th	8
		ai cdc ph	



lcq2-161-H

exp25 PROTON

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file	exp	SPECIAL	
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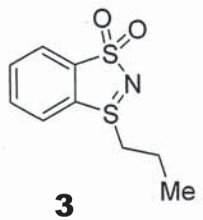
sw	7997.6	gain	not used
at	2.049	spin	not used
np	32768	hst	0.008
fb	4000	pw90	9.100
bs	2	alfa	6.600
d1	1.000	FLAGS	
nt	12	il	n
ct	12	in	n
TRANSMITTER		dp	y
tn	H1	hs	nn
sfrq	499.859	PROCESSING	
tof	499.9	fn	not used
tpwr	53	DISPLAY	
pw	4.550	sp	-140.9
DECOUPLER		wp	4396.6
dn	C13	rfl	4632.4
dof	0	rfp	3629.0
dm	nnn	rp	27.9
decwave	W40_5mm3Gi~	lp	2.2
	dp	PLOT	
dpwr	47	wc	250
dmf	32258	sc	0
		vs	30
		th	3
		ai cdc ph	



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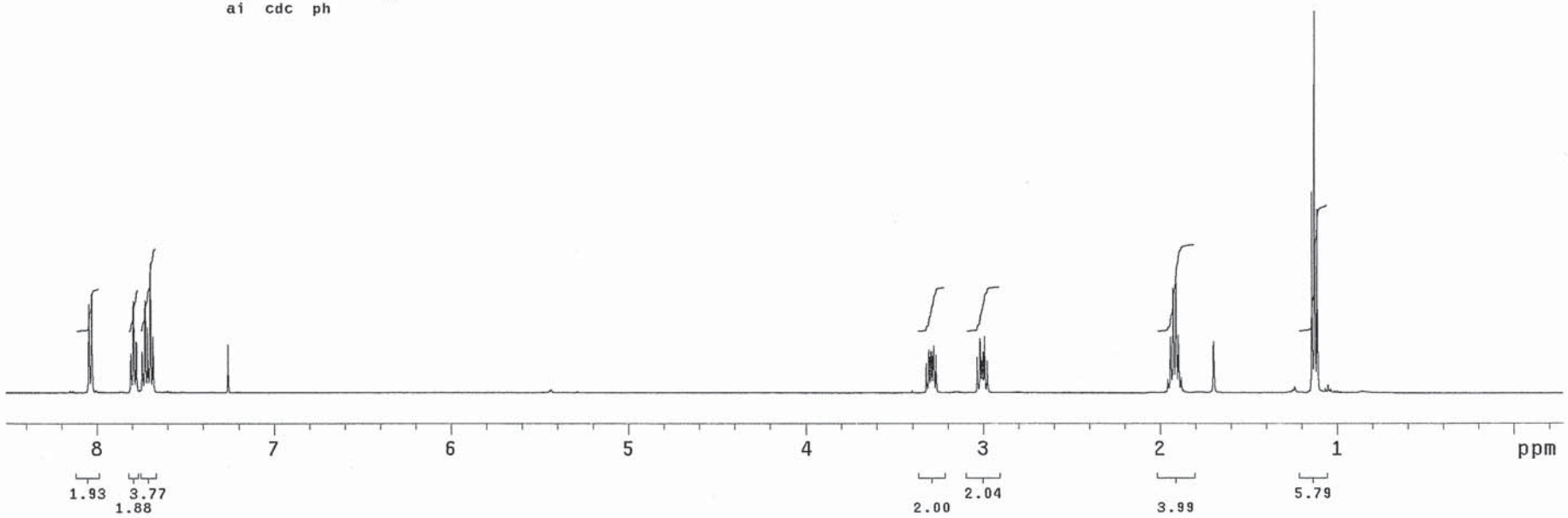

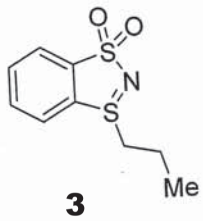

3

lcq2-161-13C

exp25 CARBON

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file	exp	spin	not used
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np	73498	FLAGS	
fb	16000	il	n
bs	2	in	n
d1	3.000	dp	y
nt	10000	hs	nn
ct	196	PROCESSING	
TRANSMITTER		lb	0.50
tn	C13	lsfid	2
sfrq	125.702	fn	not used
tof	865.4	DISPLAY	
tpwr	56	sp	-502.0
pw	13.500	wp	19445.9
DECOUPLER		rfl	11041.5
dn	H1	rfp	9678.0
dof	0	rp	-179.4
dm	nny	lp	-911.4
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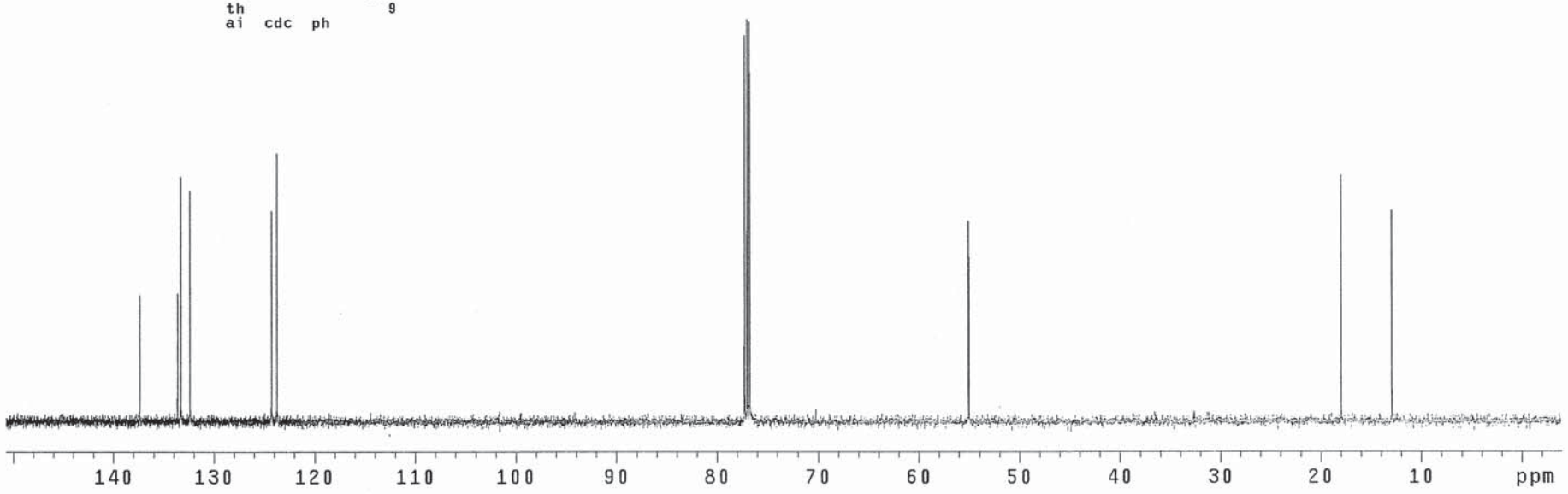
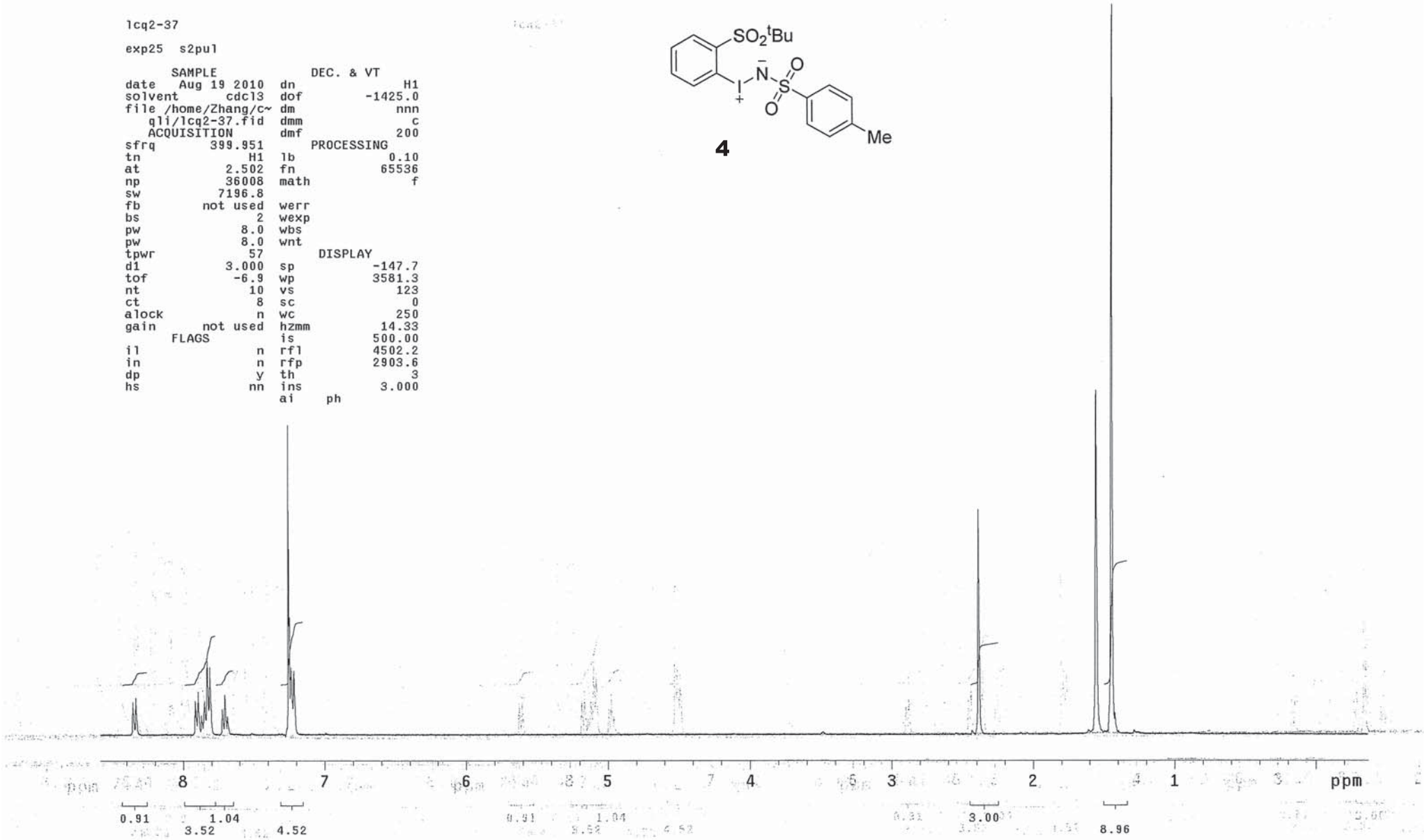
dmf	11101	sc	0
		vs	554
		th	9
		ai cdc ph	




lcq2-37
exp25 s2pul
SAMPLE
date Aug 19 2010
solvent cdcl3
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fb not used
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pw 8.0
tpwr 57
d1 3.000
tof -6.9
nt 10
ct 8
alock n
gain not used
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dp y
hs nn
DEC. & VT
dn H1
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dmm c
dmf 200
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math f
werr
wexp
wbs
wnt
DISPLAY
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wp 3581.3
vs 123
sc 0
wc 250
hzmm 14.33
is 500.00
rfl 4502.2
rfp 2903.6
th 3
ins 3.000
ai ph
SO2tBu
Me
4
8
7
6
5
4
3
2
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ppm
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3.52
4.52
3.00
8.96

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lcq2-37-13C

exp25  CARBON

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file            exp
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np              73498
fb              16000
bs                  2
d1              3.000
nt              10000
ct                266
   TRANSMITTER
tn                C13
sfrq          125.702
tof             865.4
tpwr               56
pw             13.500
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dn                 H1
dof                 0
dm                nny
decwave
dpwr               36
dmf             11101

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temp         not used
gain               54
spin         not used
hst               0.008
pw90              9.200
alfa             10.000
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il                    n
in                    n
dp                    y
hs                   nn
   PROCESSING
lb                 0.50
lsfid                 2
fn           not used
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sp              -944.4
wp             21005.9
rfl            11036.3
rfp             9678.0
rp               -36.1
lp              -833.6
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sc                    0
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th                    5
ai  cdc  ph
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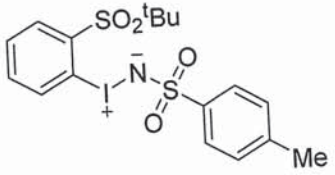

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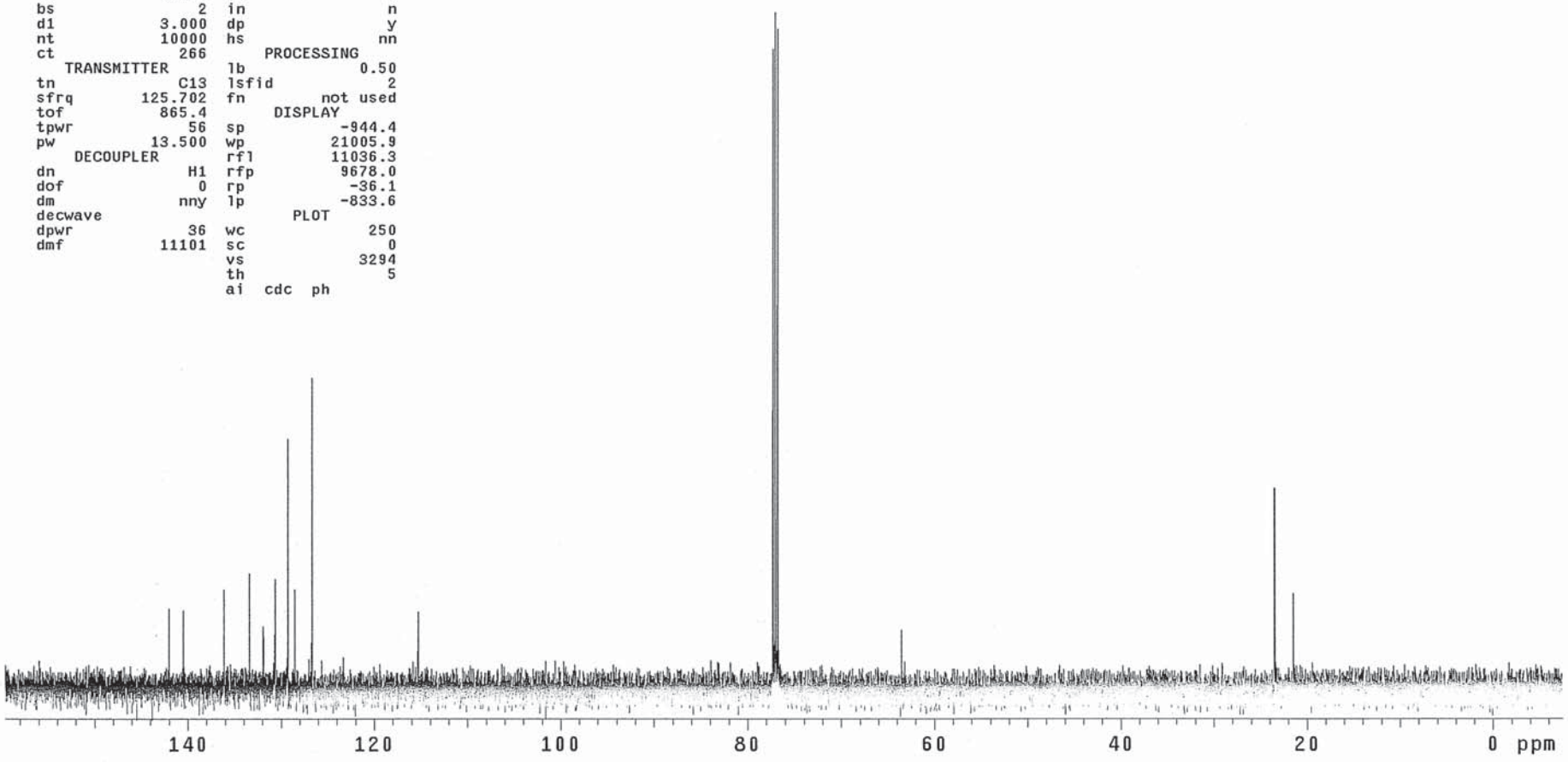

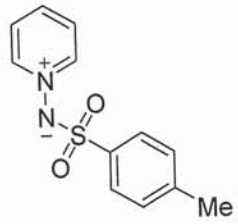

5

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lcq2-114-1

exp25  s2pul

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bs                2
pw              8.0
pw              8.0
tpwr             57
d1              3.000
tof              -6.9
nt                10
ct                10
alock              n
gain       not used
      FLAGS
il                 n
in                 n
dp                 y
hs                nn

      DEC. & VT
dn              H1
dof         -1425.0
dm              nnn
dmm               c
dmf             200
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lb             0.10
fn            65536
math              f
werr
wexp
wbs
wnt
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wp           3766.4
vs               44
sc                0
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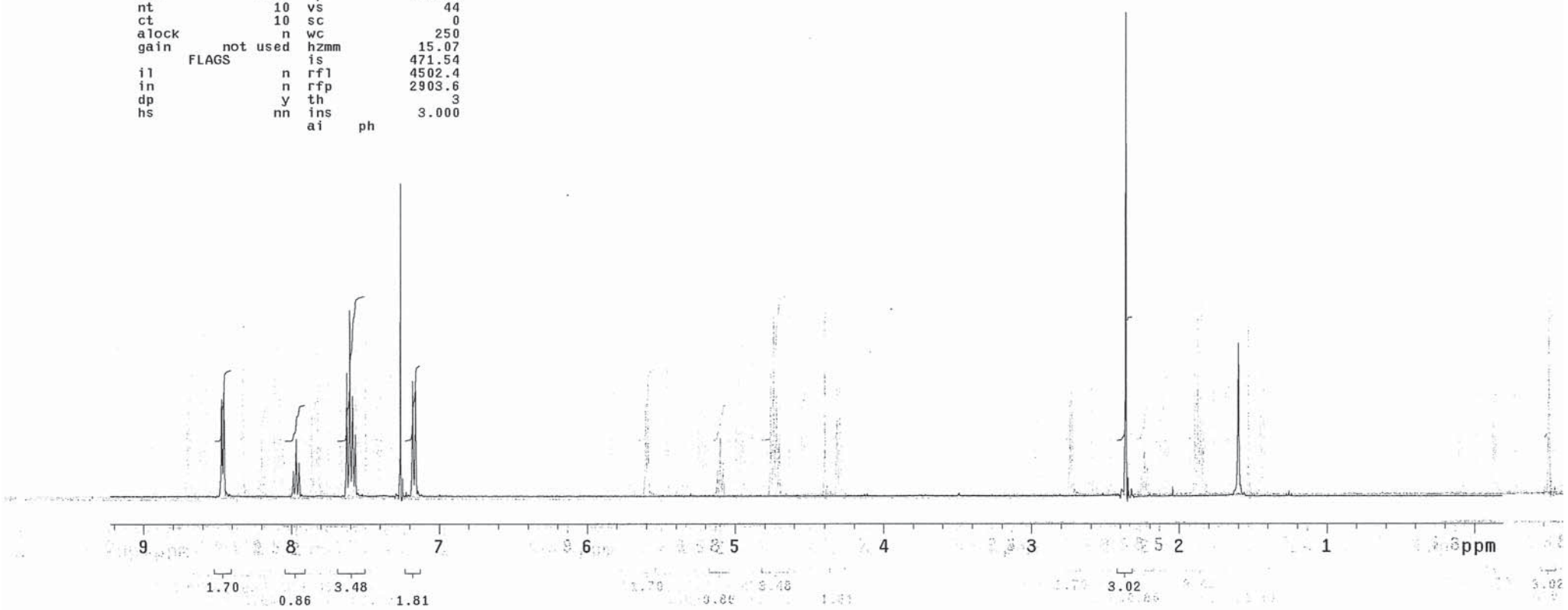
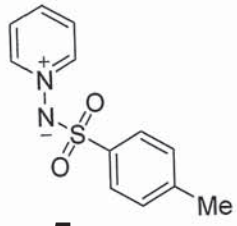
is           471.54
rfl          4502.4
rfp          2903.6
th                3
ins           3.000
ai    ph
```





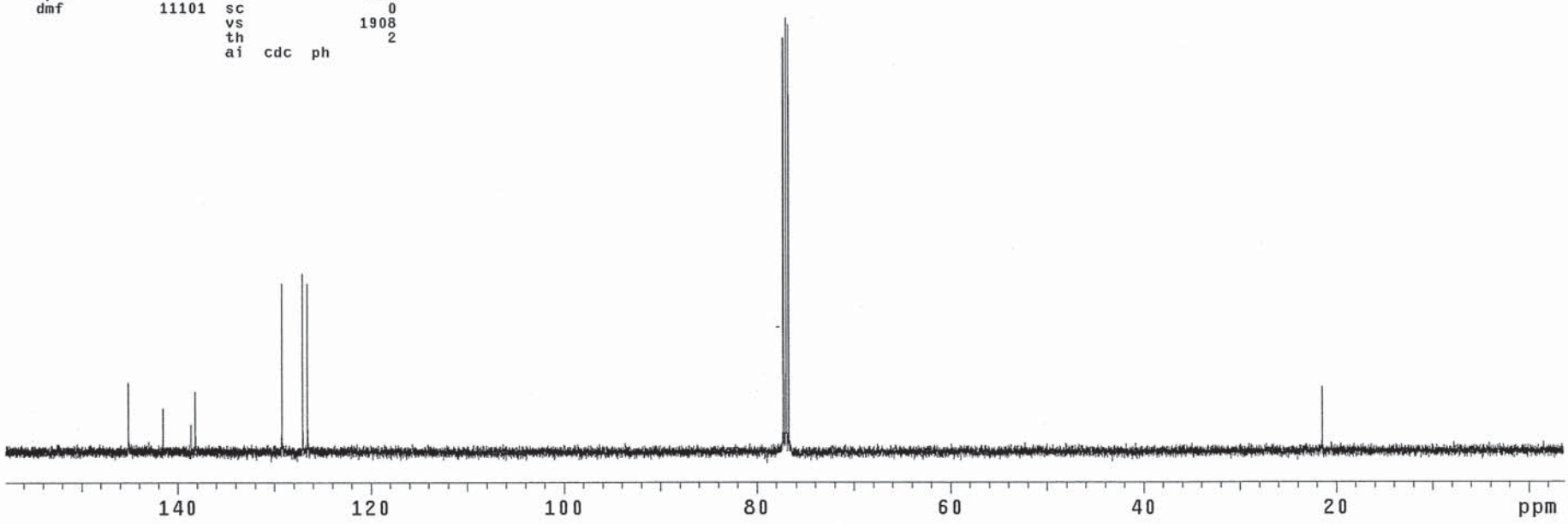
5

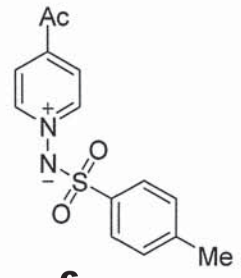
```
lcq2-114-13C

exp25  CARBON

      SAMPLE
date    Dec 17 2010
solvent       cdcl3
file            exp
   ACQUISITION
sw          28258.6
at              1.300
np              73498
fb              16000
bs                  2
d1              3.000
nt              10000
ct                826
   TRANSMITTER
tn                C13
sfrq          125.702
tof             865.4
tpwr               56
pw             13.500
    DECOUPLER
dn                  H1
dof                  0
dm                 nny
decwave
dpwr               36
dmf             11101

      SPECIAL
temp        not used
gain              54
spin        not used
hst              0.008
pw90             9.200
alfa            10.000
        FLAGS
il                   n
in                   n
dp                   y
hs                  nn
     PROCESSING
lb                0.50
lsfid                2
fn          not used
      DISPLAY
sp             -462.7
wp            20307.4
rfl           11035.5
rfp            9678.0
rp               38.2
lp            -1008.5
        PLOT
wc                 250
sc                   0
vs                1908
th                   2
ai  cdc  ph
```





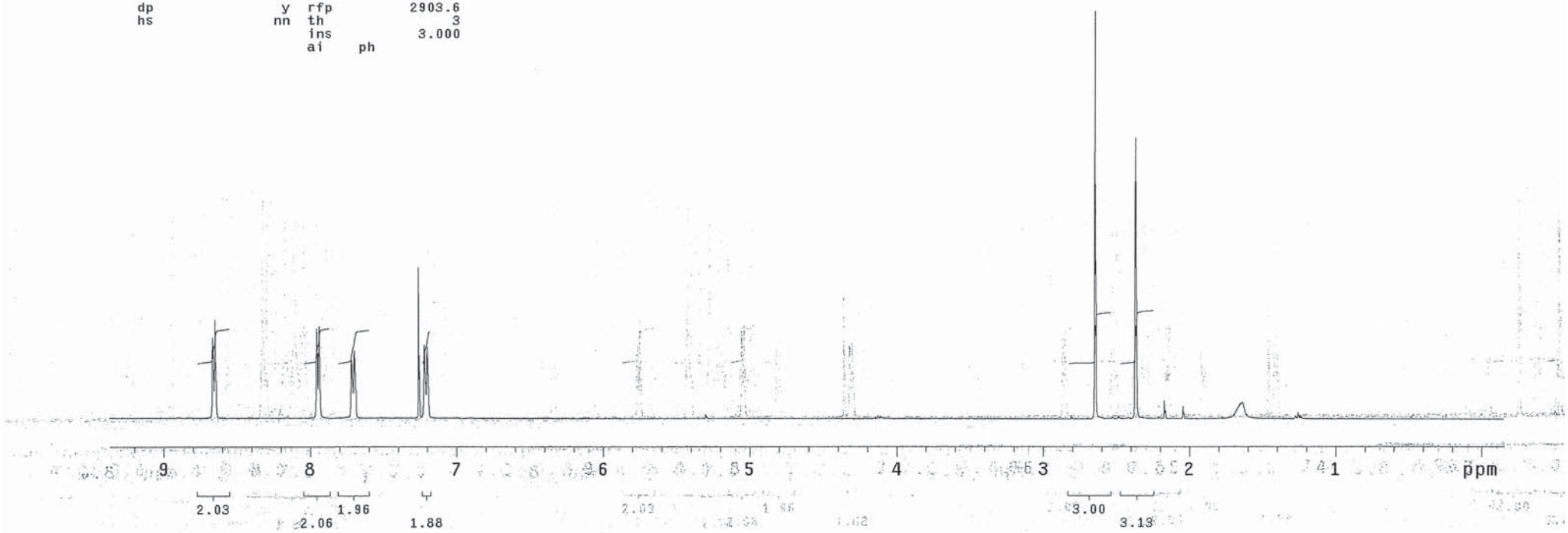
6

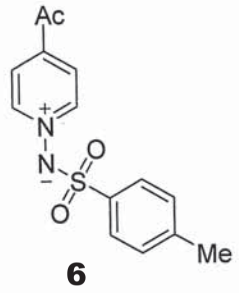
```
lcq2-215-H

exp25  s2pul

      SAMPLE
date    Dec 31 2010
solvent       cdcl3
file            exp
   ACQUISITION
sfrq        399.951
tn               H1
at           2.502
np           36008
sw          7196.8
fb        not used
bs                2
pw              8.0
pw              8.0
tpwr             57
d1            3.000
tof            -6.9
nt               16
ct               16
alock             n
gain      not used
      FLAGS
il                n
in                n
dp                y
hs               nn

      DEC. & VT
dn               H1
dof         -1425.0
dm              nnn
dmm               c
dmf             200
      PROCESSING
lb             0.10
fn            65536
math              f
werr
wexp
wbs
wnt
      DISPLAY
sp            -61.6
wp           3808.4
vs               54
sc                0
wc              250
hzmm          15.23
is           257.71
rfl         4504.0
rfp         2903.6
th                3
ins           3.000
ai    ph
```





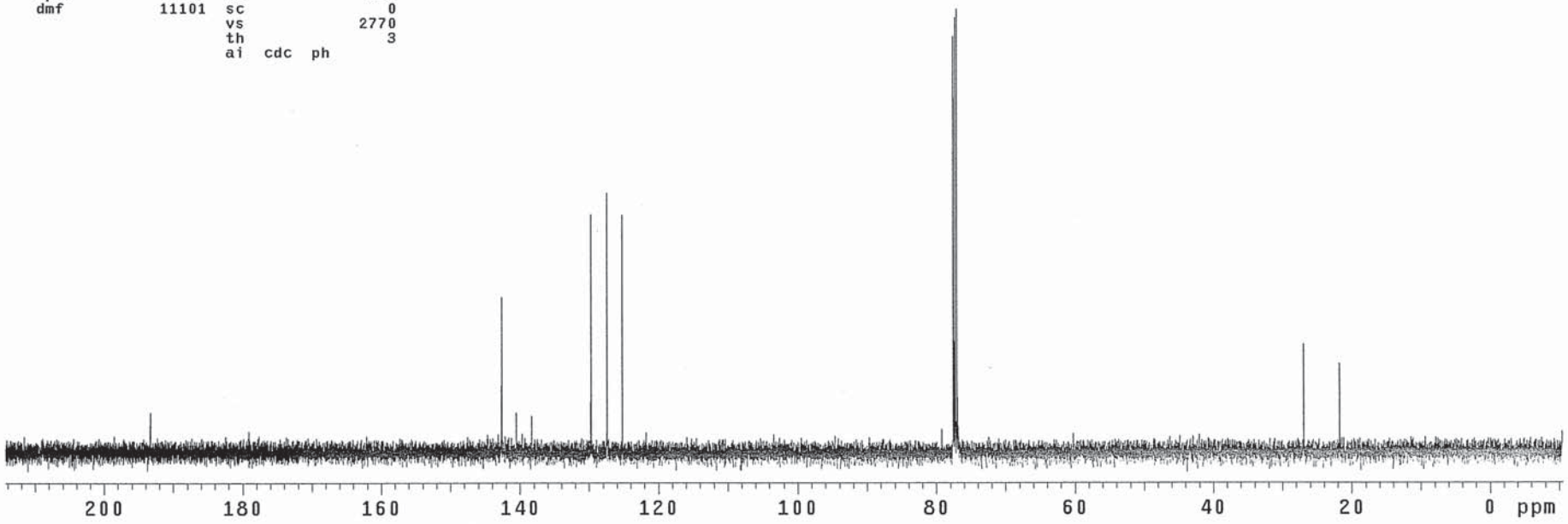
6

```
lcq2-115-13C

exp25  CARBON

      SAMPLE
date    Dec 17 2010
solvent       cdcl3
file            exp
   ACQUISITION
sw          28258.6
at              1.300
np              73498
fb              16000
bs                  2
d1              3.000
nt              10000
ct                446
   TRANSMITTER
tn                C13
sfrq          125.702
tof             865.4
tpwr               56
pw             13.500
    DECOUPLER
dn                 H1
dof                 0
dm                nny
decwave
dpwr               36
dmf             11101

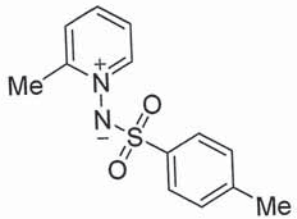
      SPECIAL
temp         not used
gain               54
spin         not used
hst             0.008
pw90            9.200
alfa           10.000
        FLAGS
il                  n
in                  n
dp                  y
hs                 nn
     PROCESSING
lb               0.50
lsfid               2
fn           not used
      DISPLAY
sp           -1326.0
wp           28258.1
rfl          11004.4
rfp           9678.0
rp               3.2
lp            -926.2
       PLOT
wc                250
sc                  0
vs               2770
th                  3
ai  cdc  ph
```



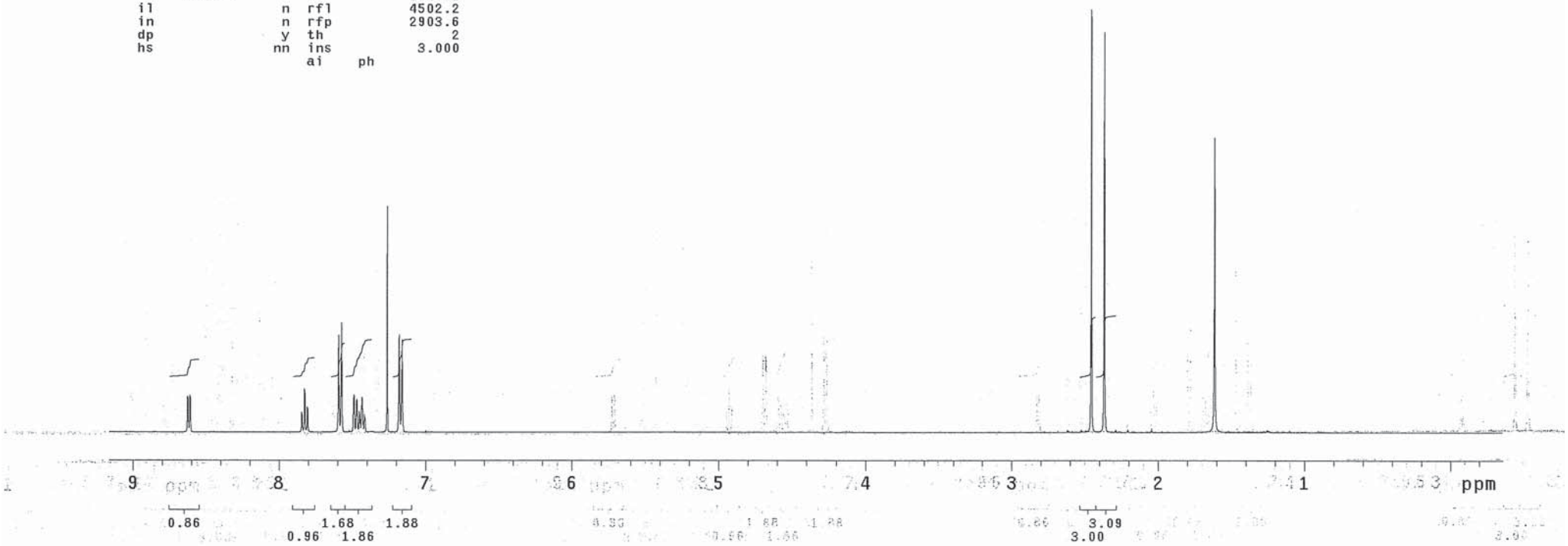
lcq2-226

exp25 s2pul

SAMPLE		DEC. & VT	
date	Oct 20 2010	dn	H1
solvent	cdcl3	dof	-1425.0
file	/home/Zhang/c~ qli/lcq2-226.fid	dm	nnn
		dmm	c
ACQUISITION		dmf	200
sfrq	399.951	PROCESSING	
tn	H1	lb	0.10
at	2.502	fn	65536
np	36008	math	f
sw	7196.8		
fb	not used	werr	
bs	2	wexp	
pw	8.0	wbs	
pw	8.0	wnt	
tpwr	57	DISPLAY	
d1	3.000	sp	-144.0
tof	-6.9	wp	3808.4
nt	16	vs	56
ct	14	sc	0
alock	n	wc	250
gain	not used	hzmm	15.23
FLAGS		is	384.92
il	n	rfl	4502.2
in	n	rfp	2903.6
dp	y	th	2
hs	nn	ins	3.000
		ai ph	



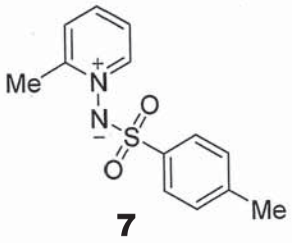
7



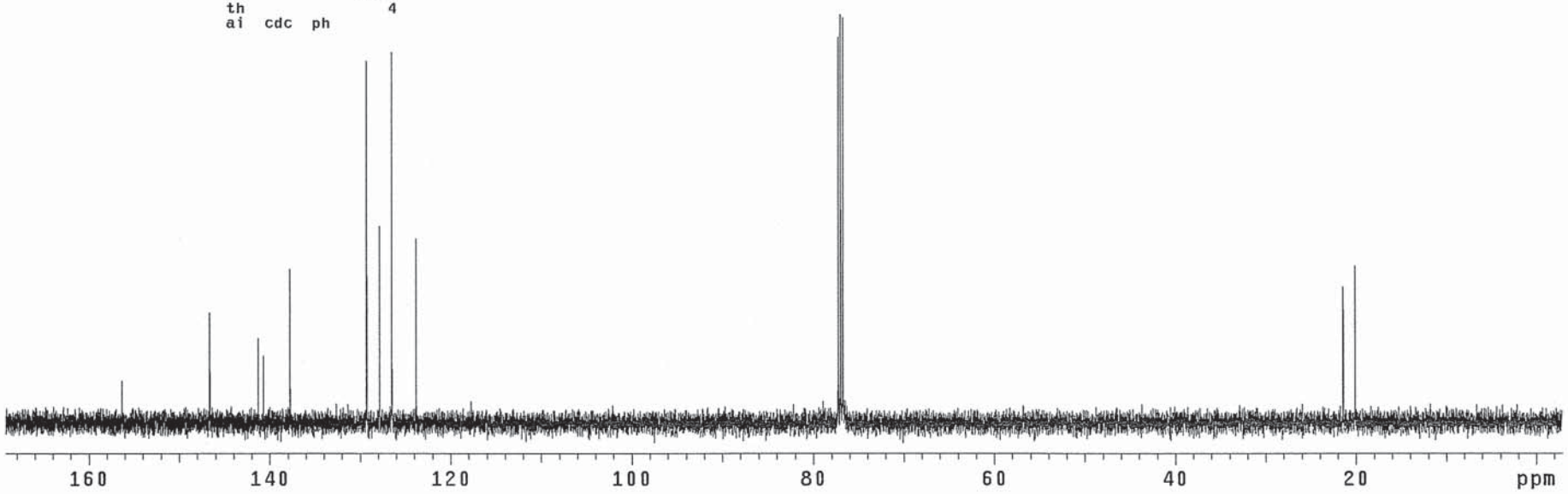
lcq2-226-13C

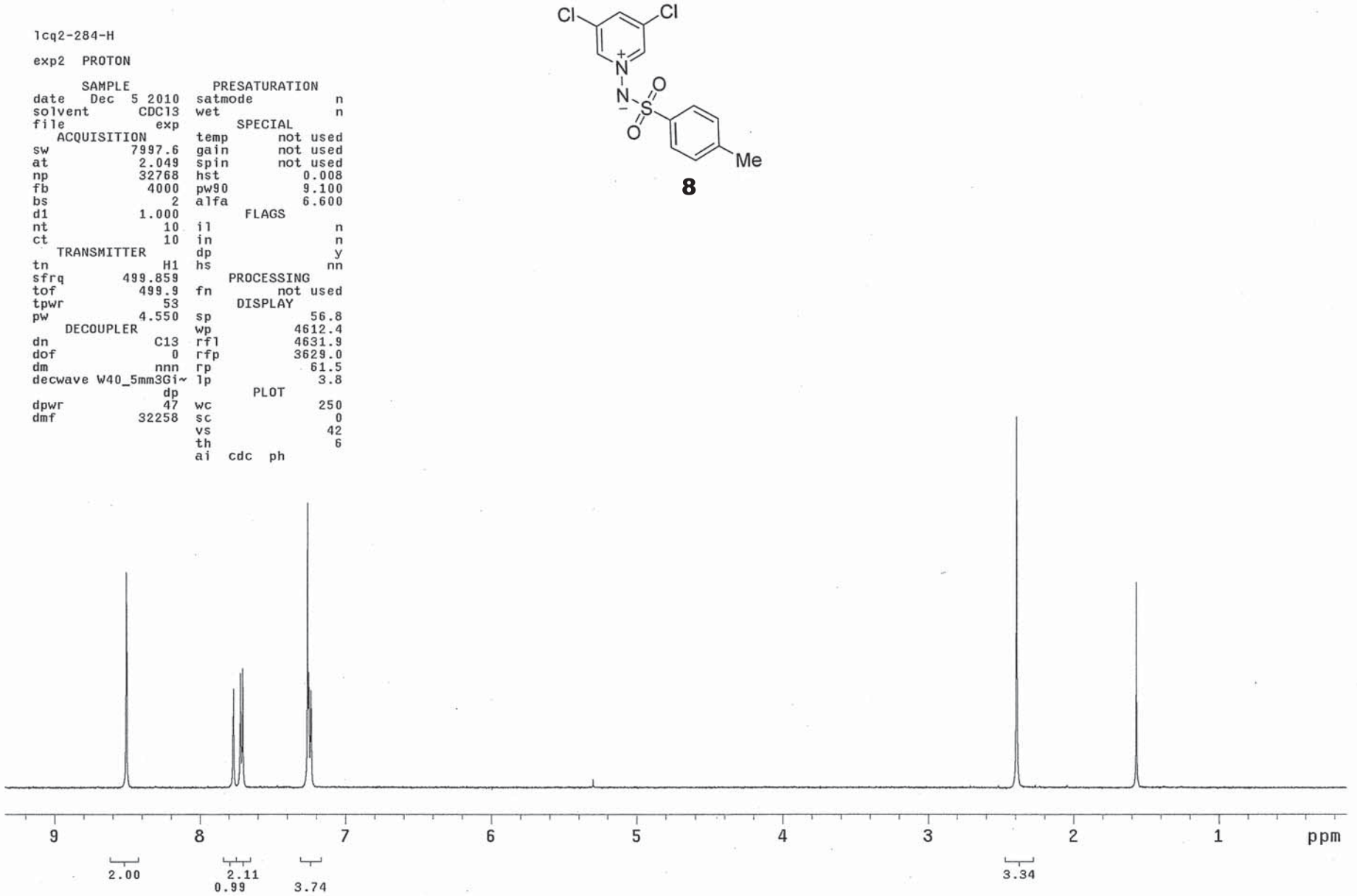
exp25 CARBON

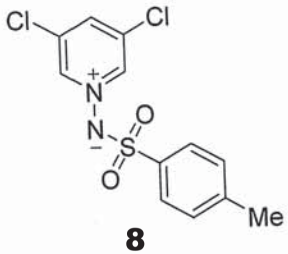
SAMPLE		SPECIAL	
date	Dec 17 2010	temp	not used
solvent	cdcl3	gain	54
file	exp	spin	not used
ACQUISITION		hst	0.008
sw	28258.6	pw90	9.200
at	1.300	alfa	10.000
np	73498	FLAGS	
fb	16000	il	n
bs	2	in	n
d1	3.000	dp	y
nt	10000	hs	nn
ct	234	PROCESSING	
TRANSMITTER		lb	0.50
tn	C13	lsfid	2
sfrq	125.702	fn	not used
tof	865.4	DISPLAY	
tpwr	56	sp	-365.7
pw	13.500	wp	21632.4
DECOUPLER		rfl	11037.6
dn	H1	rfp	9678.0
dof	0	rp	6.3
dm	nny	lp	-920.3
decwave		PLOT	
dpwr	36	wc	250
dmf	11101	sc	0
		vs	2141
		th	4
		ai cdc ph	



7




lcq2-284-H
exp2 PROTON
SAMPLE
date Dec 5 2010
solvent CDCl3
file exp
ACQUISITION
sw 7997.6
at 2.049
np 32768
fb 4000
bs 2
d1 1.000
nt 10
ct 10
TRANSMITTER
tn H1
sfrq 499.859
tof 499.9
tpwr 53
pw 4.550
DECOUPLER
dn C13
dof 0
dm nnn
decwave W40_5mm3Gi~
dp
dpwr 47
dmf 32258
PRESATURATION
satmode n
wet n
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 9.100
alfa 6.600
FLAGS
il n
in n
dp y
hs nn
PROCESSING
fn not used
DISPLAY
sp 56.8
wp 4612.4
rfl 4631.9
rfp 3629.0
rp 61.5
lp 3.8
PLOT
wc 250
sc 0
vs 42
th 6
ai cdc ph
Cl
Cl
N
N
O
O
S
O
Me
8
9
8
7
6
5
4
3
2
1
ppm
2.00
2.11
0.99
3.74
3.34

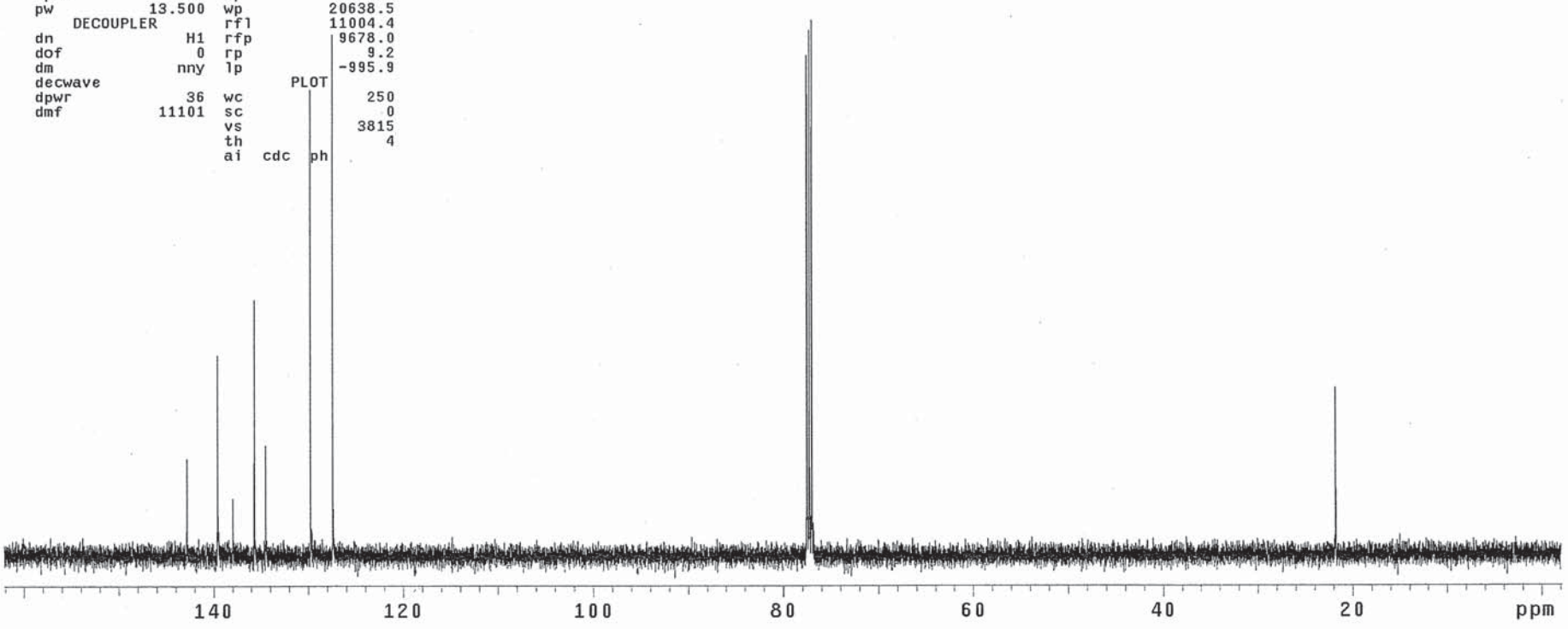


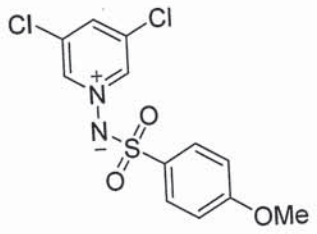
8

```
lcq2-284-13C

exp2  CARBON

      SAMPLE              SPECIAL
date    Dec  5 2010  temp       not used
solvent       cdcl3  gain            54
file            exp  spin       not used
   ACQUISITION        hst           0.008
sw          28258.6  pw90          9.200
at            1.300  alfa         10.000
np            73498          FLAGS
fb            16000  il                n
bs                2  in                n
d1            3.000  dp                y
nt            10000  hs               nn
ct              742       PROCESSING
   TRANSMITTER       lb             0.50
tn               C13  lsfid             2
sfrq        125.702  fn         not used
tof           865.4        DISPLAY
tpwr             56  sp           -266.1
pw           13.500  wp          20638.5
    DECOUPLER        rfl         11004.4
dn                H1  rfp          9678.0
dof                0  rp              9.2
dm               nny  lp           -995.9
decwave                      PLOT
dpwr              36  wc              250
dmf            11101  sc                0
                      vs             3815
                      th                4
                      ai  cdc  ph
```



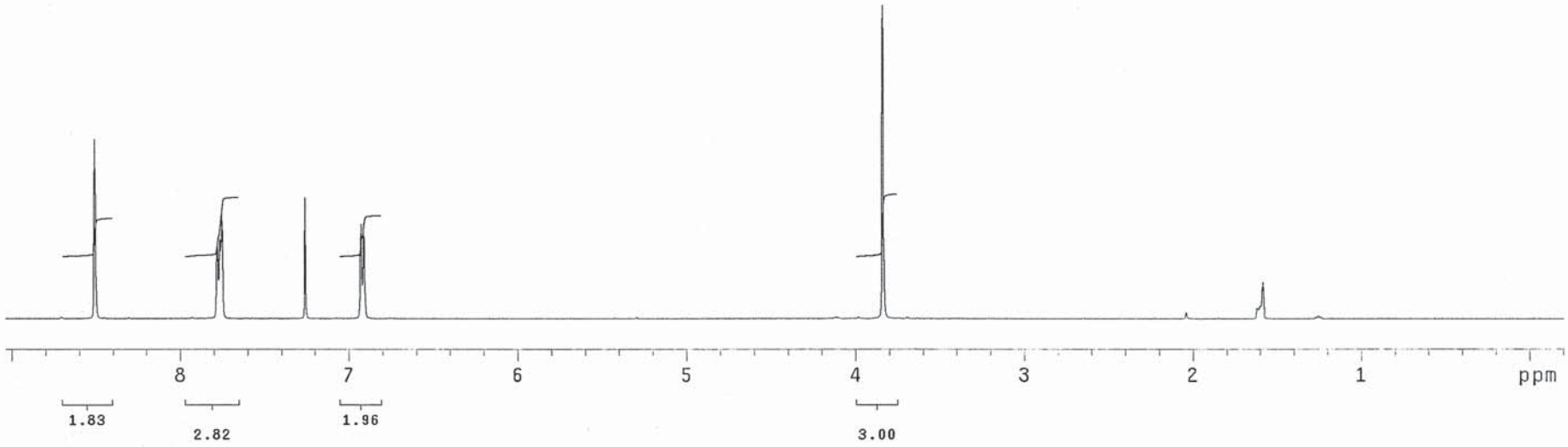



```
lcq3-120-H

exp25  PROTON

      SAMPLE
date    Dec 24 2010
solvent       CDCl3
file            exp
   ACQUISITION
sw           7997.6
at            2.049
np            32768
fb             4000
bs                2
d1            1.000
nt               16
ct               16
   TRANSMITTER
tn               H1
sfrq        499.859
tof           499.9
tpwr             53
pw            4.550
    DECOUPLER
dn              C13
dof               0
dm              nnn
decwave W40_5mm3Gi~
                dp
dpwr             47
dmf           32258

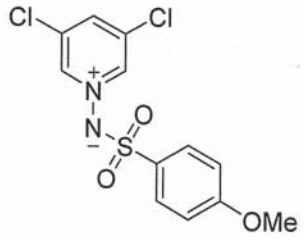
   PRESATURATION
satmode           n
wet               n
      SPECIAL
temp        not used
gain        not used
spin        not used
hst             0.008
pw90            9.100
alfa            6.600
      FLAGS
il                n
in                n
dp                y
hs               nn
    PROCESSING
fn          not used
    DISPLAY
sp             -103.8
wp             4621.7
rfl            4632.9
rfp            3629.0
rp              179.4
lp                3.4
      PLOT
wc                250
sc                  0
vs                 25
th                  3
ai  cdc  ph
```

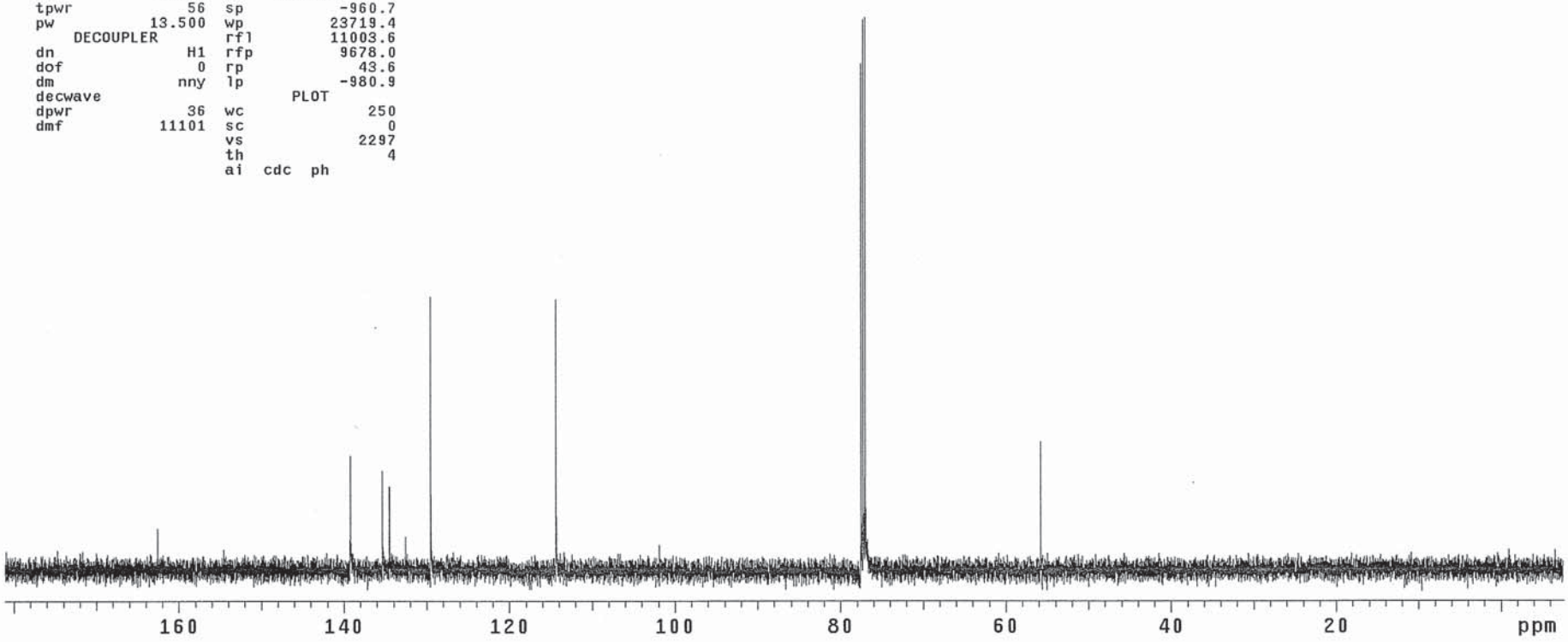


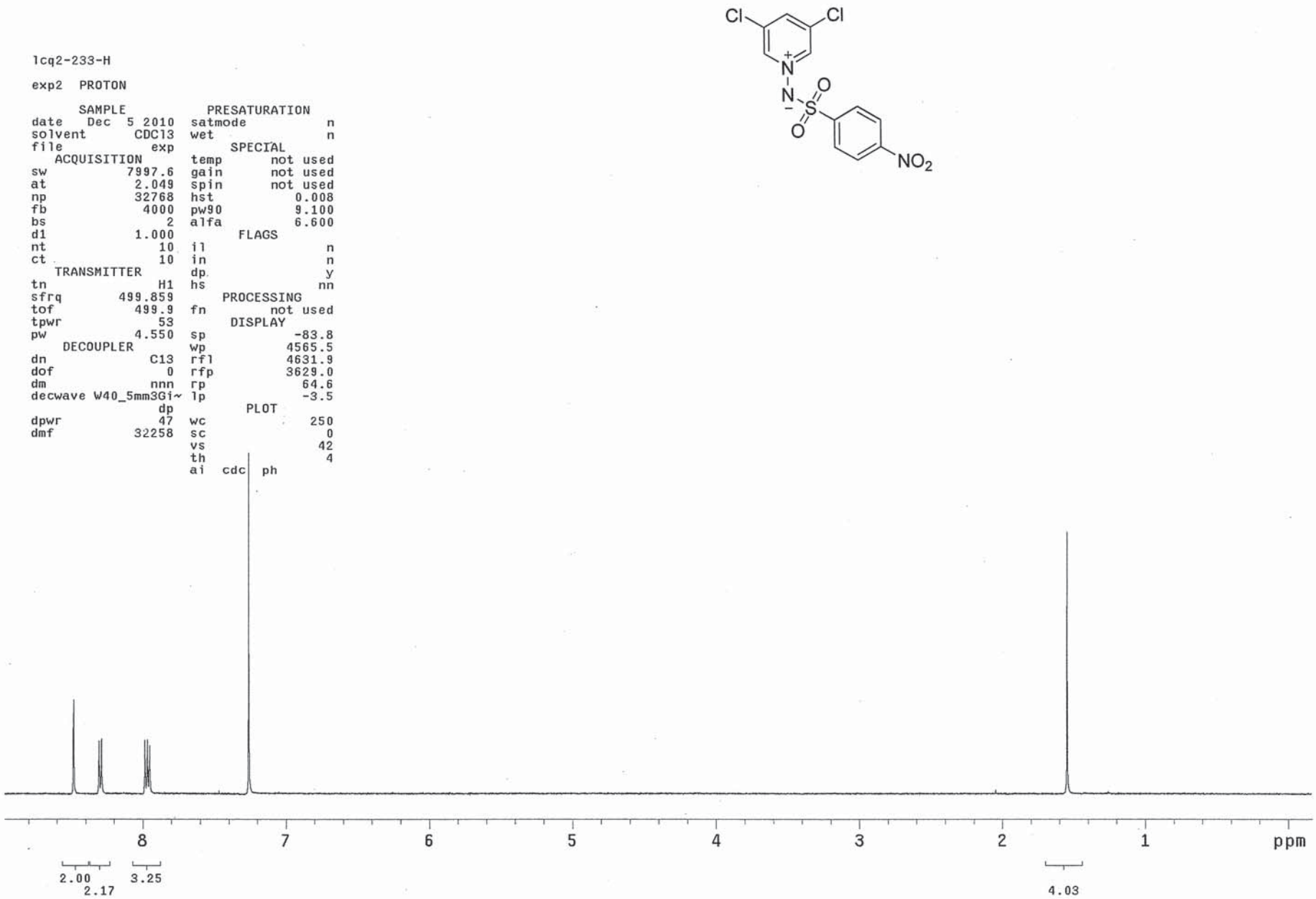
lcq3-120-13C

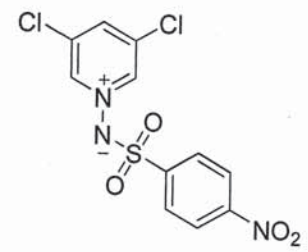
exp25 CARBON

SAMPLE		SPECIAL	
date	Dec 24 2010	temp	not used
solvent	cdcl3	gain	54
file	exp	spin	not used
ACQUISITION		hst	0.008
sw	28258.6	pw90	9.200
at	1.300	alfa	10.000
np	73498	FLAGS	
fb	16000	il	n
bs	2	in	n
d1	3.000	dp	y
nt	10000	hs	nn
ct	334	PROCESSING	
TRANSMITTER		lb	0.50
tn	C13	lsfid	2
sfrq	125.702	fn	not used
tof	865.4	DISPLAY	
tpwr	56	sp	-960.7
pw	13.500	wp	23719.4
DECOUPLER		rfl	11003.6
dn	H1	rfp	9678.0
dof	0	rp	43.6
dm	nny	lp	-980.9
decwave		PLOT	
dpwr	36	wc	250
dmf	11101	sc	0
		vs	2297
		th	4
		ai cdc ph	






lcq2-233-H
exp2 PROTON
SAMPLE
date Dec 5 2010
solvent CDCl3
file exp
ACQUISITION
sw 7997.6
at 2.049
np 32768
fb 4000
bs 2
d1 1.000
nt 10
ct 10
TRANSMITTER
tn H1
sfrq 499.859
tof 499.9
tpwr 53
pw 4.550
DECOUPLER
dn C13
dof 0
dm nnn
decwave W40_5mm3Gi~
dp
dpwr 47
dmf 32258
PRESATURATION
satmode n
wet n
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 9.100
alfa 6.600
FLAGS
il n
in n
dp y
hs nn
PROCESSING
fn not used
DISPLAY
sp -83.8
wp 4565.5
rfl 4631.9
rfp 3629.0
rp 64.6
lp -3.5
PLOT
wc 250
sc 0
vs 42
th 4
ai cdc ph
Cl
Cl
N
N
O
S
O
O
NO2
8
7
6
5
4
3
2
1
ppm
2.00
2.17
3.25
4.03

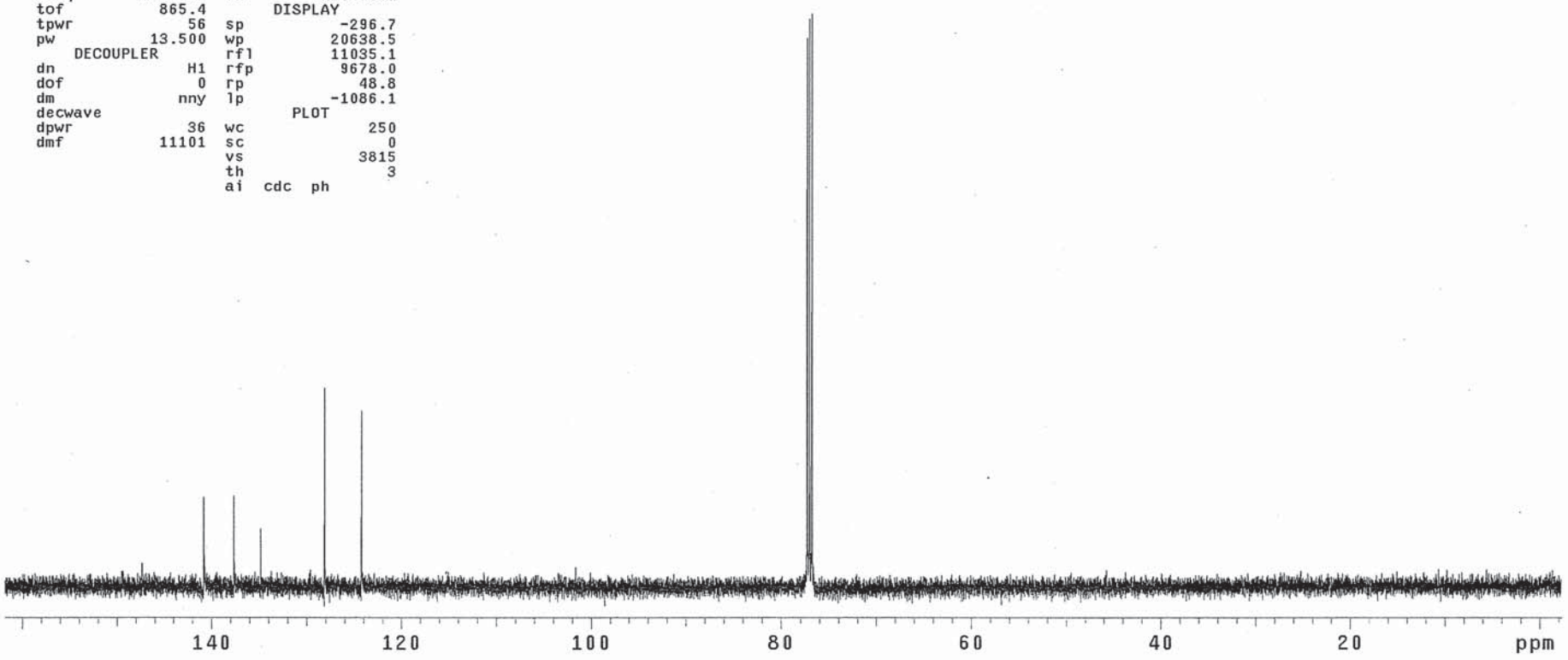


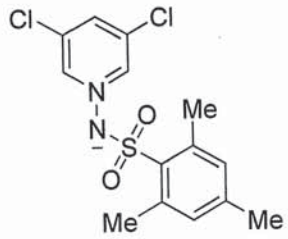

```
lcq2-233-13C

exp2  CARBON

      SAMPLE
date    Dec  5 2010
solvent       cdcl3
file            exp
   ACQUISITION
sw          28258.6
at              1.300
np              73498
fb              16000
bs                  2
d1              3.000
nt              10000
ct               1032
   TRANSMITTER
tn                C13
sfrq          125.702
tof             865.4
tpwr               56
pw             13.500
    DECOUPLER
dn                 H1
dof                 0
dm                nny
decwave
dpwr               36
dmf             11101

      SPECIAL
temp         not used
gain               54
spin         not used
hst               0.008
pw90              9.200
alfa             10.000
        FLAGS
il                    n
in                    n
dp                    y
hs                   nn
    PROCESSING
lb                 0.50
lsfid                 2
fn           not used
     DISPLAY
sp              -296.7
wp             20638.5
rfl            11035.1
rfp             9678.0
rp                48.8
lp             -1086.1
       PLOT
wc                  250
sc                    0
vs                 3815
th                    3
ai  cdc  ph
```

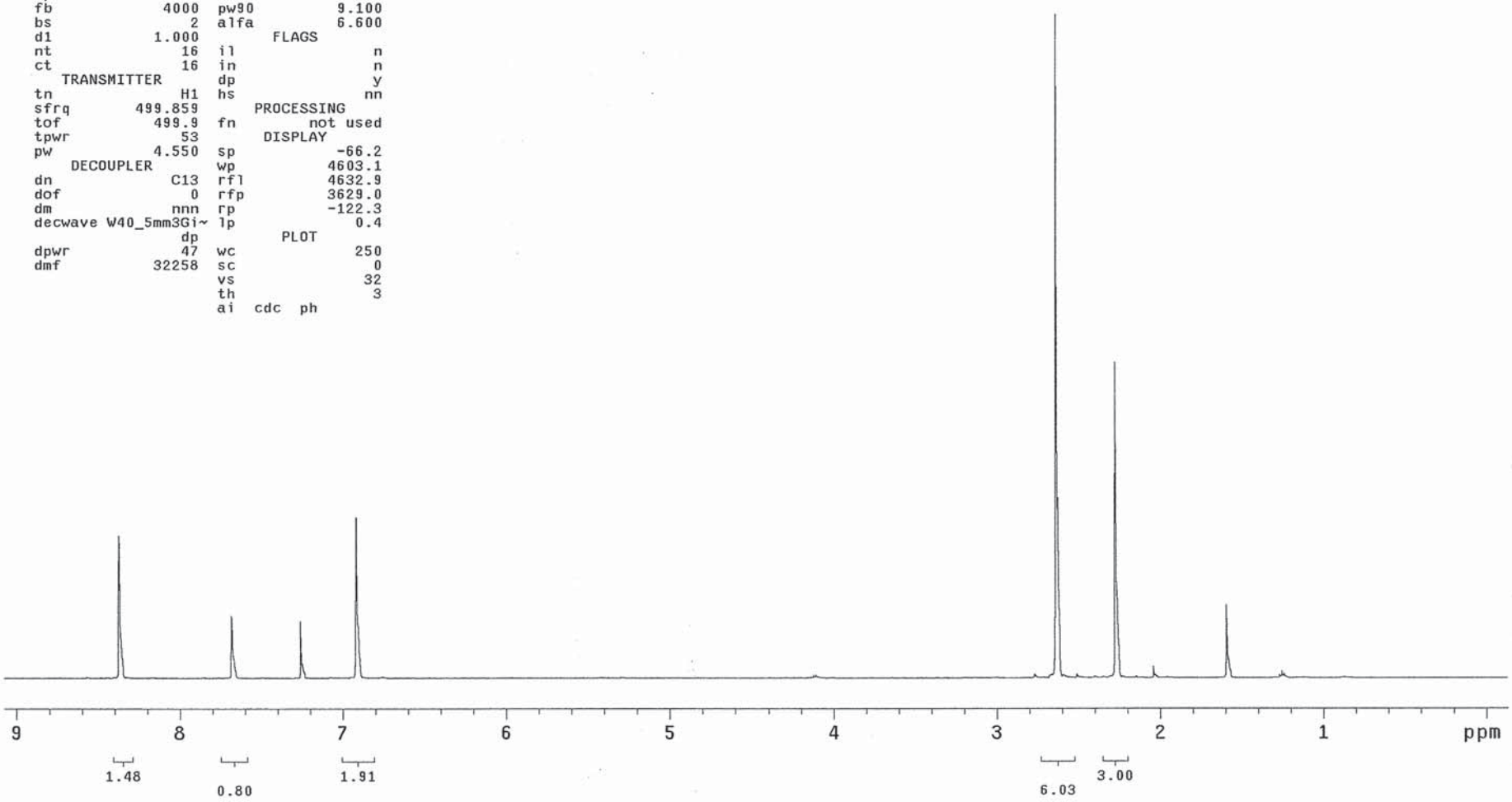


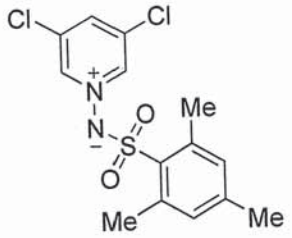


lcq3-169-H

exp1 PROTON

SAMPLE		PRESATURATION	
date	Jan 16 2011	satmode	n
solvent	CDCl3	wet	n
file	exp	SPECIAL	
ACQUISITION		temp	not used
sw	7997.6	gain	not used
at	2.049	spin	not used
np	32768	hst	0.008
fb	4000	pw90	9.100
bs	2	alfa	6.600
d1	1.000	FLAGS	
nt	16	il	n
ct	16	in	n
TRANSMITTER		dp	y
tn	H1	hs	nn
sfrq	499.859	PROCESSING	
tof	499.9	fn	not used
tpwr	53	DISPLAY	
pw	4.550	sp	-66.2
DECOUPLER		wp	4603.1
dn	C13	rfl	4632.9
dof	0	rfp	3629.0
dm	nnn	rp	-122.3
decwave	W40_5mm3Gi~	lp	0.4
	dp	PLOT	
dpwr	47	wc	250
dmf	32258	sc	0
		vs	32
		th	3
		ai cdc ph	



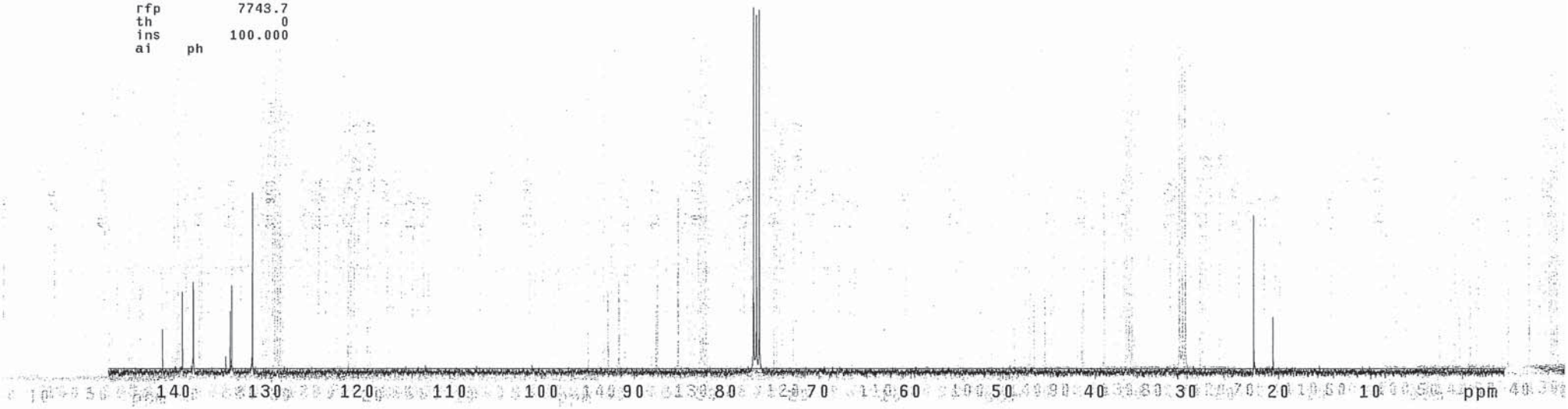



```
lcq3-169-13C

exp25  std13c

      SAMPLE
date   Jan 16 2011
solvent      cdcl3
file           exp
   ACQUISITION
sfrq       100.577
tn             C13
at             0.701
np             39216
sw          27972.0
fb         not used
bs                2
ss                4
tpwr             58
pw              7.0
d1            1.300
tof           525.7
nt           100000
ct             1596
alock             n
gain             44
      FLAGS
il                n
in                n
dp                y
hs               nn
     DISPLAY
sp           -465.8
wp          15259.6
vs             6974
sc                0
wc              250
hzmm          61.04
is           500.00
rfl         11705.9
rfp          7743.7
th                0
ins          100.000
ai    ph

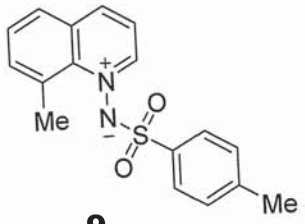
      DEC. & VT
dfrq       399.951
dn              H1
dpwr            40
dof              0
dm             nny
dmm              w
dmf           6700
dseq
dres          90.0
homo             n
     PROCESSING
lb            1.00
wtfile
proc             ft
fn           65536
math             f
werr
wexp
wbs
wnt
```



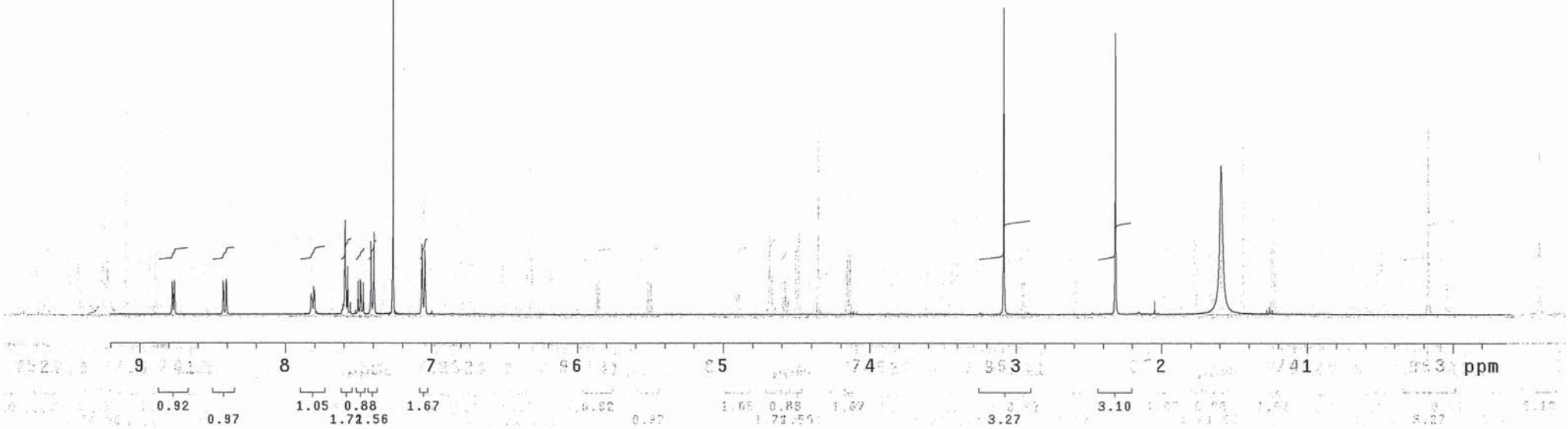
lcq2-198

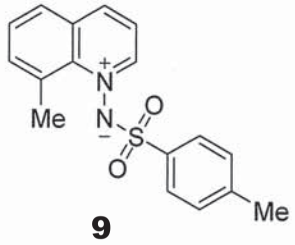
exp25 s2pul

SAMPLE		DEC. & VT	
date	Oct 13 2010	dn	H1
solvent	cdcl3	dof	-1425.0
file	/home/Zhang/c~ qli/lcq2-198.fid	dm	nnn
		dmm	c
ACQUISITION		dmf	200
sfrq	399.951	PROCESSING	
tn	H1	lb	0.10
at	2.502	fn	65536
np	36008	math	f
sw	7196.8		
fb	not used	werr	
bs	2	wexp	
pw	8.0	wbs	
pw	8.0	wnt	
tpwr	57	DISPLAY	
d1	3.000	sp	-144.6
tof	-6.9	wp	3825.3
nt	12	vs	86
ct	12	sc	0
alock	n	wc	250
gain	not used	hzmm	15.30
FLAGS		is	430.78
il	n	rfl	4502.9
in	n	rfp	2903.6
dp	y	th	3
hs	nn	ins	3.000
		ai ph	



9





9

```
lcq2-198-13C

exp25  CARBON

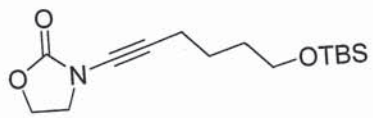
      SAMPLE
date    Dec 19 2010
solvent       cdcl3
file            exp
   ACQUISITION
sw          28258.6
at              1.300
np              73498
fb              16000
bs                  2
d1              3.000
nt              10000
ct               1000
   TRANSMITTER
tn                C13
sfrq          125.702
tof             865.4
tpwr               56
pw             13.500
    DECOUPLER
dn                 H1
dof                 0
dm                nny
decwave
dpwr               36
dmf             11101

      SPECIAL
temp         not used
gain               54
spin         not used
hst             0.008
pw90            9.200
alfa           10.000
        FLAGS
il                  n
in                  n
dp                  y
hs                 nn
     PROCESSING
lb               0.50
lsfid               2
fn           not used
      DISPLAY
sp              -562.3
wp             22063.2
rfl            11035.5
rfp             9678.0
rp               145.5
lp              -861.2
        PLOT
wc                250
sc                  0
vs               5794
th                  7
ai  cdc  ph
```

lcq3-78-H

exp2 PROTON

SAMPLE		PRESATURATION	
date	Dec 8 2010	satmode	n
solvent	CDCl3	wet	n
file	exp	SPECIAL	
ACQUISITION		temp	not used
sw	7997.6	gain	not used
at	2.049	spin	not used
np	32768	hst	0.008
fb	4000	pw90	9.100
bs	2	alfa	6.600
d1	1.000	FLAGS	
nt	20	il	n
ct	20	in	n
TRANSMITTER		dp	y
tn	H1	hs	nn
sfrq	499.859	PROCESSING	
tof	499.9	fn	not used
tpwr	53	DISPLAY	
pw	4.550	sp	-228.3
DECOUPLER		wp	4213.1
dn	C13	rfl	4632.9
dof	0	rfp	3629.0
dm	nnn	rp	47.4
decwave	W40_5mm3Gi~	lp	0.7
	dp	PLOT	
dpwr	47	wc	250
dmf	32258	sc	0
		vs	46
		th	2
		ai cdc ph	

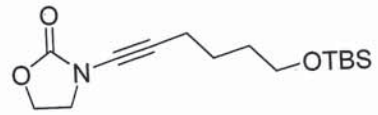


10

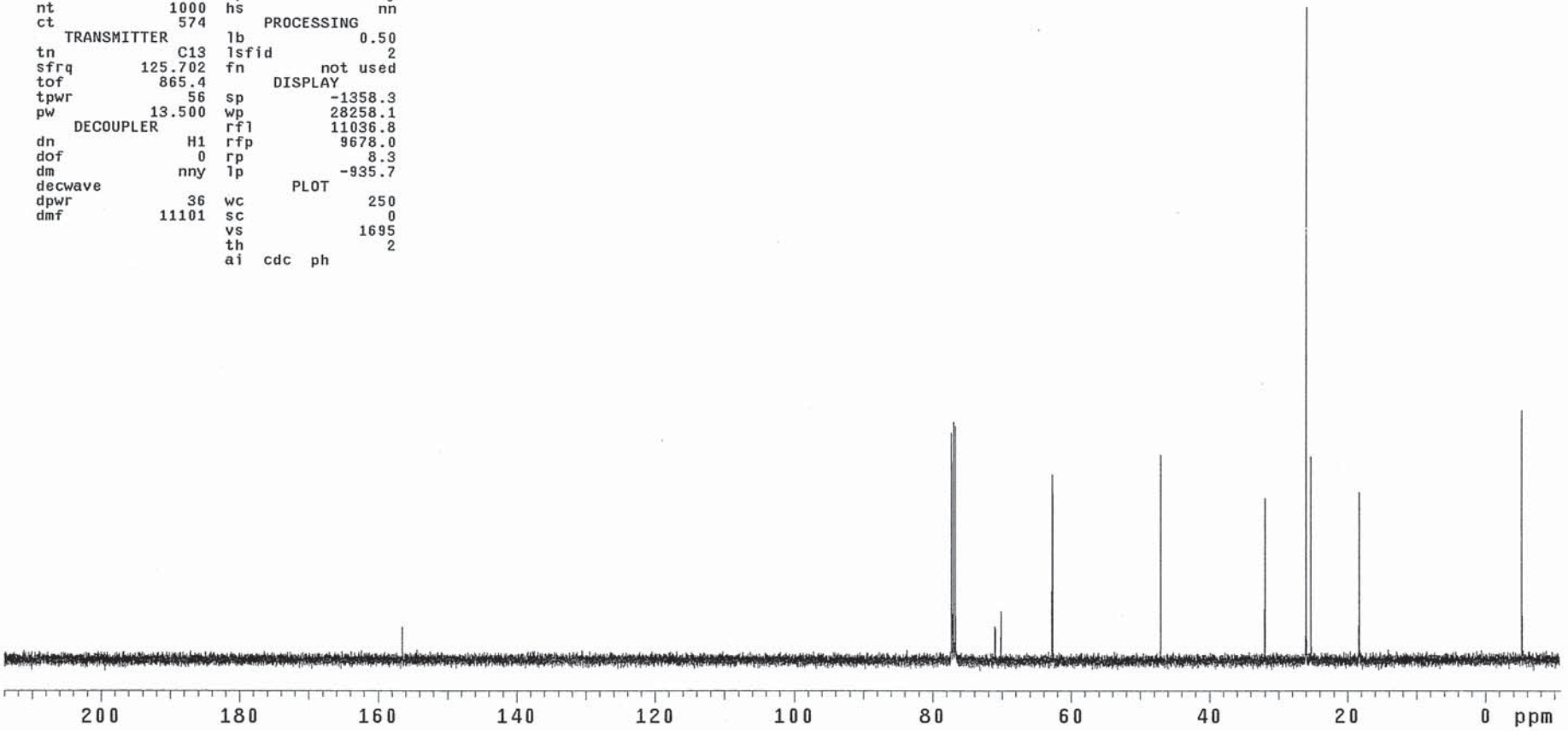
lcq3-78-13C

exp2 CARBON

SAMPLE		SPECIAL	
date	Dec 8 2010	temp	not used
solvent	cdcl3	gain	54
file	exp	spin	not used
ACQUISITION		hst	0.008
sw	28258.6	pw90	9.200
at	1.300	alfa	10.000
np	73498	FLAGS	
fb	16000	il	n
bs	2	in	n
d1	3.000	dp	y
nt	1000	hs	nn
ct	574	PROCESSING	
TRANSMITTER		lb	0.50
tn	C13	lsfid	2
sfrq	125.702	fn	not used
tof	865.4	DISPLAY	
tpwr	56	sp	-1358.3
pw	13.500	wp	28258.1
DECOUPLER		rfl	11036.8
dn	H1	rfp	9678.0
dof	0	rp	8.3
dm	nny	lp	-935.7
decwave		PLOT	
dpwr	36	wc	250
dmf	11101	sc	0
		vs	1695
		th	2
		ai cdc ph	



10

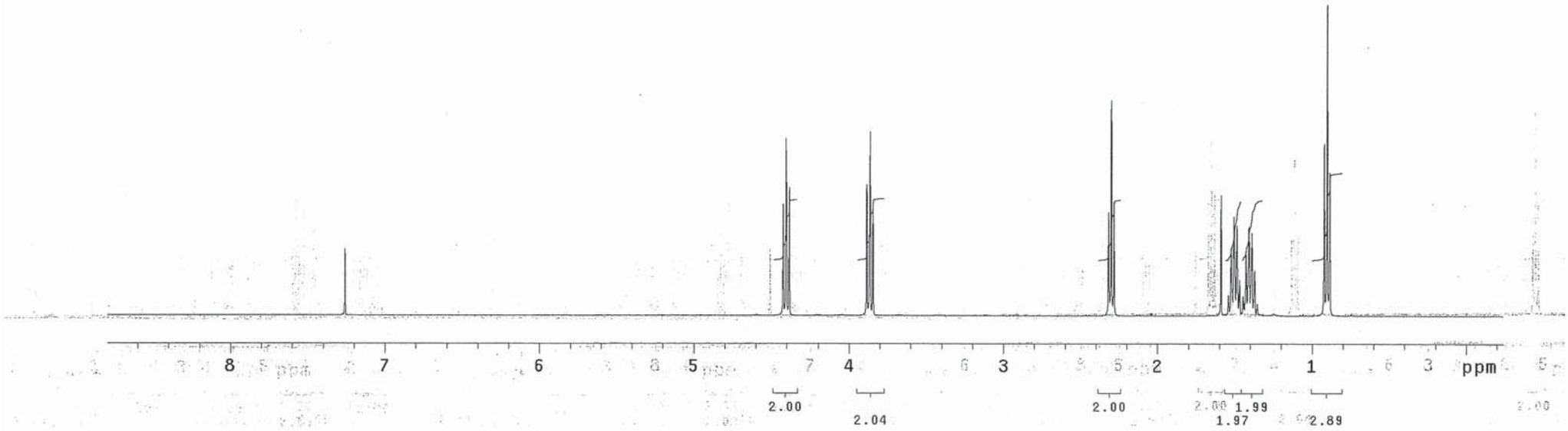


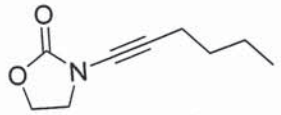
lcq2-192

exp25 s2pul

SAMPLE		DEC. & VT	
date	Oct 12 2010	dn	H1
solvent	cdcl3	dof	-1425.0
file	/home/Zhang/c~	dm	nnn
	qli/lcq2-192.fid	dmm	c
ACQUISITION		dmf	200
sfrq	399.951	temp	22.0
tn	H1	PROCESSING	
at	2.502	lb	0.10
np	36008	fn	65536
sw	7196.8	math	f
fb	not used		
bs	2	werr	
pw	8.0	wexp	
pw	8.0	wbs	
tpwr	57	wnt	
d1	3.000	DISPLAY	
tof	-6.9	sp	-97.0
nt	10	wp	3615.1
ct	8	vs	56
alock	n	sc	0
gain	not used	wc	250
FLAGS		hzmm	14.46
il	n	is	327.48
in	n	rfl	4503.7
dp	y	rfp	2903.6
hs	nn	th	44
		ins	2.000
		ai ph	

13a





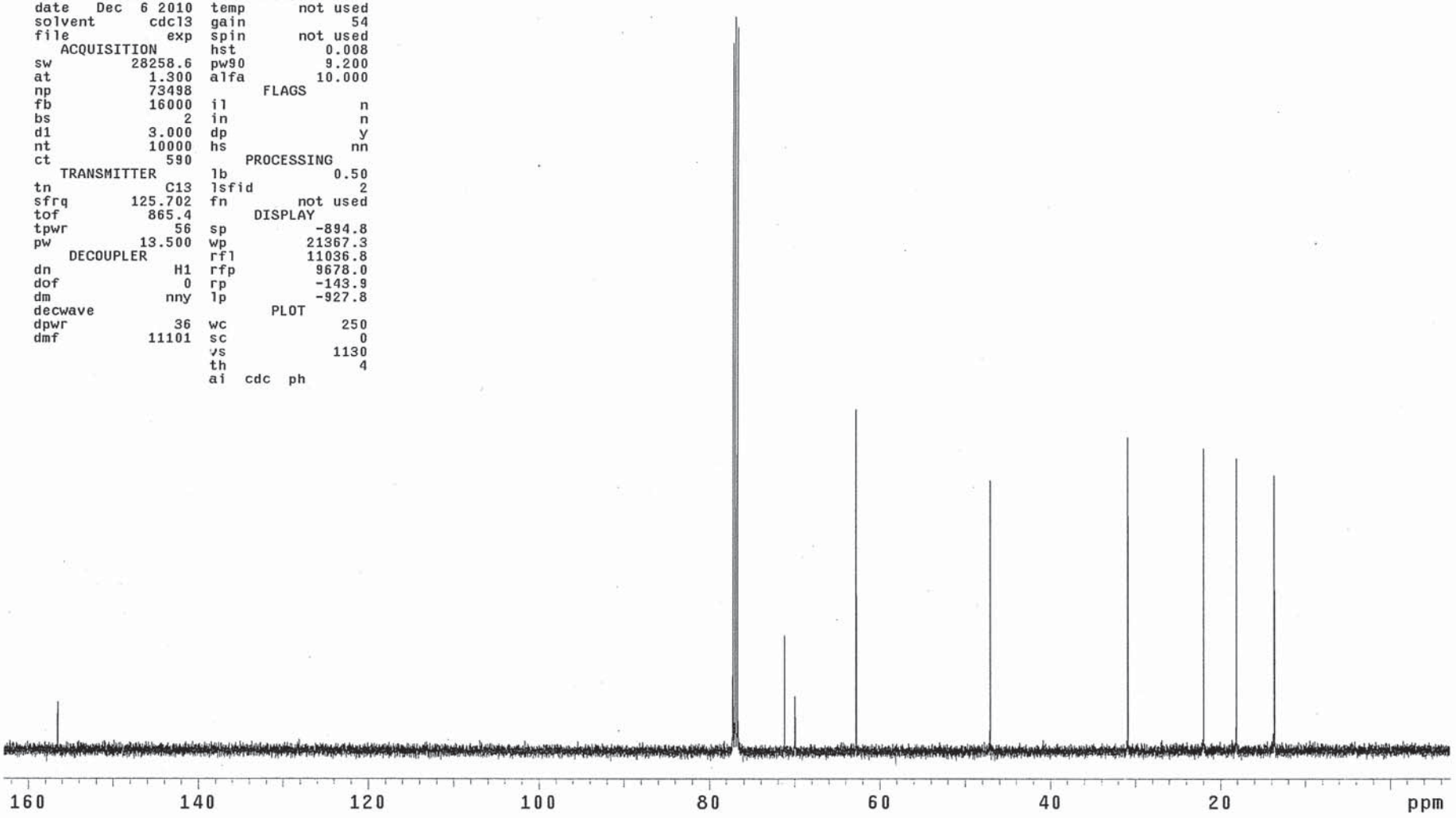
13a

```
lcq2-263-13C

exp2  CARBON

      SAMPLE
date    Dec  6 2010
solvent       cdcl3
file            exp
   ACQUISITION
sw          28258.6
at              1.300
np              73498
fb              16000
bs                  2
d1              3.000
nt              10000
ct                590
   TRANSMITTER
tn                C13
sfrq          125.702
tof             865.4
tpwr               56
pw              13.500
    DECOUPLER
dn                  H1
dof                  0
dm                 nny
decwave
dpwr                36
dmf             11101

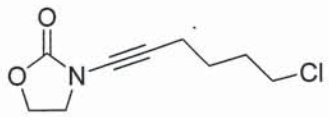
      SPECIAL
temp          not used
gain                54
spin          not used
hst                0.008
pw90               9.200
alfa              10.000
        FLAGS
il                     n
in                     n
dp                     y
hs                    nn
     PROCESSING
lb                  0.50
lsfid                  2
fn            not used
       DISPLAY
sp                -894.8
wp               21367.3
rfl              11036.8
rfp               9678.0
rp                -143.9
lp                -927.8
          PLOT
wc                   250
sc                     0
vs                  1130
th                     4
ai  cdc  ph
```



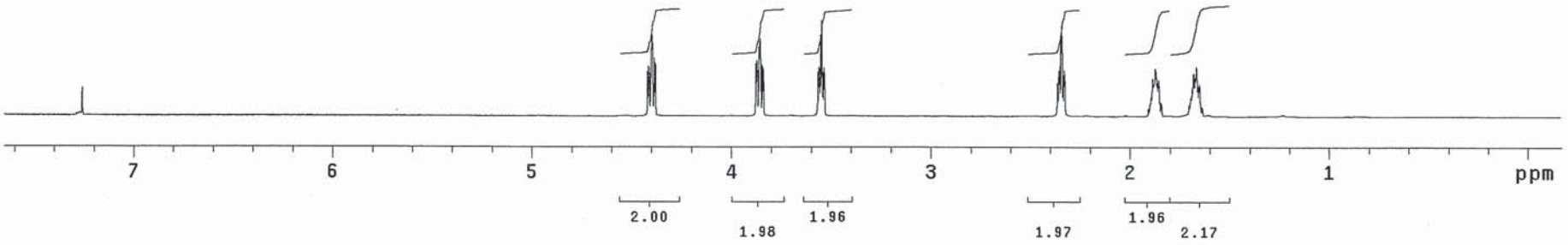
lcq3-106-H

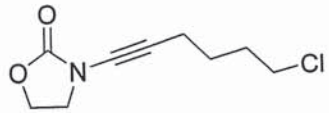
exp25 PROTON

SAMPLE		PRESATURATION	
date	Dec 14 2010	satmode	n
solvent	CDCl3	wet	n
file	exp	SPECIAL	
ACQUISITION		temp	not used
sw	7997.6	gain	not used
at	2.049	spin	not used
np	32768	hst	0.008
fb	4000	pw90	9.100
bs	2	alfa	6.600
d1	1.000	FLAGS	
nt	12	il	n
ct	12	in	n
TRANSMITTER		dp	y
tn	H1	hs	nn
sfrq	499.859	PROCESSING	
tof	499.9	fn	not used
tpwr	53	DISPLAY	
pw	4.550	sp	-84.3
DECOUPLER		wp	3909.5
dn	C13	rfl	4632.4
dof	0	rfp	3629.0
dm	nnn	rp	57.2
decwave	W40_5mm3Gi~dp	lp	-4.6
dpwr	47	PLOT	
dmf	32258	wc	250
		sc	0
		vs	24
		th	2
		ai cdc ph	



13b



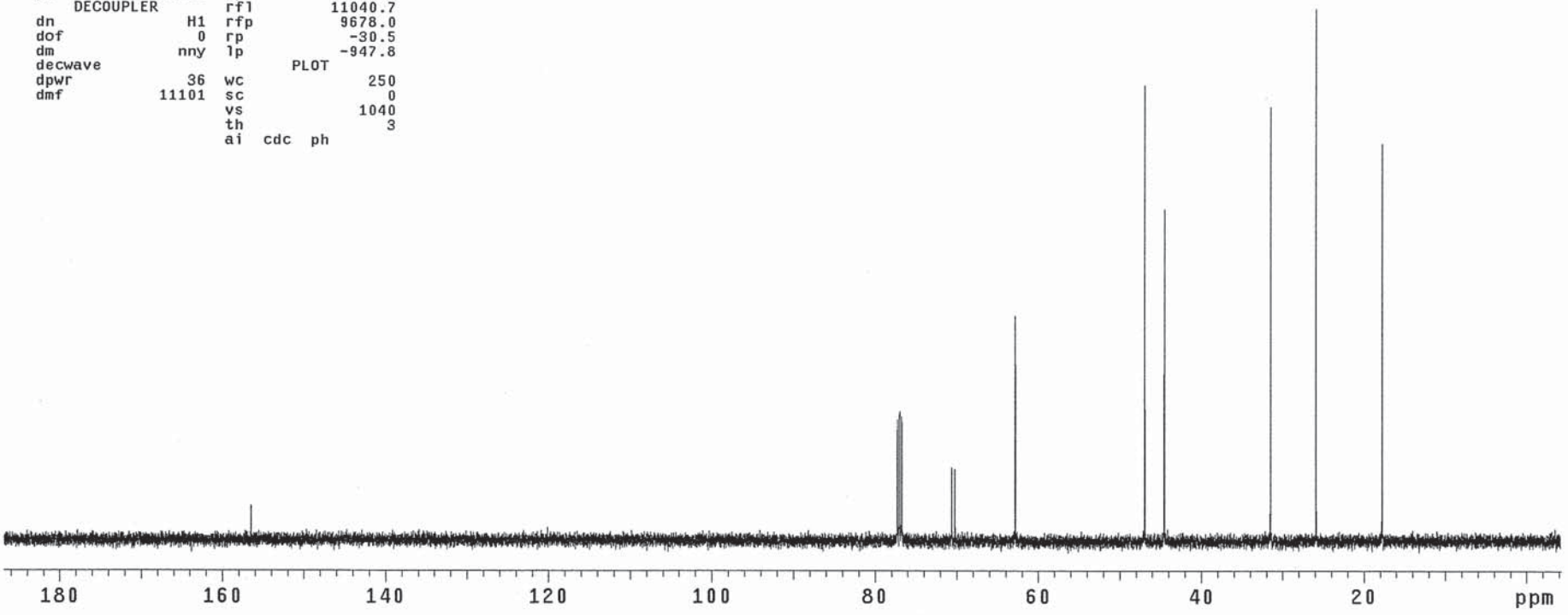


13b

lcq3-106-13C

exp25 CARBON

SAMPLE		SPECIAL	
date	Dec 14 2010	temp	not used
solvent	cdcl3	gain	54
file	exp	spin	not used
ACQUISITION		hst	0.008
sw	28258.6	pw90	9.200
at	1.300	alfa	10.000
np	73498	FLAGS	
fb	16000	il	n
bs	2	in	n
d1	3.000	dp	y
nt	10000	hs	nn
ct	184	PROCESSING	
TRANSMITTER		lb	0.50
tn	C13	lsfid	2
sfrq	125.702	fn	not used
tof	865.4	DISPLAY	
tpwr	56	sp	-534.3
pw	13.500	wp	24017.4
DECOUPLER		rfl	11040.7
dn	H1	rfp	9678.0
dof	0	rp	-30.5
dm	nny	lp	-947.8
decwave		PLOT	
dpwr	36	wc	250
dmf	11101	sc	0
		vs	1040
		th	3
		ai cdc ph	

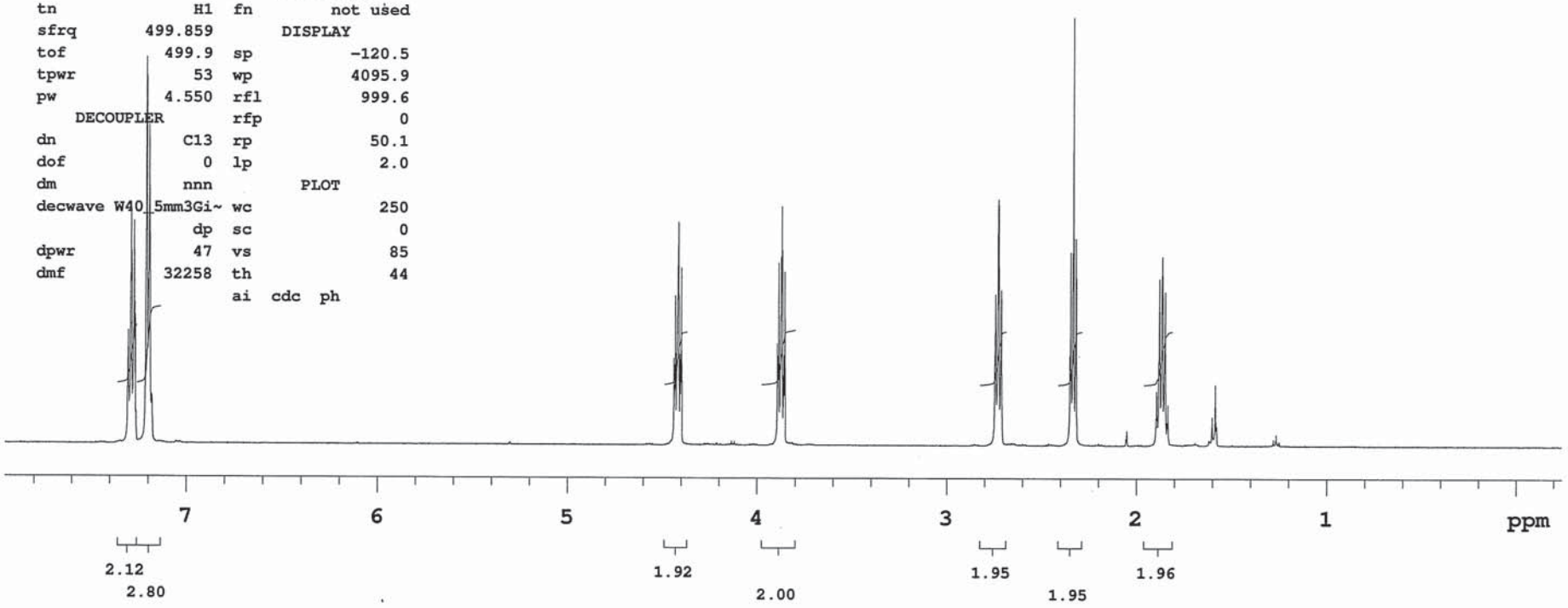


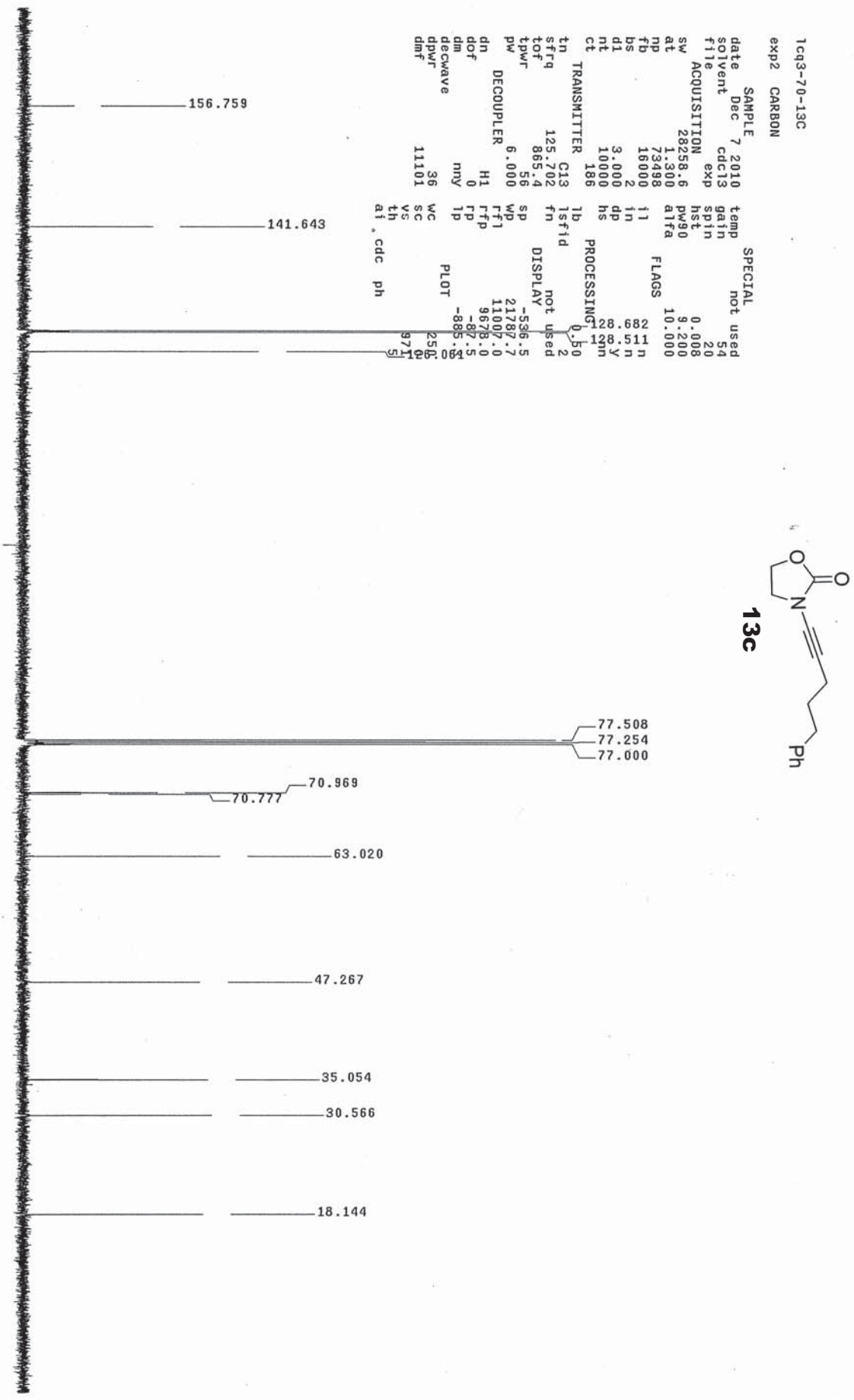
lcq3-70-h

exp1 PROTON

SAMPLE		PRESATURATION	
date	Dec 6 2010	satmode	n
solvent	CDCl3	wet	n
file	/nmr500/Zhang~	SPECIAL	
/cqli/lcq3-70-h.fi~	d	temp	not used
		gain	not used
ACQUISITION		spin	not used
sw	7997.6	hst	0.008
at	2.049	pw90	9.100
np	32768	alfa	6.600
fb	4000	FLAGS	
bs	2	il	n
d1	1.000	in	n
nt	16	dp	y
ct	16	hs	nn
TRANSMITTER		PROCESSING	
tn	H1	fn	not used
sfrq	499.859	DISPLAY	
tof	499.9	sp	-120.5
tpwr	53	wp	4095.9
pw	4.550	rfl	999.6
DECOUPLER		rfp	0
dn	C13	rp	50.1
dof	0	lp	2.0
dm	nnn	PLOT	
decwave	W40_5mm3Gi~	wc	250
	dp	sc	0
dpwr	47	vs	85
dmf	32258	th	44
		ai cdc ph	

13c




lcq3-70-13C
exp2 CARBON
SAMPLE
date Dec 7 2010
solvent cdcl3
file exp
ACQUISITION
sw 28258.6
at 1.300
np 73498
fb 16000
bs 2
d1 3.000
nt 10000
ct 186
TRANSMITTER
tn C13
sfrq 125.702
tof 865.4
tpwr 56
pw 6.000
DECOUPLER
dn H1
dof 0
dm nny
decwave
dpwr
dmf
PLOT
wc
sc
vs
th
ai
cdc ph
temp
gain
spin
hst
pw90
alfa
FLAGS
il
in
dp
hs
PROCESSING
lb
lsfid
fn
DISPLAY
sp
wp
rfl
rfp
rp
lp
SPECIAL
not used
54
20
0.008
9.200
10.000
128.682
128.511
not used
not used
156.759
141.643
77.508
77.254
77.000
70.969
70.777
63.020
47.267
35.054
30.566
18.144
13c
O
O
N
Ph

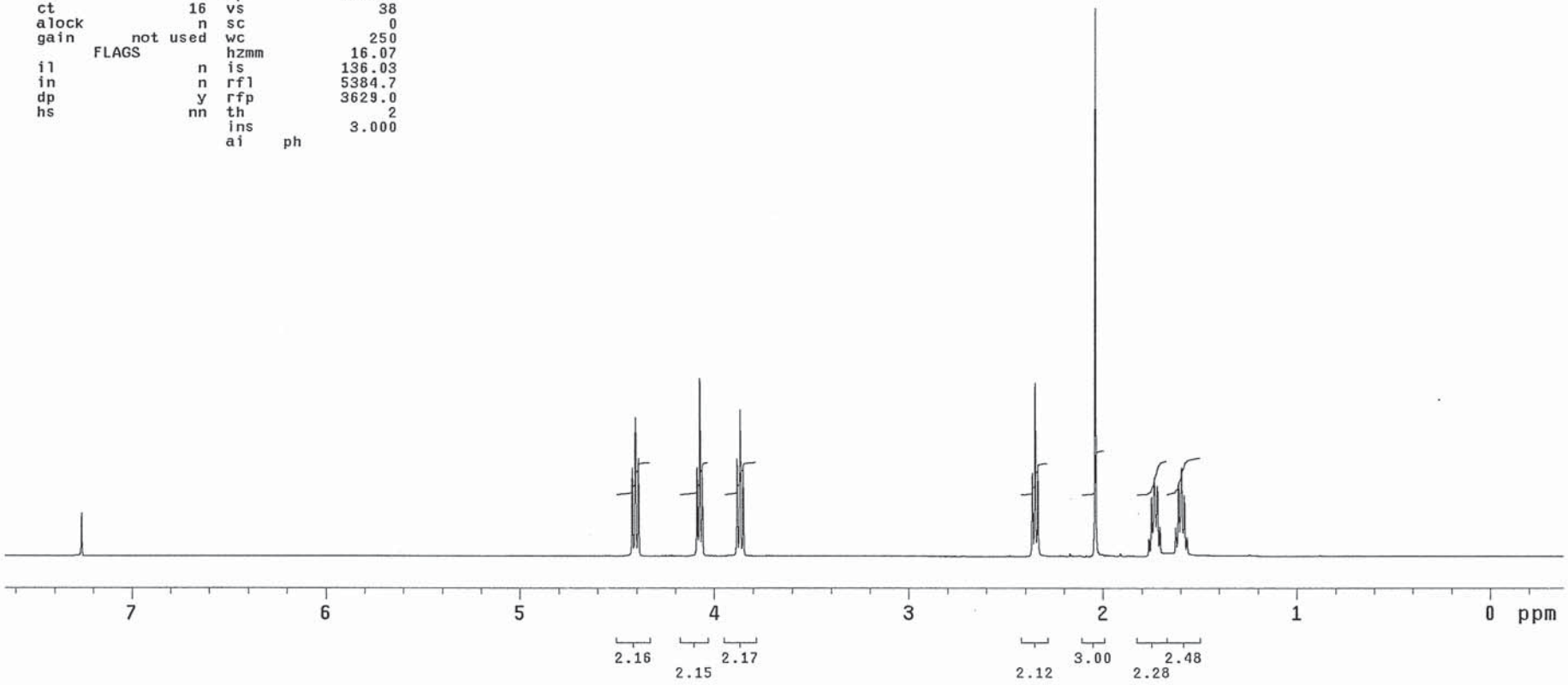
13d

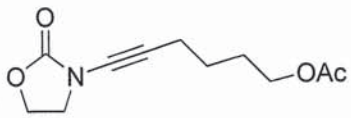
```
lcq3-92

exp25  s2pul

      SAMPLE
date    Dec 10 2010
solvent       CDCl3
file            exp
   ACQUISITION
sfrq        499.859
tn               H1
at             2.500
np             42518
sw            8503.4
fb         not used
bs                 2
pw               7.8
pw               7.8
tpwr              57
d1             4.800
tof                0
nt                16
ct                16
alock              n
gain       not used
      FLAGS
il                 n
in                 n
dp                 y
hs                nn

      DEC. & VT
dn                C13
dof                0
dm               nnn
dmm                c
dmf              200
      PROCESSING
lb              0.20
fn             32768
math               i
werr
wexp
wbs
wnt
      DISPLAY
sp             -190.4
wp             4017.1
vs                 38
sc                  0
wc                250
hzmm            16.07
is             136.03
rfl            5384.7
rfp            3629.0
th                  2
ins             3.000
ai     ph
```





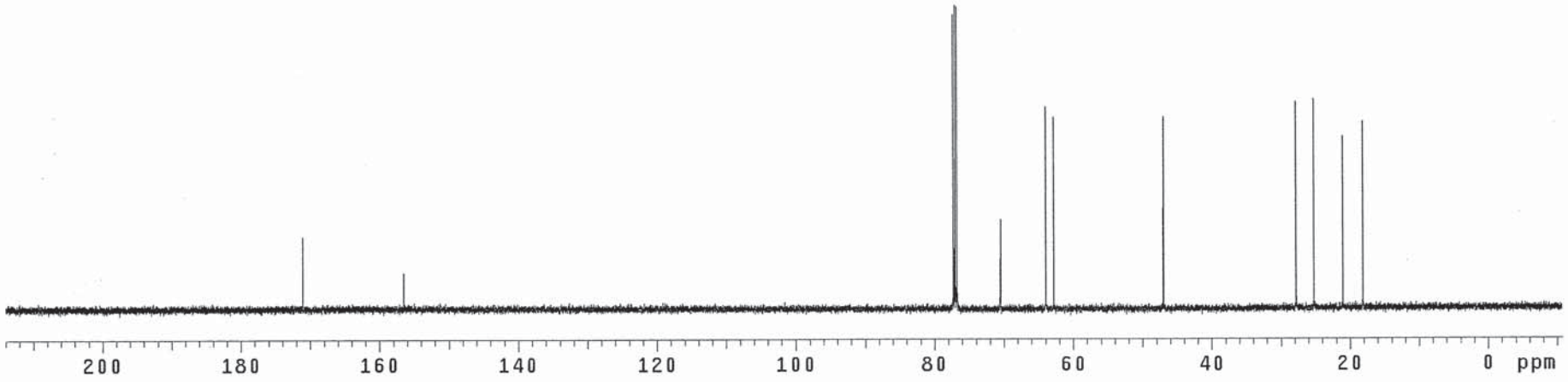
13d

```
lcq3-92-13C

exp25  CARBON

      SAMPLE
date    Dec 10 2010
solvent       cdcl3
file            exp
   ACQUISITION
sw          28258.6
at              1.300
np              73498
fb              16000
bs                  4
d1              3.000
nt              10000
ct                372
   TRANSMITTER
tn                C13
sfrq          125.702
tof             865.4
tpwr               56
pw             13.500
    DECOUPLER
dn                 H1
dof                 0
dm                nny
decwave
dpwr               36
dmf             11101

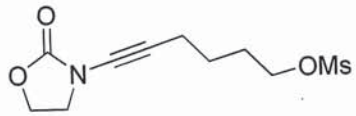
      SPECIAL
temp          not used
gain                54
spin          not used
hst                0.008
pw90               9.200
alfa              10.000
      FLAGS
il                    n
in                    n
dp                    y
hs                   nn
   PROCESSING
lb                 0.50
lsfid                 2
fn            not used
     DISPLAY
sp              -1359.2
wp              28258.1
rfl             11037.6
rfp              9678.0
rp               -119.8
lp               -907.0
       PLOT
wc                  250
sc                    0
vs                  581
th                    7
ai  cdc  ph
```



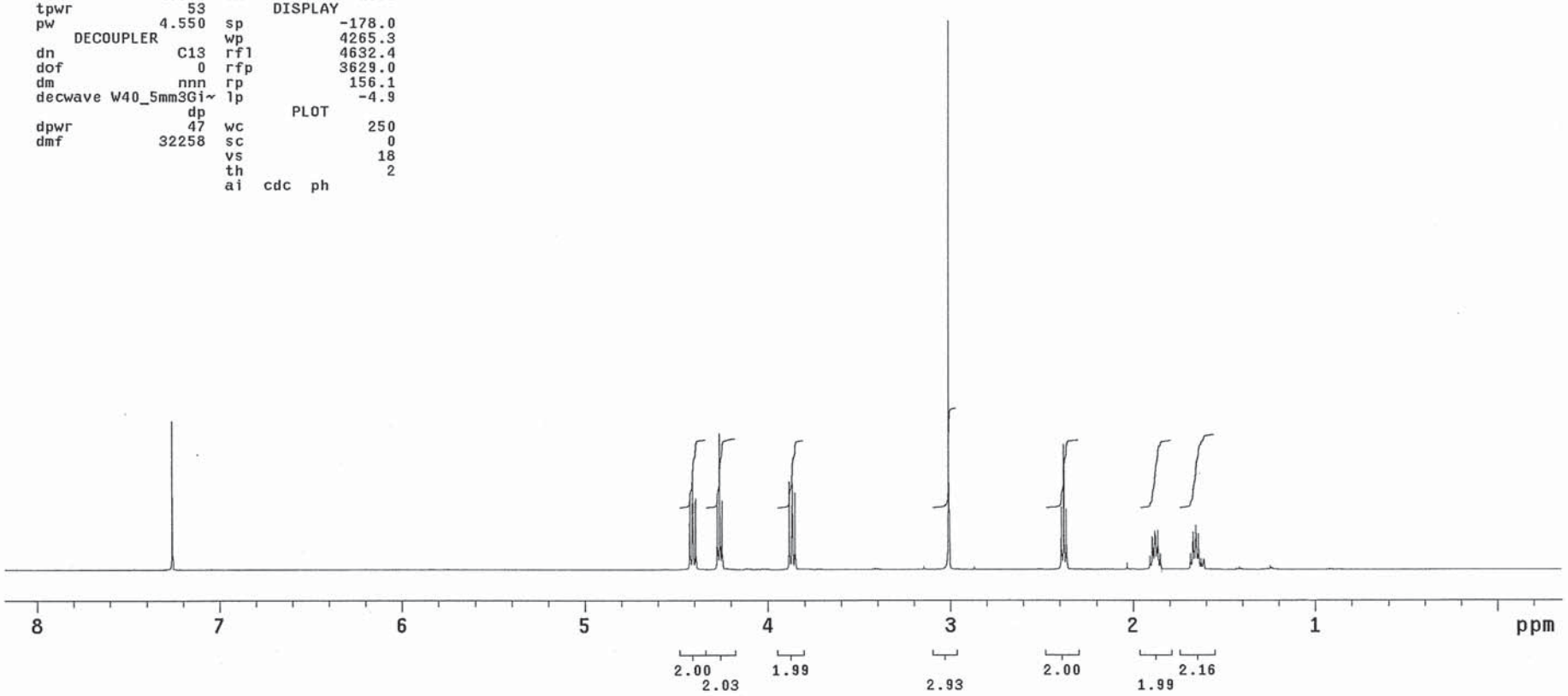
lcq3-110-H

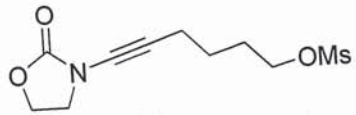
exp25 PROTON

SAMPLE		PRESATURATION	
date	Dec 27 2010	satmode	n
solvent	CDCl3	wet	n
file	exp	SPECIAL	
ACQUISITION		temp	not used
sw	7997.6	gain	not used
at	2.049	spin	not used
np	32768	hst	0.008
fb	4000	pw90	9.100
bs	2	alfa	6.600
d1	1.000	FLAGS	
nt	16	il	n
ct	16	in	n
TRANSMITTER		dp	y
tn	H1	hs	nn
sfrq	499.859	PROCESSING	
tof	499.9	fn	not used
tpwr	53	DISPLAY	
pw	4.550	sp	-178.0
DECOUPLER		wp	4265.3
dn	C13	rfl	4632.4
dof	0	rfp	3629.0
dm	nnn	rp	156.1
decwave	W40_5mm3Gi~	lp	-4.9
	dp	PLOT	
dpwr	47	wc	250
dmf	32258	sc	0
		vs	18
		th	2
		ai cdc ph	



13e





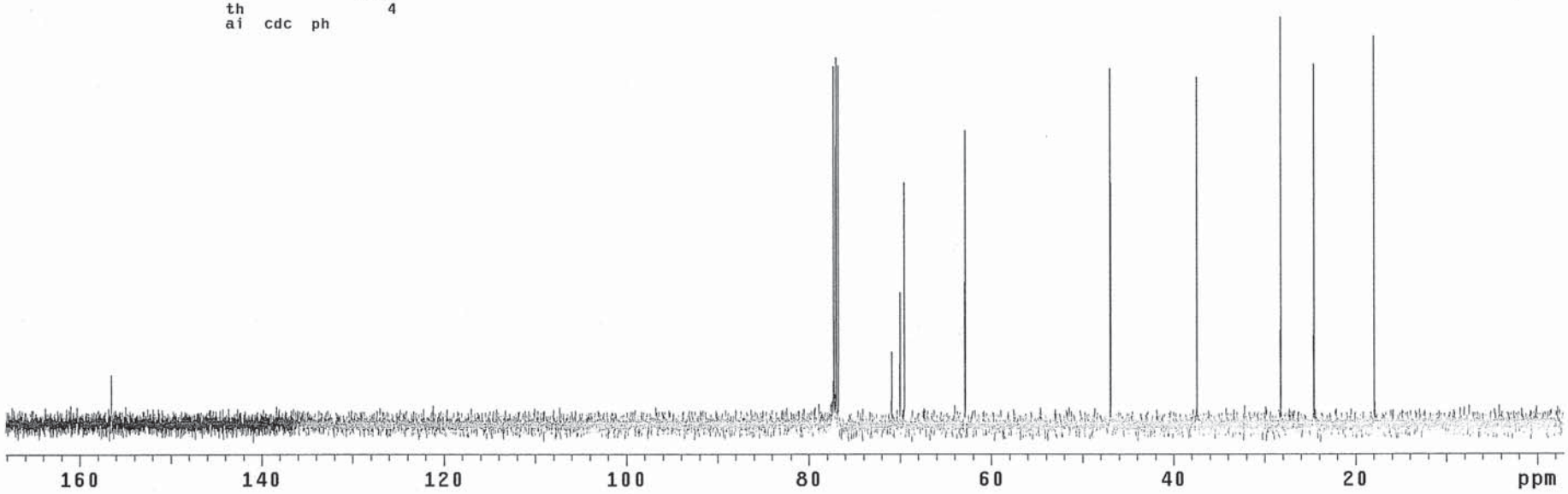
13e

```
lcq3-110-13C

exp25  CARBON

      SAMPLE
date    Dec 27 2010
solvent       cdcl3
file            exp
   ACQUISITION
sw          28258.6
at              1.300
np              73498
fb              16000
bs                  2
d1              3.000
nt              10000
ct                210
   TRANSMITTER
tn                C13
sfrq          125.702
tof             865.4
tpwr               56
pw             13.500
    DECOUPLER
dn                 H1
dof                 0
dm                nny
decwave
dpwr               36
dmf             11101

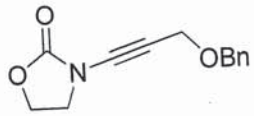
      SPECIAL
temp        not used
gain              54
spin        not used
hst              0.008
pw90             9.200
alfa            10.000
        FLAGS
il                   n
in                   n
dp                   y
hs                  nn
     PROCESSING
lb                0.50
lsfid                2
fn          not used
      DISPLAY
sp             -367.4
wp            21499.6
rfl           11039.4
rfp            9678.0
rp               33.7
lp             -898.5
        PLOT
wc                 250
sc                   0
vs                1695
th                   4
ai  cdc  ph
```



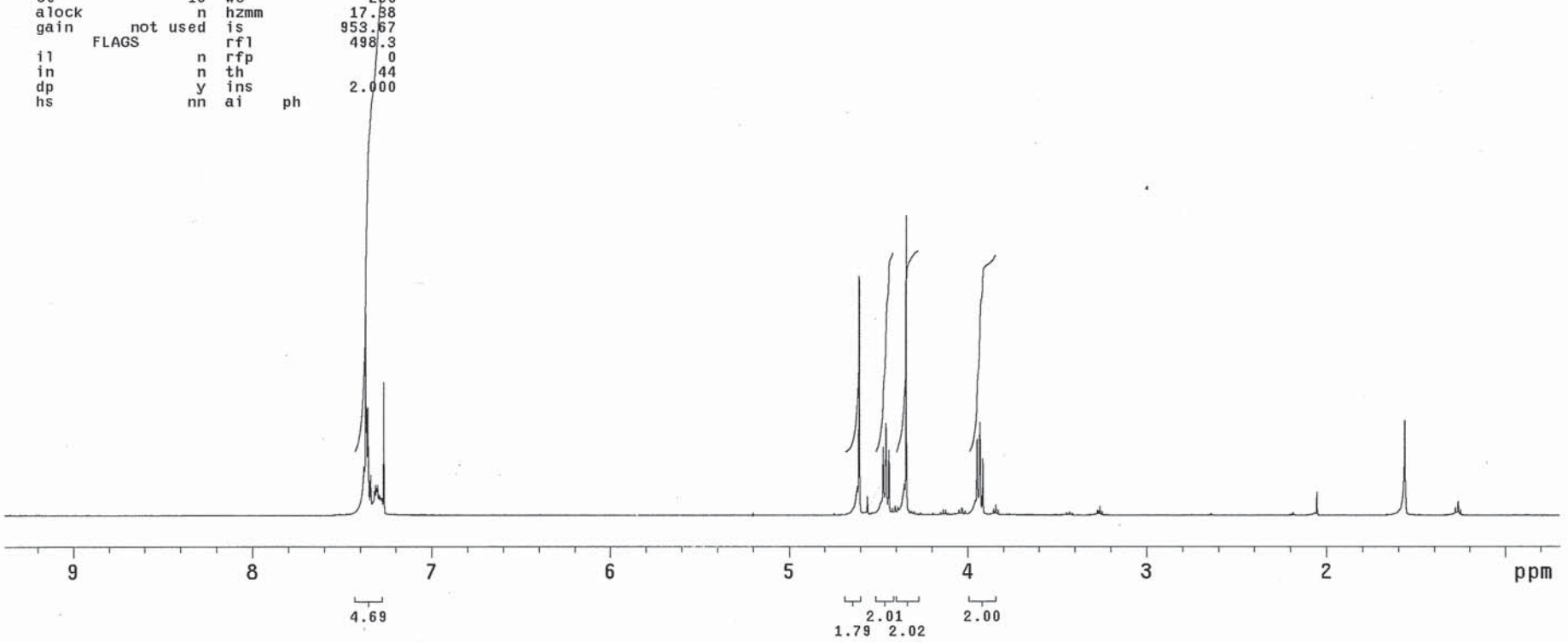
lb-II-249-2

exp3 s2pul

SAMPLE		DEC. & VT	
date	Oct 17 2010	dn	F19
solvent	CDCl3	dof	0
file	/nmr500/Zhang~	dm	nnn
/biaolu/lb-II-249-~	2.fid	dmm	c
		dmf	200
ACQUISITION		PROCESSING	
sfrq	499.859	lb	0.20
tn	H1	fn	32768
at	2.669	math	i
np	32000		
sw	5995.2	werr	
fb	not used	wexp	
bs	2	wbs	
pw	9.0	wnt	
pw	9.0	DISPLAY	
tpwr	57	sp	345.5
d1	3.000	wp	4346.0
tof	0	vs	49
nt	16	sc	0
ct	16	wc	250
alock	n	hzmm	17.38
gain	not used	is	953.67
FLAGS		rfl	498.3
il	n	rfp	0
in	n	th	44
dp	y	ins	2.000
hs	nn	ai ph	



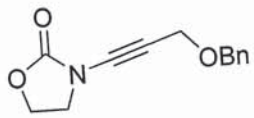
13f



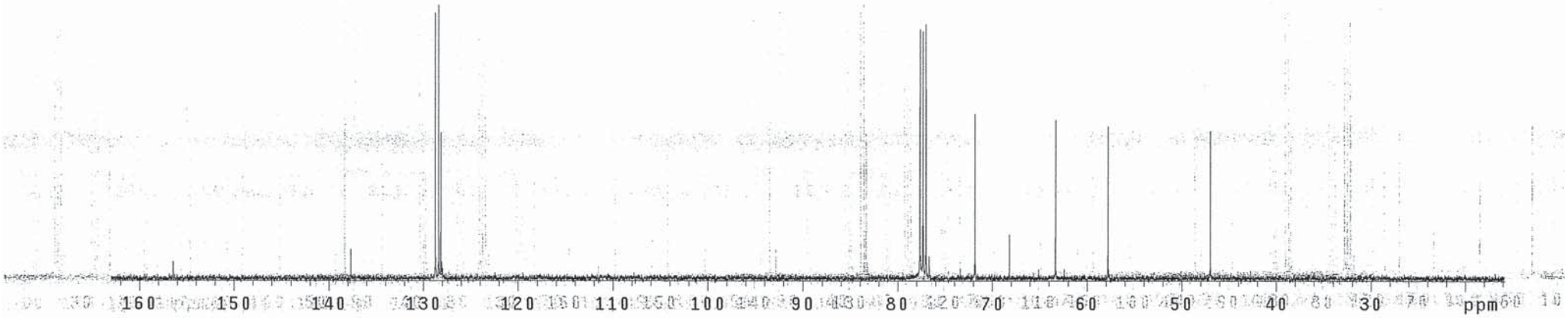
lu2-249-13C

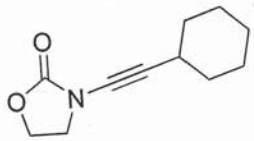
exp25 std13c

SAMPLE		DEC. & VT	
date	Jan 17 2011	dfrq	399.951
solvent	cdcl3	dn	H1
file	exp	dpwr	40
ACQUISITION		dof	0
sfrq	100.577	dm	nny
tn	C13	dmm	w
at	0.701	dmf	6700
np	39216	dseq	
sw	27972.0	dres	90.0
fb	not used	homo	n
bs	2	PROCESSING	
ss	4	lb	1.00
tpwr	58	wtfile	
pw	7.0	proc	ft
d1	1.300	fn	65536
tof	525.7	math	f
nt	10000		
ct	1530	werr	
alock	n	wexp	
gain	44	wbs	
FLAGS		wnt	
il	n		
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	1589.8		
wp	14802.1		
vs	5517		
sc	0		
wc	250		
hzmm	59.21		
is	500.00		
rfl	11643.6		
rfp	7743.7		
th	0		
ins	100.000		
ai	ph		



13f





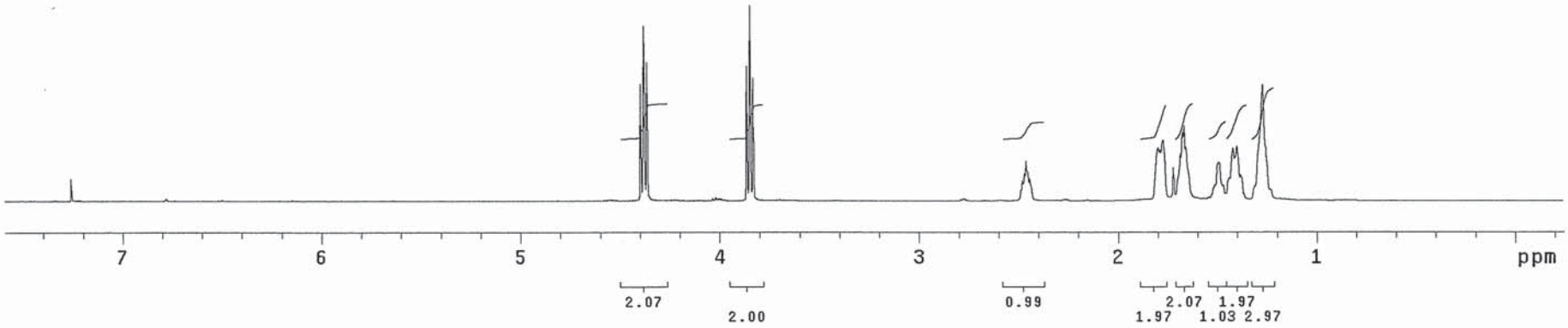
13g

```
lcq2-200-H

exp25  PROTON

      SAMPLE
date    Dec 16 2010
solvent      CDCl3
file           exp
   ACQUISITION
sw          7997.6
at           2.049
np           32768
fb            4000
bs               2
d1           1.000
nt              16
ct              16
   TRANSMITTER
tn              H1
sfrq       499.859
tof          499.9
tpwr            53
pw           4.550
    DECOUPLER
dn             C13
dof              0
dm             nnn
decwave W40_5mm3Gi~
                dp
dpwr            47
dmf          32258

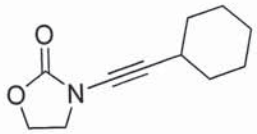
   PRESATURATION
satmode          n
wet              n
      SPECIAL
temp       not used
gain       not used
spin       not used
hst           0.008
pw90          9.100
alfa          6.600
       FLAGS
il               n
in               n
dp               y
hs              nn
    PROCESSING
fn         not used
     DISPLAY
sp           -122.4
wp           3918.7
rfl          4632.9
rfp          3629.0
rp             53.3
lp              0.6
       PLOT
wc              250
sc                0
vs               30
th                2
ai  cdc  ph
```



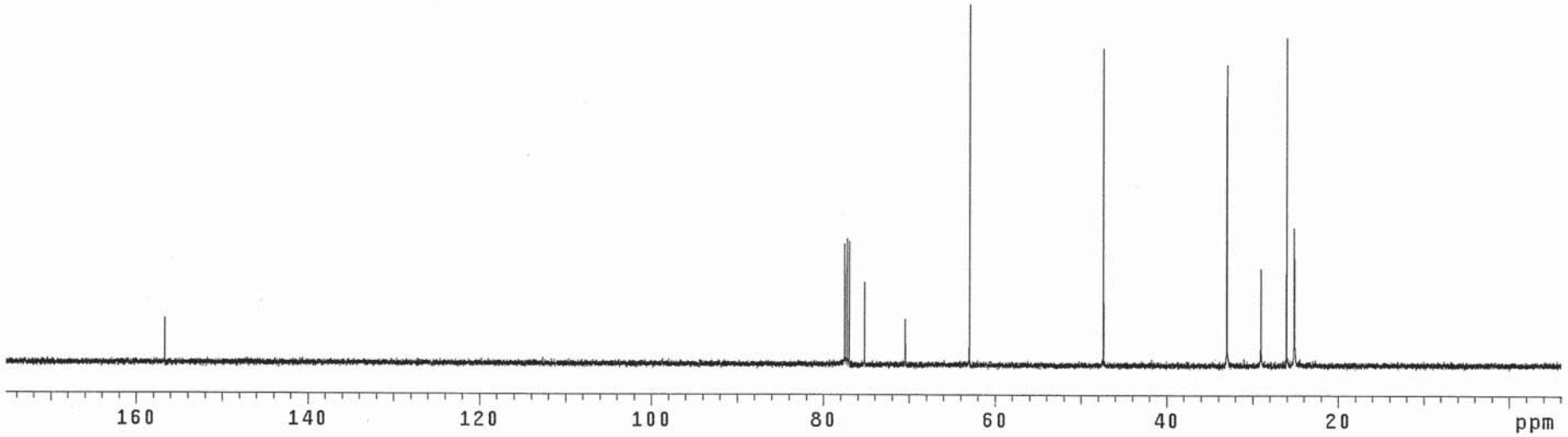
lcq2-200-13C

exp25 CARBON

SAMPLE		SPECIAL	
date	Dec 16 2010	temp	not used
solvent	cdcl3	gain	54
file	exp	spin	not used
ACQUISITION		hst	0.008
sw	28258.6	pw90	9.200
at	1.300	alfa	10.000
np	73498	**FLAGS**	
fb	16000	il	n
bs	2	in	n
d1	3.000	dp	y
nt	10000	hs	nn
ct	224	**PROCESSING**	
TRANSMITTER		lb	0.50
tn	C13	lsfid	2
sfrq	125.702	fn	not used
tof	865.4	**DISPLAY**	
tpwr	56	sp	-769.3
pw	13.500	wp	22791.9
DECOUPLER		rfl	11010.9
dn	H1	rfp	9678.0
dof	0	rp	-58.1
dm	nny	lp	-869.8
decwave		**PLOT**	
dpwr	36	wc	250
dmf	11101	sc	0
		vs	478
		th	3
		ai cdc ph	



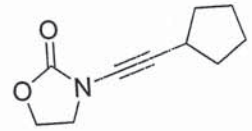
13g



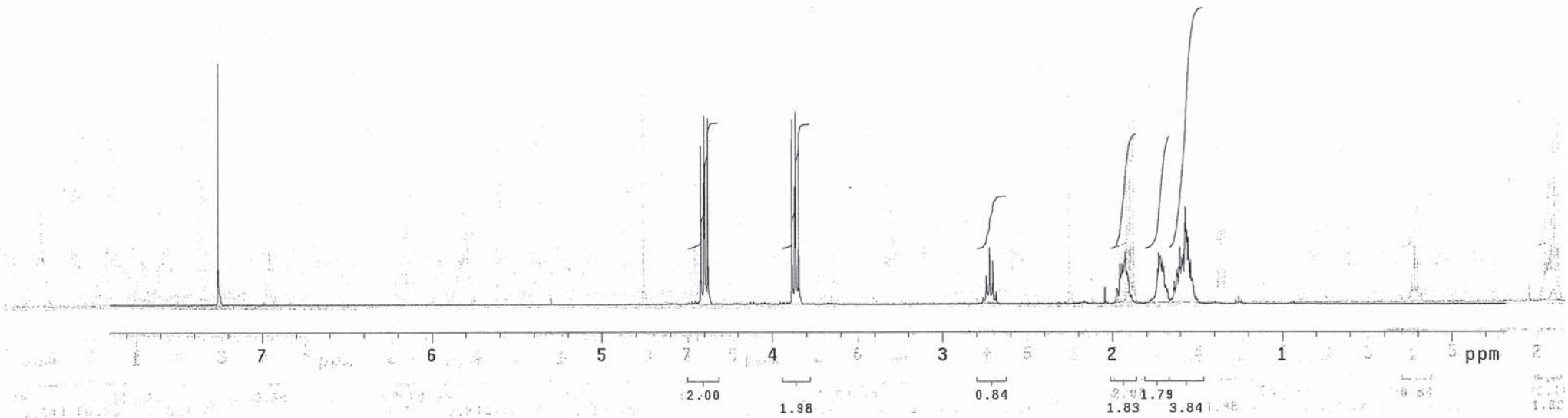
lcq2-253

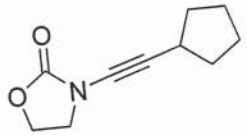
exp25 s2pul

SAMPLE		DEC. & VT	
date	Oct 28 2010	dn	H1
solvent	cdcl3	dof	-1425.0
file	/home/Zhang/c~	dm	nnn
	qli/lcq2-253.fid	dmm	c
ACQUISITION		dmf	200
sfrq	399.951	PROCESSING	
tn	H1	lb	0.10
at	2.500	fn	65536
np	35984	math	f
sw	7196.8		
fb	not used	werr	
bs	2	wexp	
pw	6.7	wbs	
pw	6.7	wnt	
tpwr	57	DISPLAY	
d1	4.800	sp	-128.8
tof	-6.9	wp	3287.2
nt	10	vs	57
ct	10	sc	0
alock	n	wc	250
gain	not used	hzmm	13.15
FLAGS		is	770.72
il	n	rfl	4502.0
in	n	rfp	2903.6
dp	y	th	35
hs	nn	ins	2.000
		ai ph	



13h





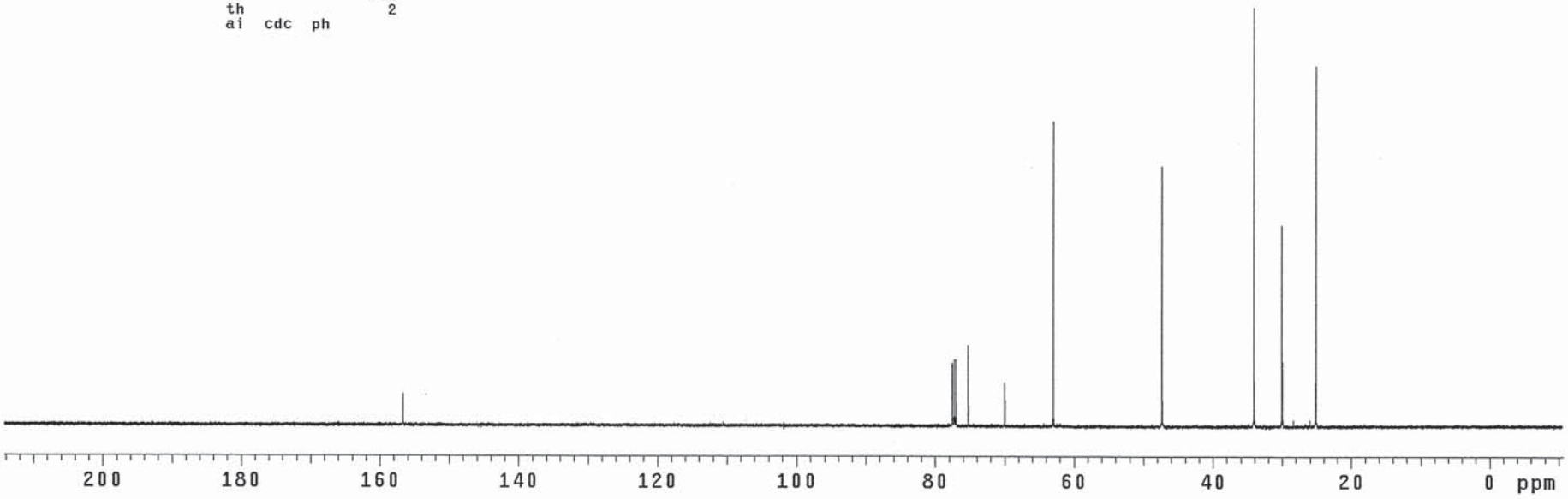
13h

```
lcq-2-253-C13

exp2  CARBON

      SAMPLE
date    Dec 15 2010
solvent       cdcl3
file            exp
    ACQUISITION
sw          28258.6
at              1.300
np              73498
fb              16000
bs                  4
d1              3.000
nt              10000
ct                692
   TRANSMITTER
tn                C13
sfrq          125.702
tof             865.4
tpwr               56
pw             13.500
    DECOUPLER
dn                  H1
dof                  0
dm                 nny
decwave
dpwr               36
dmf             11101

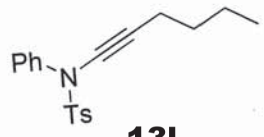
      SPECIAL
temp         not used
gain               54
spin               20
hst             0.008
pw90            9.200
alfa           10.000
       FLAGS
il                   n
in                   n
dp                   y
hs                  nn
    PROCESSING
lb                0.50
lsfid                2
fn           not used
     DISPLAY
sp            -1334.6
wp            28258.1
rfl           11013.1
rfp            9678.0
rp                6.5
lp             -942.7
       PLOT
wc                 250
sc                   0
vs                 502
th                   2
ai  cdc  ph
```



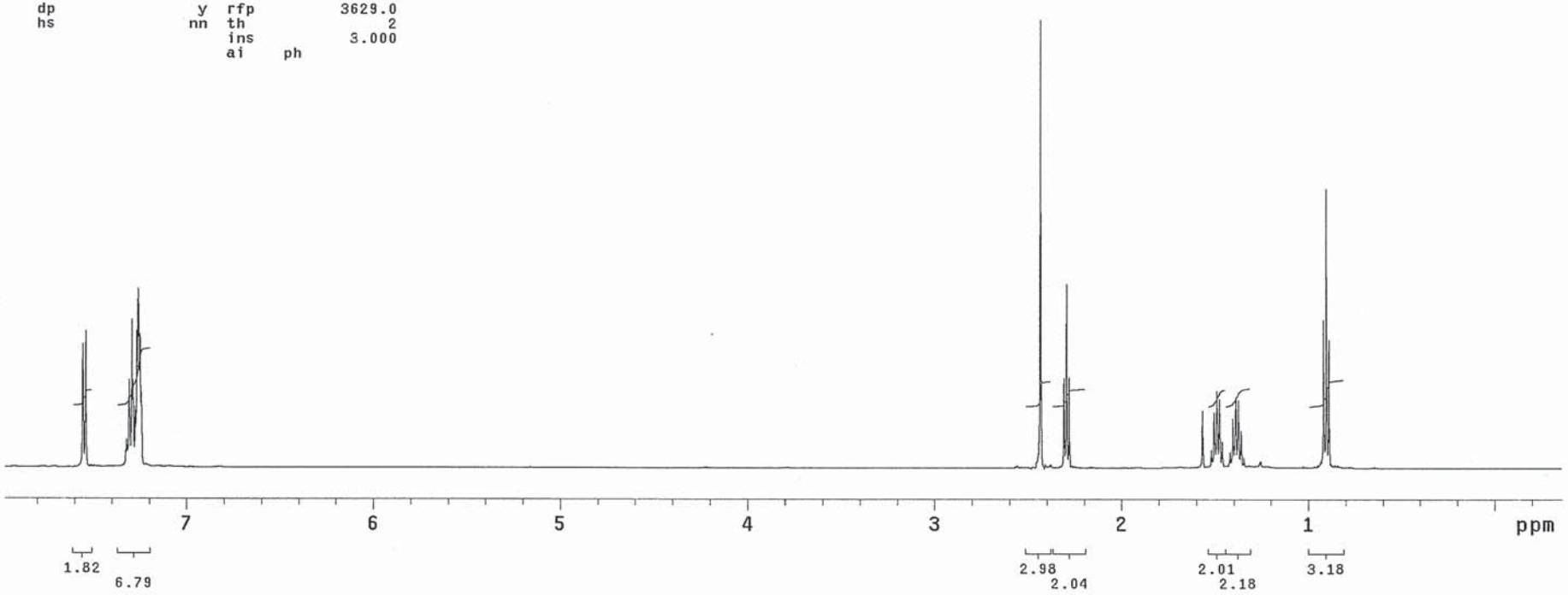
lcq3-24-H

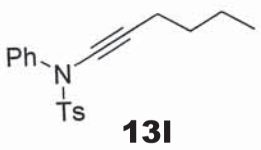
exp25 s2pul

SAMPLE		DEC. & VT	
date	Dec 10 2010	dn	C13
solvent	CDCl3	dof	0
file	exp	dm	nnn
ACQUISITION		dmm	c
sfrq	499.859	dmf	200
tn	H1	PROCESSING	
at	2.500	lb	0.20
np	42518	fn	32768
sw	8503.4	math	i
fb	not used		
bs	2	werr	
pw	7.8	wexp	
pw	7.8	wbs	
tpwr	57	wnt	
d1	4.800	DISPLAY	
tof	0	sp	-181.1
nt	16	wp	4166.6
ct	16	vs	38
alock	n	sc	0
gain	not used	wc	250
FLAGS		hzmm	16.67
il	n	is	89.78
in	n	rfl	5385.2
dp	y	rfp	3629.0
hs	nn	th	2
		ins	3.000
		ai ph	



13l



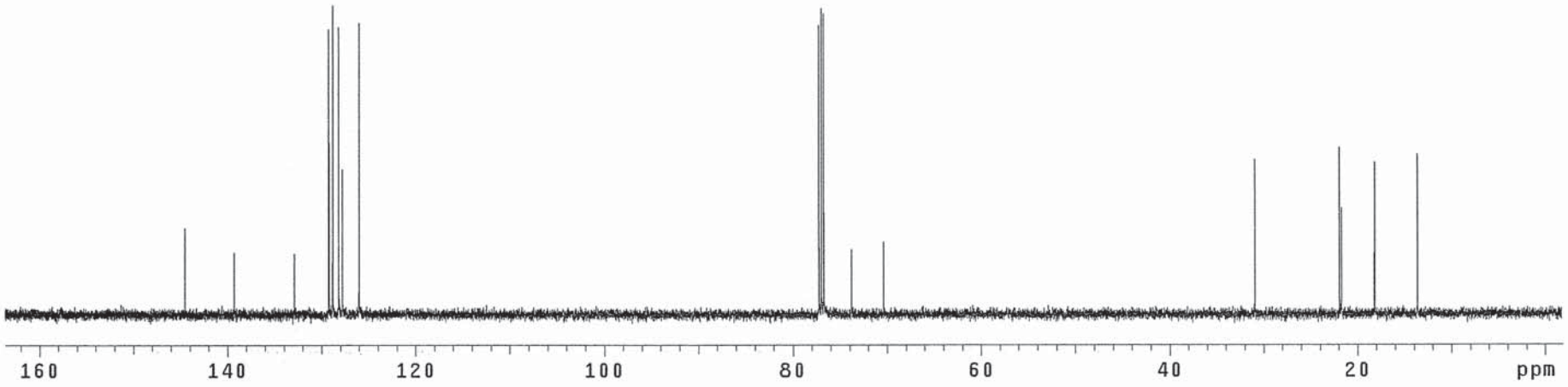


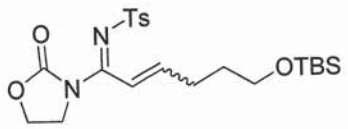
13l

```
lcq3-24-13C

exp25  CARBON

      SAMPLE              SPECIAL
date    Dec 10 2010  temp       not used
solvent       cdcl3  gain             54
file            exp  spin       not used
   ACQUISITION        hst           0.008
sw          28258.6  pw90          9.200
at              1.300  alfa         10.000
np              73498          FLAGS
fb              16000  il                n
bs                  4  in                n
d1              3.000  dp                y
nt              10000  hs               nn
ct                148          PROCESSING
   TRANSMITTER         lb             0.50
tn                C13  lsfid             2
sfrq         125.702  fn         not used
tof            865.4          DISPLAY
tpwr               56  sp           -231.6
pw             13.500  wp          20804.1
    DECOUPLER          rfl         11036.3
dn                 H1  rfp          9678.0
dof                 0  rp           -108.2
dm                nny  lp           -929.3
decwave                      PLOT
dpwr               36  wc               250
dmf            11101  sc                 0
                      vs               581
                      th                 3
                      ai  cdc  ph
```



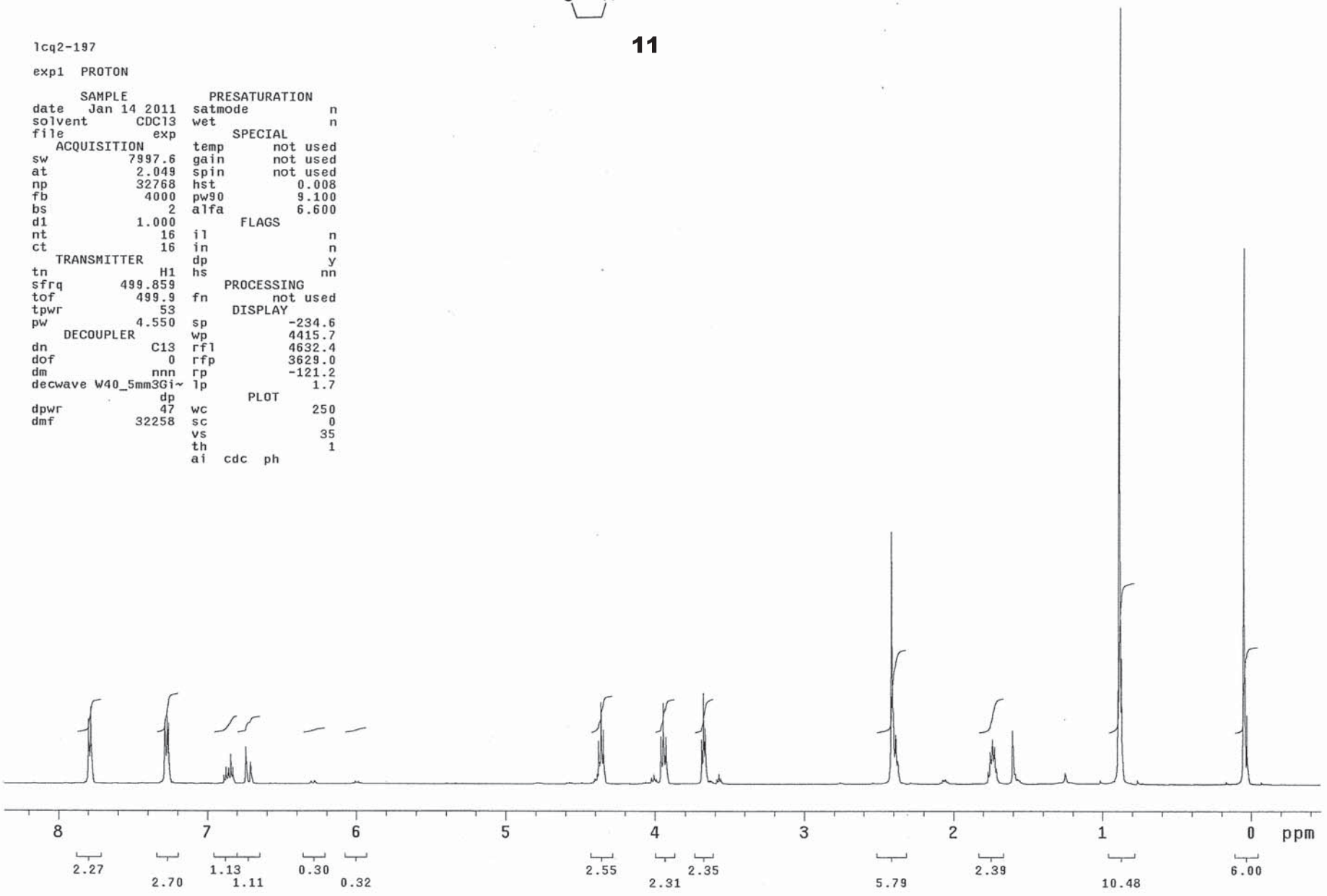


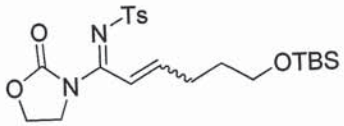
11

lcq2-197

exp1 PROTON

SAMPLE		PRESATURATION	
date	Jan 14 2011	satmode	n
solvent	CDCl3	wet	n
file	exp	SPECIAL	
ACQUISITION		temp	not used
sw	7997.6	gain	not used
at	2.049	spin	not used
np	32768	hst	0.008
fb	4000	pw90	9.100
bs	2	alfa	6.600
d1	1.000	FLAGS	
nt	16	il	n
ct	16	in	n
TRANSMITTER		dp	y
tn	H1	hs	nn
sfrq	499.859	PROCESSING	
tof	499.9	fn	not used
tpwr	53	DISPLAY	
pw	4.550	sp	-234.6
DECOUPLER		wp	4415.7
dn	C13	rfl	4632.4
dof	0	rfp	3629.0
dm	nnn	rp	-121.2
decwave	W40_5mm3Gi~	lp	1.7
	dp	PLOT	
dpwr	47	wc	250
dmf	32258	sc	0
		vs	35
		th	1
		ai cdc ph	





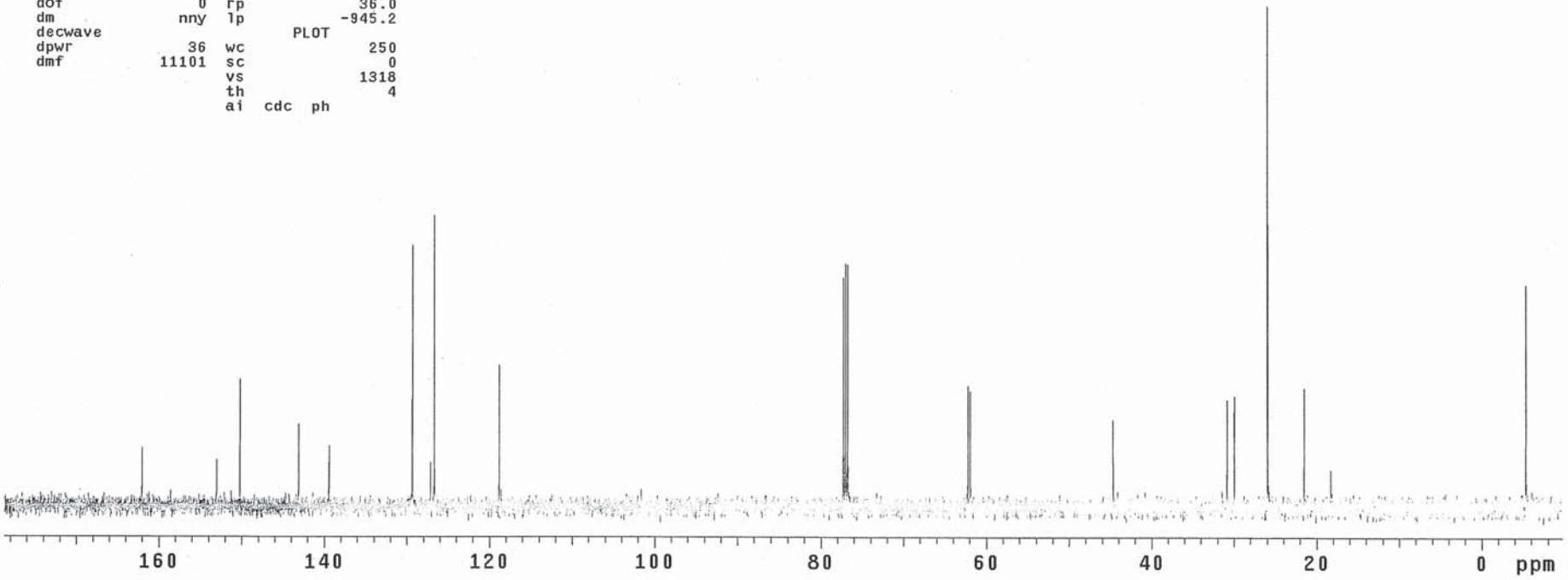
11

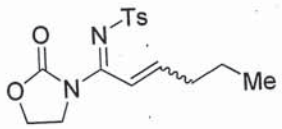
```
lcq3-126-13C

exp2  CARBON

      SAMPLE
date    Dec 30 2010
solvent       cdcl3
file            exp
   ACQUISITION
sw          28258.6
at            1.300
np            73498
fb            16000
bs                2
d1            3.000
nt            10000
ct              216
   TRANSMITTER
tn              C13
sfrq        125.702
tof           865.4
tpwr             56
pw            13.500
    DECOUPLER
dn                H1
dof                0
dm               nny
decwave
dpwr              36
dmf            11101

      SPECIAL
temp        not used
gain              54
spin        not used
hst              0.008
pw90             9.200
alfa            10.000
       FLAGS
il                   n
in                   n
dp                   y
hs                  nn
    PROCESSING
lb                0.50
lsfid                2
fn          not used
     DISPLAY
sp            -1224.6
wp            23686.2
rfl           11035.5
rfp            9678.0
rp               36.0
lp             -945.2
       PLOT
wc                 250
sc                   0
vs                1318
th                   4
ai  cdc  ph
```





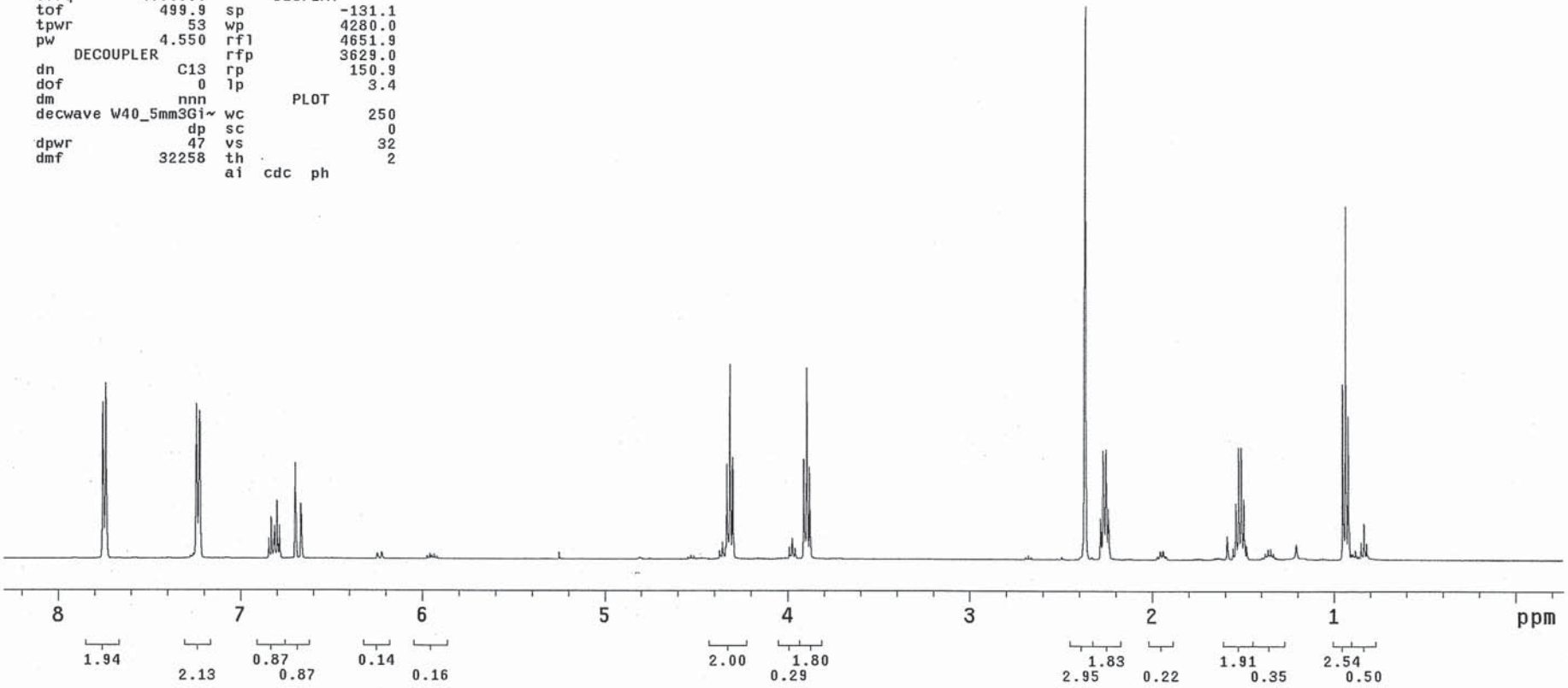
14a

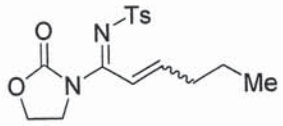
```
lcq3-14-H

exp2  PROTON

      SAMPLE
date    Dec 30 2010
solvent       CDCl3
file /home/Zhang/c~
qli/lcq3-14-2-H.fi~
                  d
   ACQUISITION
sw             7997.6
at              2.049
np              32768
fb               4000
bs                  2
d1              1.000
nt                 16
ct                 16
   TRANSMITTER
tn                 H1
sfrq          499.859
tof             499.9
tpwr               53
pw              4.550
    DECOUPLER
dn                C13
dof                 0
dm                nnn
decwave W40_5mm3Gi~
                  dp
dpwr               47
dmf             32258

   PRESATURATION
satmode             n
wet                 n
      SPECIAL
temp          not used
gain          not used
spin          not used
hst               0.008
pw90              9.100
alfa              6.600
       FLAGS
il                  n
in                  n
dp                  y
hs                 nn
     PROCESSING
fn            not used
     DISPLAY
sp               -131.1
wp               4280.0
rfl              4651.9
rfp              3629.0
rp                150.9
lp                  3.4
       PLOT
wc                  250
sc                    0
vs                   32
th                    2
ai  cdc  ph
```



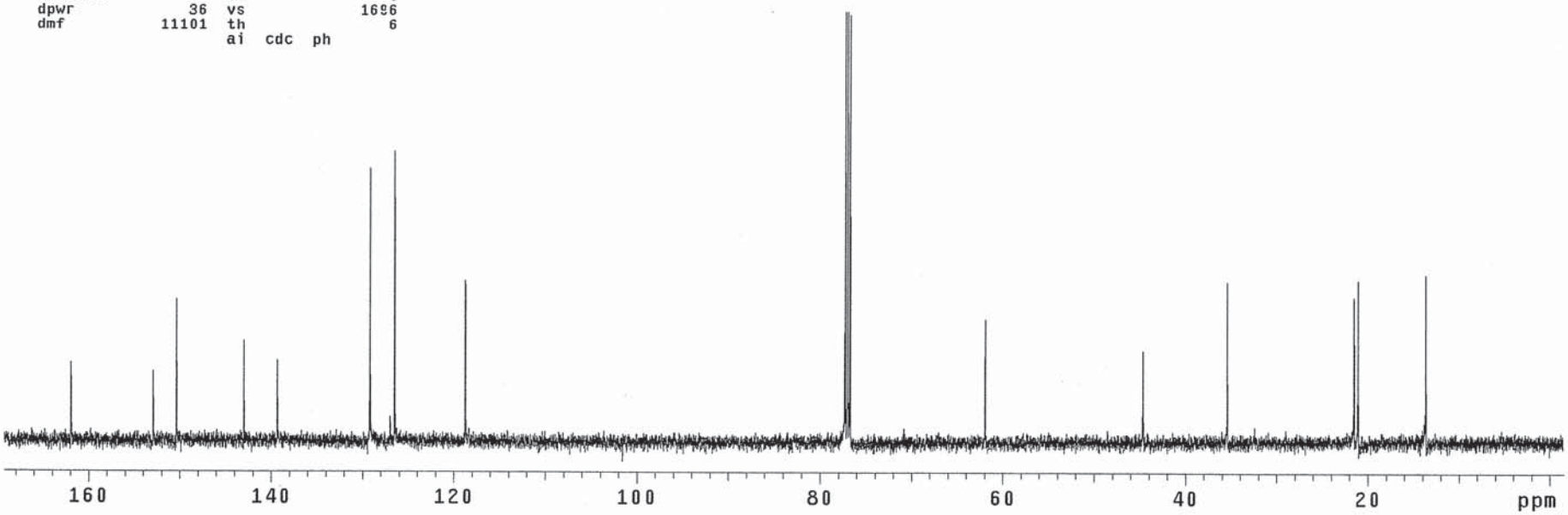


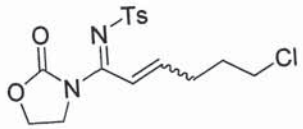
14a

lcq3-14a

exp2 CARBON

SAMPLE		SPECIAL	
date	Nov 16 2010	temp	not used
solvent	cdcl3	gain	54
file	/home/Zhang/c~	spin	not used
	qli/lcq3-14a13C.fi~	hst	0.008
	d	pw90	9.200
ACQUISITION		alfa	10.000
sw	28258.6	FLAGS	
at	1.300	il	n
np	73498	in	n
fb	16000	dp	y
bs	2	hs	nn
d1	3.000	PROCESSING	
nt	1000	lb	1.00
ct	172	lsfid	2
TRANSMITTER		fn	not used
tn	C13	DISPLAY	
sfrq	125.702	sp	-194.1
tof	865.4	wp	21466.9
tpwr	56	rfl	11044.1
pw	6.000	rfp	9678.0
DECOUPLER		rp	1.2
dn	H1	lp	-938.3
dof	0	PLOT	
dm	nny	wc	250
decwave		sc	0
dpwr	36	vs	1696
dmf	11101	th	6
		ai cdc ph	



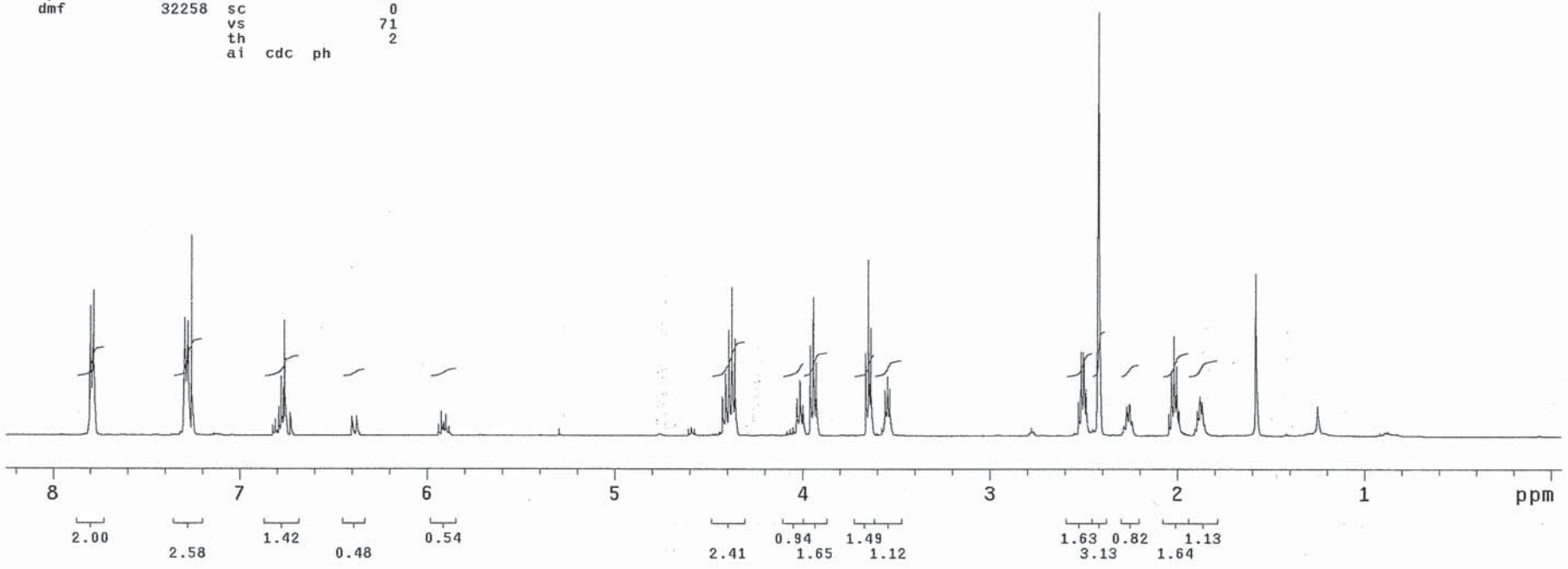


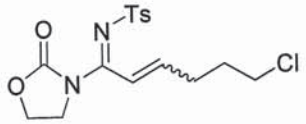
14b

lcq3-113

exp1 PROTON

SAMPLE		PRESATURATION	
date	Jan 14 2011	satmode	n
solvent	CDCl3	wet	n
file	exp	SPECIAL	
ACQUISITION		temp	not used
sw	7997.6	gain	not used
at	2.049	spin	not used
np	32768	hst	0.008
fb	4000	pw90	9.100
bs	2	alfa	6.600
d1	1.000	FLAGS	
nt	16	il	n
ct	16	in	n
TRANSMITTER		dp	y
tn	H1	hs	nn
sfrq	499.859	PROCESSING	
tof	499.9	fn	not used
tpwr	53	DISPLAY	
pw	4.550	sp	-28.2
DECOUPLER		wp	4153.1
dn	C13	rfl	4632.4
dof	0	rfp	3629.0
dm	nnn	rp	-126.0
decwave	W40_5mm3Gi~	lp	-0.4
	dp	PLOT	
dpwr	47	wc	250
dmf	32258	sc	0
		vs	71
		th	2
		ai cdc ph	



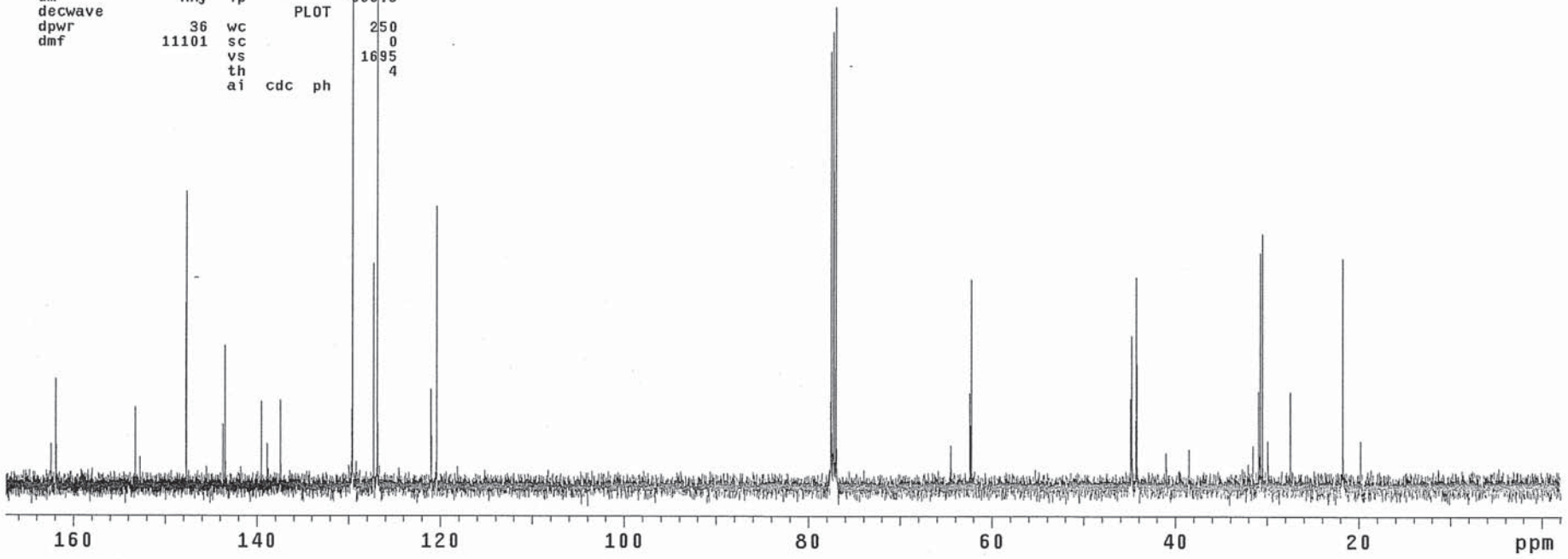


14b

lcq3-113-13C

exp2 CARBON

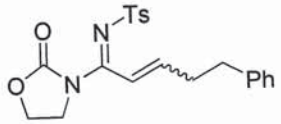
SAMPLE		SPECIAL	
date	Dec 28 2010	temp	not used
solvent	cdcl3	gain	54
file	exp	spin	not used
ACQUISITION		hst	0.008
sw	28258.6	pw90	9.200
at	1.300	alfa	10.000
np	73498	**FLAGS**	
fb	16000	il	n
bs	2	in	n
d1	3.000	dp	y
nt	10000	hs	nn
ct	216	**PROCESSING**	
TRANSMITTER		lb	0.50
tn	C13	lsfid	2
sfrq	125.702	fn	not used
tof	865.4	**DISPLAY**	
tpwr	56	sp	-265.7
pw	13.500	wp	21800.9
DECOUPLER		rfl	11004.0
dn	H1	rfp	9678.0
dof	0	rp	46.5
dm	nny	lp	-966.5
decwave		**PLOT**	
dpwr	36	wc	250
dmf	11101	sc	0
		vs	1695
		th	4
		ai cdc ph	



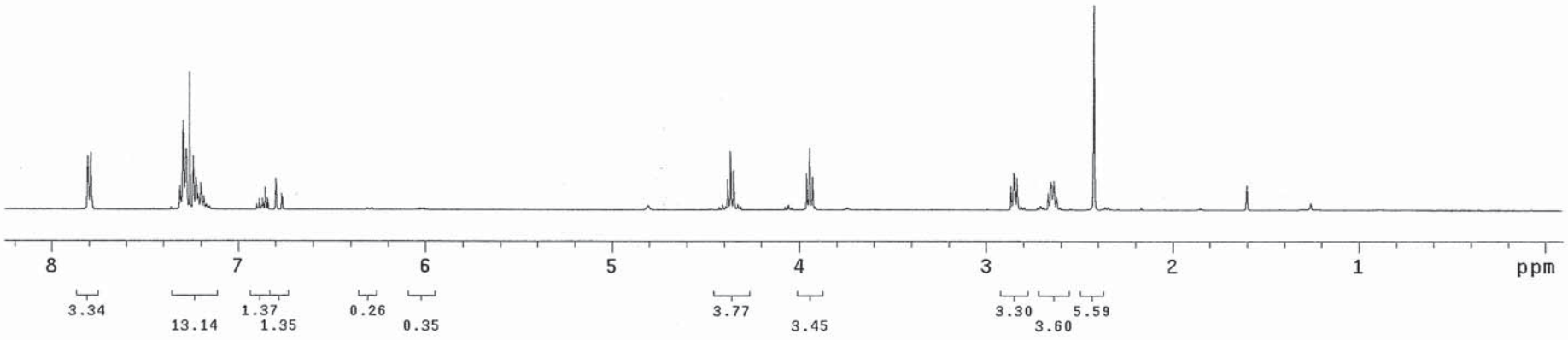
lcq3-78

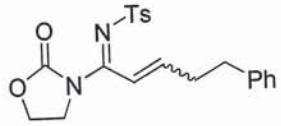
exp1 PROTON

SAMPLE		PRESATURATION	
date	Jan 16 2011	satmode	n
solvent	CDCl3	wet	n
file	exp	SPECIAL	
ACQUISITION		temp	not used
sw	7997.6	gain	not used
at	2.049	spin	not used
np	32768	hst	0.008
fb	4000	pw90	9.100
bs	2	alfa	6.600
d1	1.000	FLAGS	
nt	16	il	n
ct	16	in	n
TRANSMITTER		dp	y
tn	H1	hs	nn
sfrq	499.859	PROCESSING	
tof	499.9	fn	not used
tpwr	53	DISPLAY	
pw	4.550	sp	-46.2
DECOUPLER		wp	4171.6
dn	C13	rfl	4631.9
dof	0	rfp	3629.0
dm	nnn	rp	-121.0
decwave	W40_5mm3Gi~	lp	1.2
	dp	PLOT	
dpwr	47	wc	250
dmf	32258	sc	0
		vs	13
		th	7
		ai cdc ph	



14c



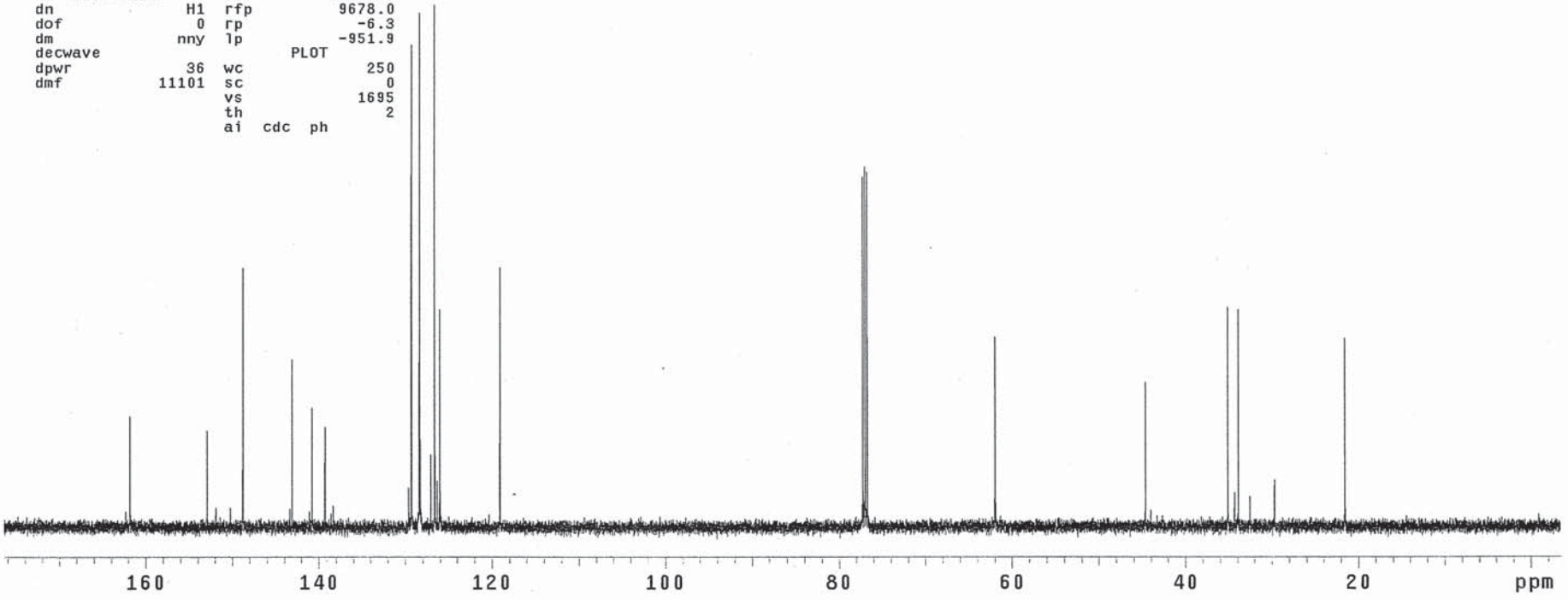


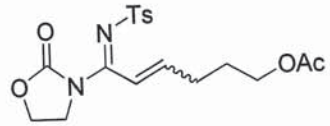
14c

lcq3-78

exp2 CARBON

SAMPLE		SPECIAL	
date	Dec 7 2010	temp	not used
solvent	cdcl3	gain	54
file	exp	spin	not used
ACQUISITION		hst	0.008
sw	28258.6	pw90	9.200
at	1.300	alfa	10.000
np	73498	FLAGS	
fb	16000	il	n
bs	2	in	n
d1	3.000	dp	y
nt	10000	hs	nn
ct	472	PROCESSING	
TRANSMITTER		lb	0.50
tn	C13	lsfid	2
sfrq	125.702	fn	not used
tof	865.4	DISPLAY	
tpwr	56	sp	-438.1
pw	13.500	wp	22613.0
DECOUPLER		rfl	11040.7
dn	H1	rfp	9678.0
dof	0	rp	-6.3
dm	nny	lp	-951.9
decwave		PLOT	
dpwr	36	wc	250
dmf	11101	sc	0
		vs	1695
		th	2
		ai cdc ph	





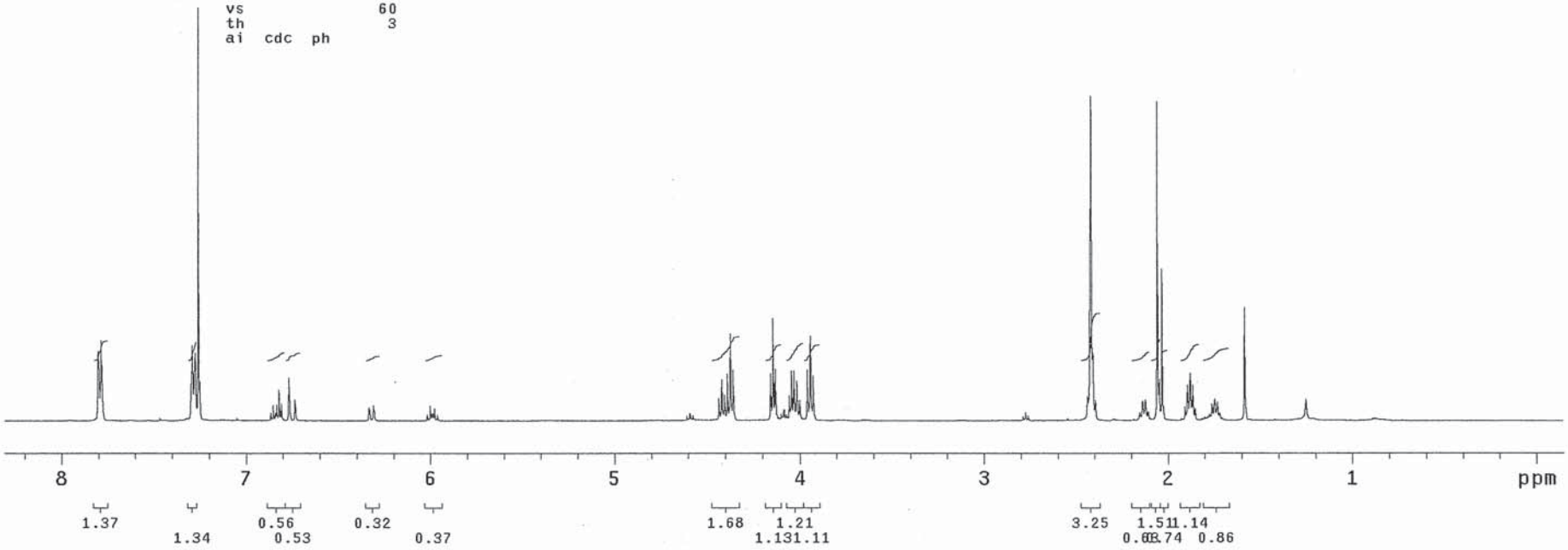
14d

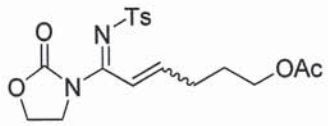
```
lcq3-101

exp1  PROTON

      SAMPLE
date   Jan 16 2011
solvent      CDCl3
file           exp
   ACQUISITION
sw          7997.6
at           2.049
np           32768
fb            4000
bs               2
d1           1.000
nt              16
ct              16
   TRANSMITTER
tn              H1
sfrq       499.859
tof          499.9
tpwr            53
pw           4.550
    DECOUPLER
dn             C13
dof              0
dm             nnn
decwave W40_5mm3Gi~
                dp
dpwr            47
dmf          32258

   PRESATURATION
satmode          n
wet              n
      SPECIAL
temp       not used
gain       not used
spin       not used
hst           0.008
pw90          9.100
alfa          6.600
       FLAGS
il               n
in               n
dp               y
hs              nn
    PROCESSING
fn         not used
     DISPLAY
sp            -74.5
wp           4228.2
rfl          4631.9
rfp          3629.0
rp           -126.2
lp             -2.3
       PLOT
wc             250
sc               0
vs              60
th               3
ai  cdc  ph
```



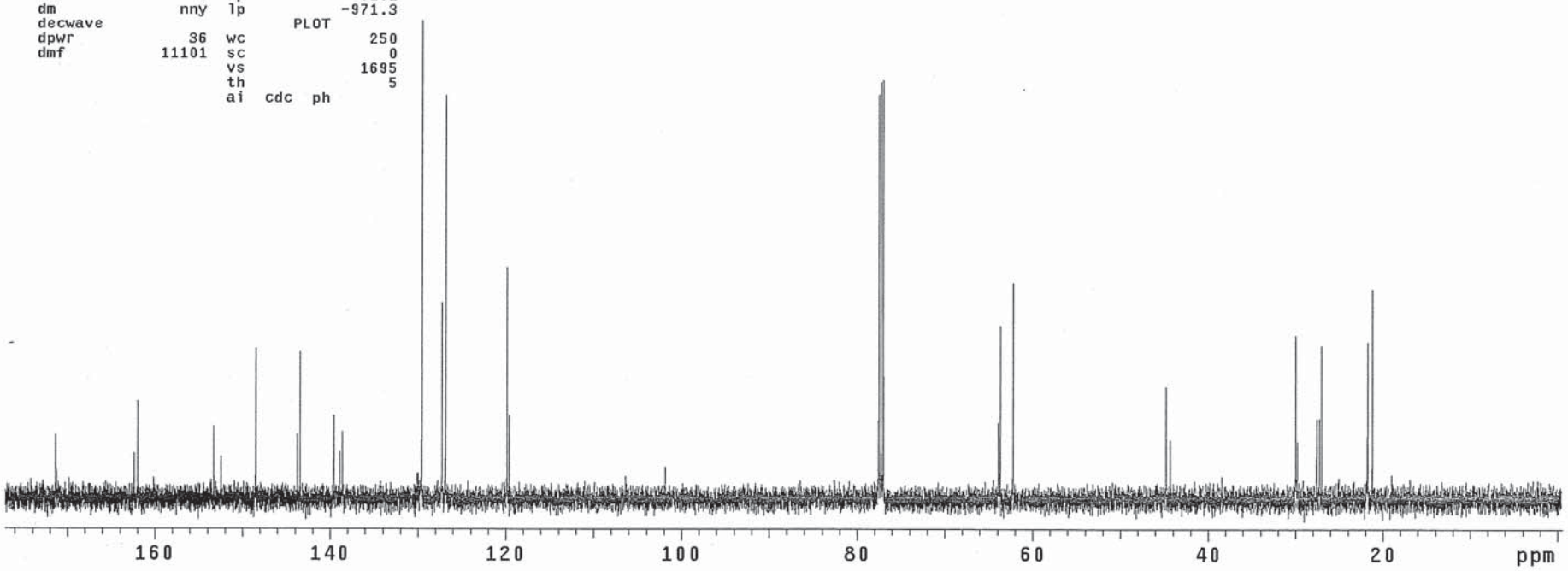


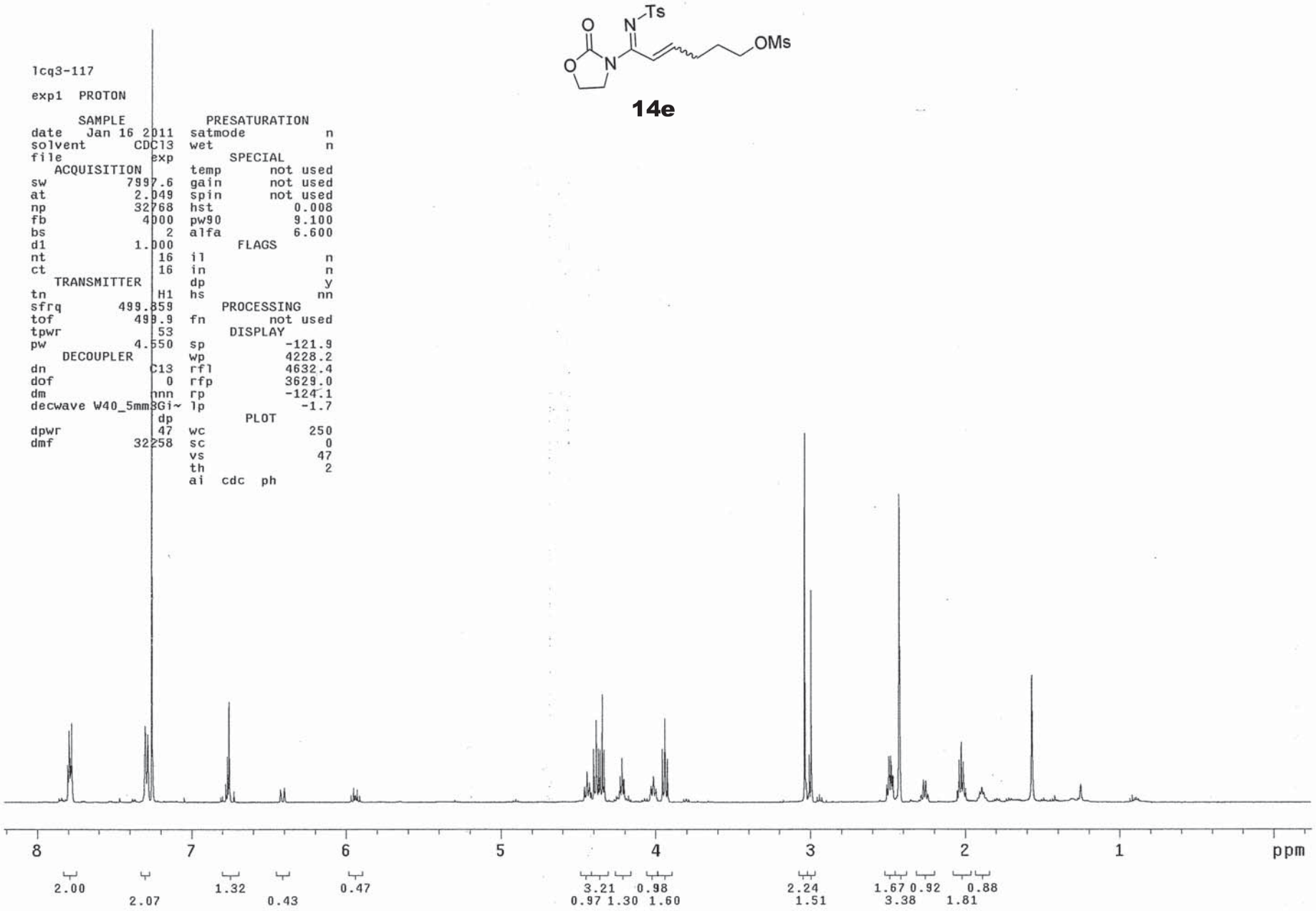
14d

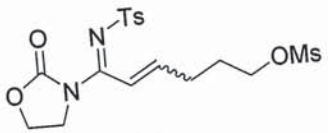
lcq-1-217-C13

exp2 CARBON

SAMPLE		SPECIAL	
date	Dec 28 2010	temp	not used
solvent	cdcl3	gain	54
file	exp	spin	not used
ACQUISITION		hst	0.008
sw	28258.6	pw90	9.200
at	1.300	alfa	10.000
np	73498	**FLAGS**	
fb	16000	il	n
bs	2	in	n
d1	3.000	dp	y
nt	10000	hs	nn
ct	174	**PROCESSING**	
TRANSMITTER		lb	0.50
tn	C13	lsfid	2
sfrq	125.702	fn	not used
tof	865.4	**DISPLAY**	
tpwr	56	sp	-67.7
pw	13.500	wp	22328.0
DECOUPLER		rfl	11004.9
dn	H1	rfp	9678.0
dof	0	rp	62.1
dm	nny	lp	-971.3
decwave		**PLOT**	
dpwr	36	wc	250
dmf	11101	sc	0
		vs	1695
		th	5
		ai cdc ph	




lcq3-117
exp1 PROTON
SAMPLE
date Jan 16 2011
solvent CDCl3
file exp
ACQUISITION
sw 7997.6
at 2.049
np 32768
fb 4000
bs 2
d1 1.000
nt 16
ct 16
TRANSMITTER
tn H1
sfrq 499.859
tof 499.9
tpwr 53
pw 4.550
DECOUPLER
dn C13
dof 0
dm nnn
decwave W40_5mm3Gi~
dp
dpwr 47
dmf 32258
PRESATURATION
satmode n
wet n
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 9.100
alfa 6.600
FLAGS
il n
in n
dp y
hs nn
PROCESSING
fn not used
DISPLAY
sp -121.9
wp 4228.2
rfl 4632.4
rfp 3629.0
rp -124.1
lp -1.7
PLOT
wc 250
sc 0
vs 47
th 2
ai cdc ph
O
N
Ts
O
N
OMs
14e
8
7
6
5
4
3
2
1
ppm
2.00
2.07
1.32
0.43
0.47
3.21
0.97
1.30
0.98
1.60
2.24
1.51
1.67
3.38
0.92
0.88
1.81

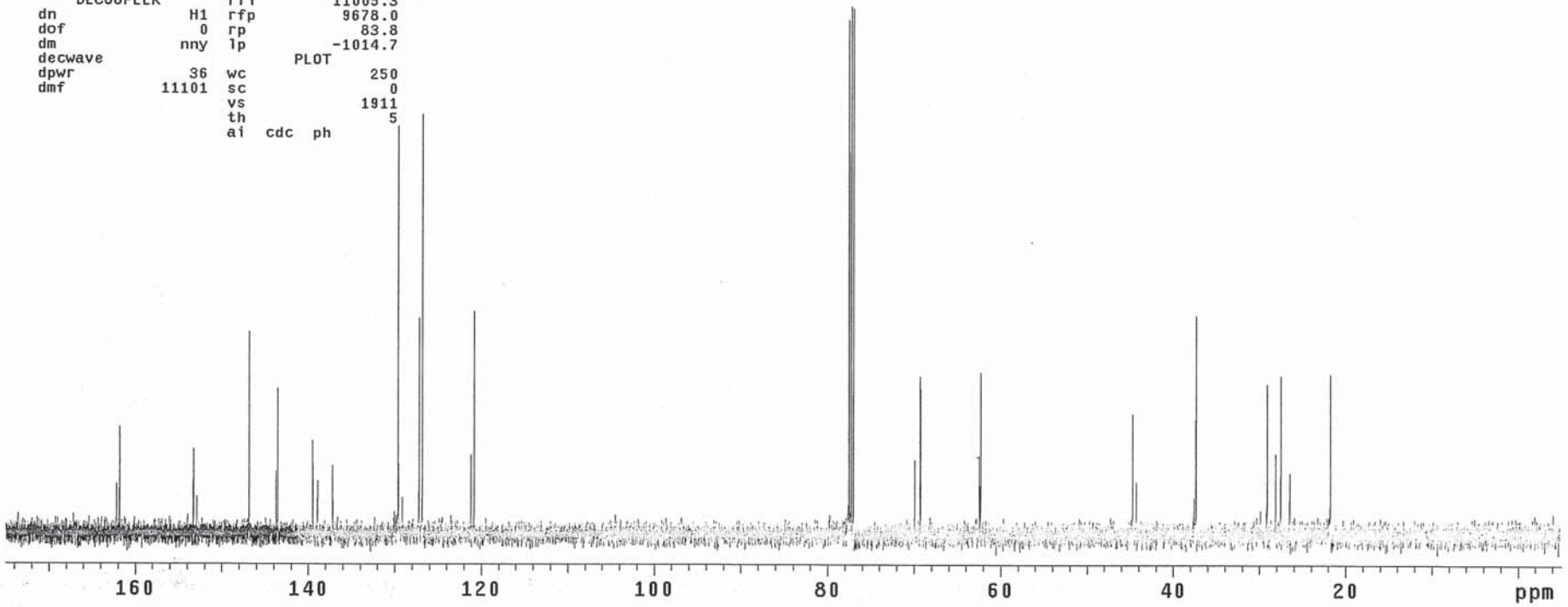


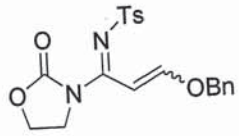
14e

lcq3-117-13C

exp2 CARBON

SAMPLE		SPECIAL	
date	Dec 30 2010	temp	not used
solvent	cdcl3	gain	54
file	exp	spin	not used
ACQUISITION		hst	0.008
sw	28258.6	pw90	9.200
at	1.300	alfa	10.000
np	73498	FLAGS	
fb	16000	il	n
bs	2	in	n
d1	3.000	dp	y
nt	10000	hs	nn
ct	250	PROCESSING	
TRANSMITTER		lb	0.50
tn	C13	lsfid	2
sfrq	125.702	fn	not used
tof	865.4	DISPLAY	
tpwr	56	sp	-631.3
pw	13.500	wp	22626.3
DECOUPLER		rfl	11005.3
dn	H1	rfp	9678.0
dof	0	rp	83.8
dm	nny	lp	-1014.7
decwave		PLOT	
dpwr	36	wc	250
dmf	11101	sc	0
		vs	1911
		th	5
		ai cdc ph	



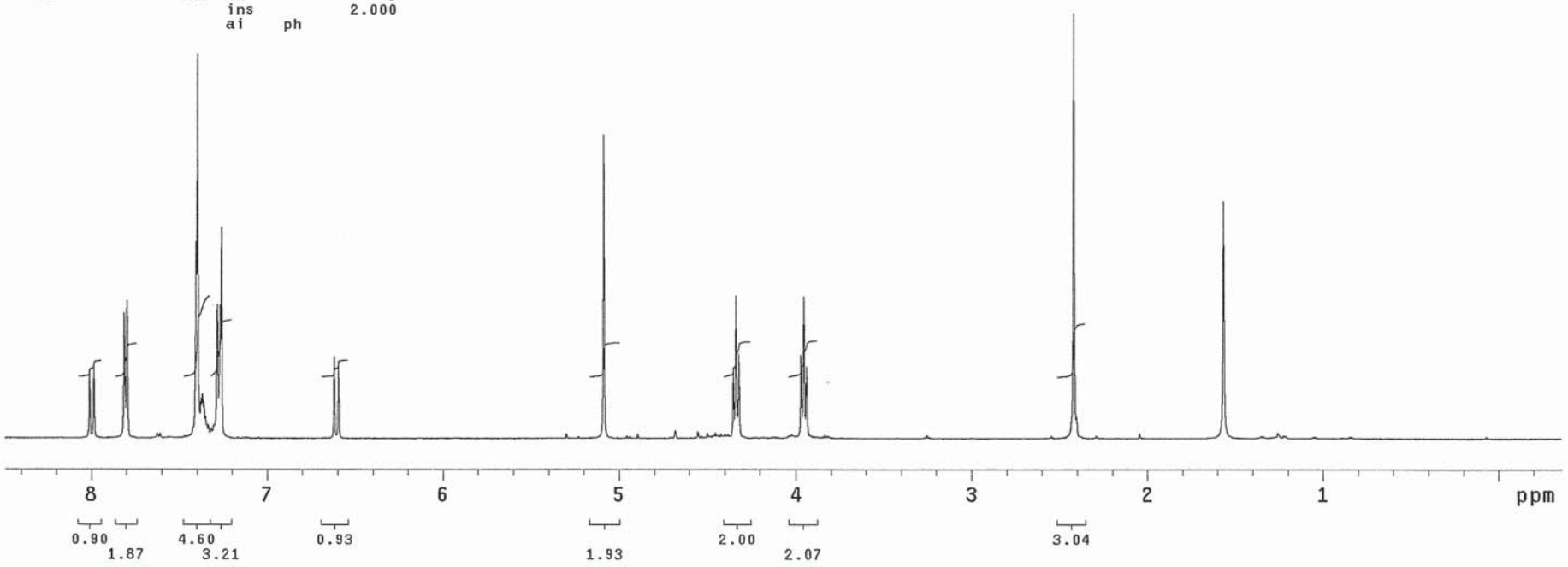


14f

```
lcq2-303-H

exp25  s2pul

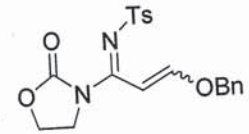
      SAMPLE              DEC. & VT
date    Dec 10 2010  dn              C13
solvent      CDCl3   dof               0
file           exp   dm              nnn
   ACQUISITION       dmm               c
sfrq       499.859   dmf             200
tn              H1       PROCESSING
at           2.500   lb             0.20
np           42518   fn            32768
sw          8503.4   math             i
fb        not used
bs               2   werr
pw             7.8   wexp
pw             7.8   wbs
tpwr            57   wnt
d1           4.800        DISPLAY
tof              0   sp          -181.1
nt              16   wp          4425.6
ct              16   vs              73
alock            n   sc               0
gain      not used   wc             250
      FLAGS         hzmm         17.70
il               n   is          259.57
in               n   rfl         5385.2
dp               y   rfp         3629.0
hs              nn   th               3
                     ins          2.000
                     ai    ph
```



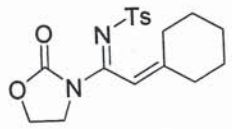
lcq2-303-13C

exp25 CARBON

SAMPLE		SPECIAL	
date	Dec 10 2010	temp	not used
solvent	cdcl3	gain	54
file	exp	spin	not used
ACQUISITION		hst	0.008
sw	28258.6	pw90	9.200
at	1.300	alfa	10.000
np	73498	FLAGS	
fb	16000	il	n
bs	4	in	n
d1	3.000	dp	y
nt	10000	hs	nn
ct	600	PROCESSING	
TRANSMITTER		lb	0.50
tn	C13	lsfid	2
sfrq	125.702	fn	not used
tof	865.4	DISPLAY	
tpwr	56	sp	-396.3
pw	13.500	wp	24050.6
DECOUPLER		rfl	11035.5
dn	H1	rfp	9678.0
dof	0	rp	-99.0
dm	nny	lp	-958.5
decwave		PLOT	
dpwr	36	wc	250
dmf	11101	sc	0
		vs	2557
		th	6
		ai cdc ph	



14f



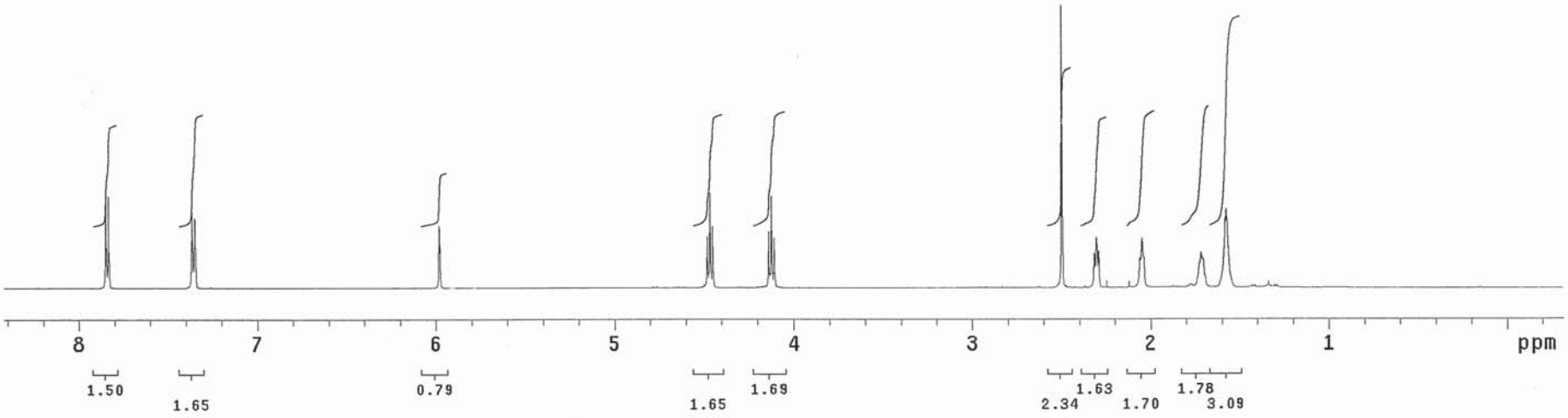
14g

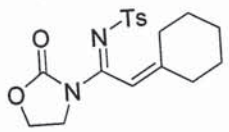
```
lcq2-265-H

exp25  PROTON

      SAMPLE
date    Dec 27 2010
solvent       CDCl3
file             exp
   ACQUISITION
sw            7997.6
at             2.049
np             32768
fb              4000
bs                 2
d1             1.000
nt                12
ct                12
   TRANSMITTER
tn                H1
sfrq         499.859
tof            499.9
tpwr              53
pw             4.550
    DECOUPLER
dn               C13
dof                0
dm               nnn
decwave W40_5mm3Gi~
                  dp
dpwr              47
dmf            32258

   PRESATURATION
satmode            n
wet                n
      SPECIAL
temp         not used
gain         not used
spin         not used
hst             0.008
pw90            9.100
alfa            6.600
       FLAGS
il                 n
in                 n
dp                 y
hs                nn
    PROCESSING
fn           not used
     DISPLAY
sp             -159.0
wp             4368.8
rfl            4585.1
rfp            3629.0
rp              157.1
lp               -1.3
      PLOT
wc                250
sc                  0
vs                 22
th                  4
ai  cdc  ph
```





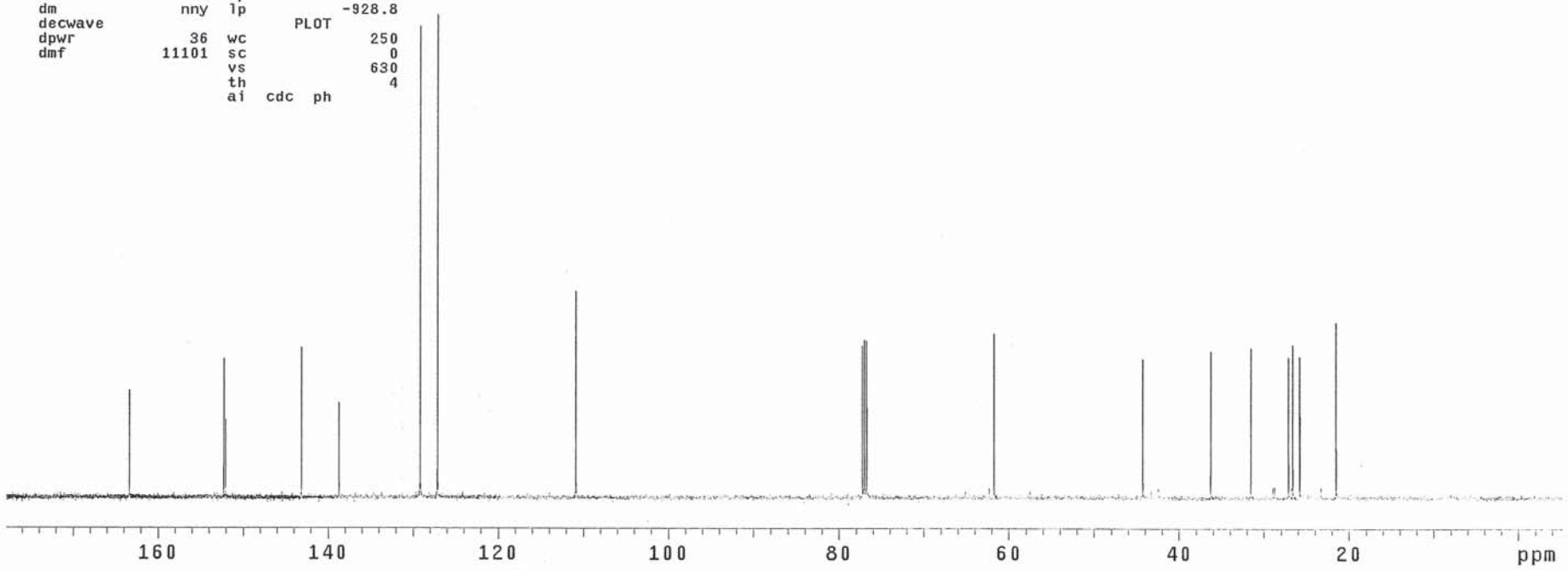
14g

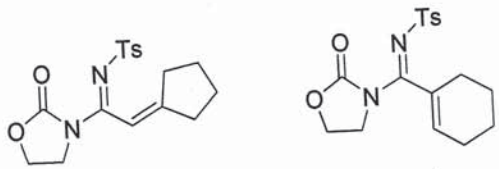
```
lcq2-265-13C

exp25  CARBON

      SAMPLE
date    Dec 27 2010
solvent       cdcl3
file            exp
   ACQUISITION
sw          28258.6
at              1.300
np              73498
fb              16000
bs                  2
d1              3.000
nt              10000
ct                296
   TRANSMITTER
tn                C13
sfrq          125.702
tof             865.4
tpwr               56
pw             13.500
    DECOUPLER
dn                 H1
dof                 0
dm                nny
decwave
dpwr               36
dmf             11101

      SPECIAL
temp        not used
gain              54
spin        not used
hst             0.008
pw90            9.200
alfa           10.000
        FLAGS
il                  n
in                  n
dp                  y
hs                 nn
     PROCESSING
lb              0.50
lsfid              2
fn          not used
       DISPLAY
sp            -668.4
wp           23023.9
rfl          11042.4
rfp           9678.0
rp              29.8
lp            -928.8
         PLOT
wc                250
sc                  0
vs                630
th                  4
ai  cdc  ph
```





(major)

(minor)

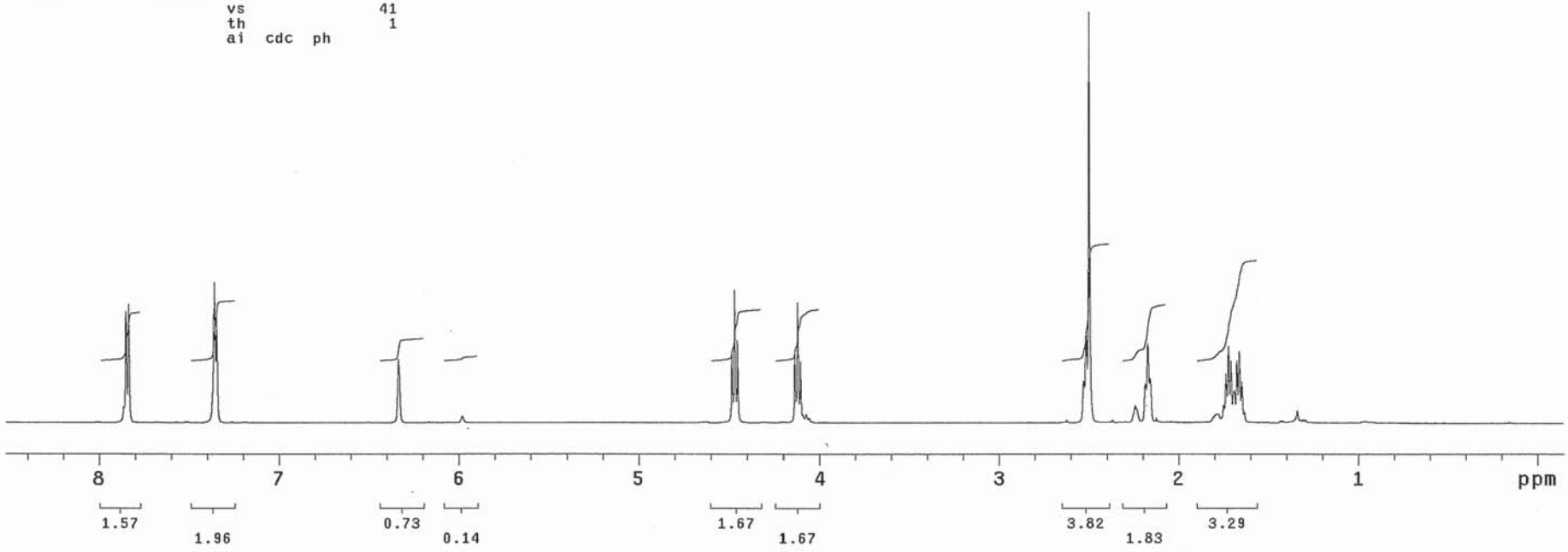
14h

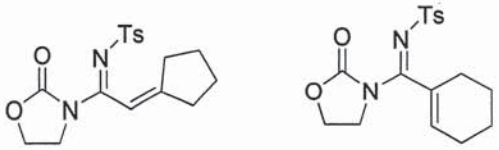
```
lcq2-266-2-H

exp25  PROTON

      SAMPLE
date    Dec 28 2010
solvent       CDCl3
file            exp
   ACQUISITION
sw           7997.6
at            2.049
np            32768
fb             4000
bs                2
d1            1.000
nt               16
ct               16
   TRANSMITTER
tn               H1
sfrq        499.859
tof           499.9
tpwr             53
pw            4.550
    DECOUPLER
dn               C13
dof                0
dm               nnn
decwave W40_5mm3Gi~
                dp
dpwr             47
dmf           32258

   PRESATURATION
satmode           n
wet               n
      SPECIAL
temp       not used
gain       not used
spin       not used
hst           0.008
pw90          9.100
alfa          6.600
       FLAGS
il                n
in                n
dp                y
hs               nn
    PROCESSING
fn         not used
     DISPLAY
sp            -72.9
wp           4331.2
rfl          3944.6
rfp          2990.1
rp            156.1
lp              2.7
      PLOT
wc              250
sc                0
vs               41
th                1
ai  cdc  ph
```





(major)

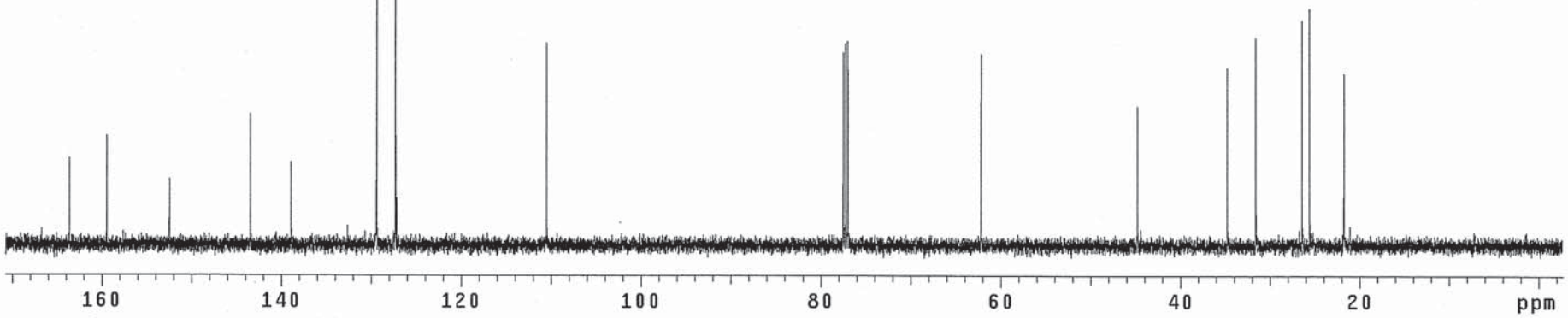
(minor)

14h

```
lcq2-266-13C

exp25  CARBON

      SAMPLE                SPECIAL
date    Dec 27 2010   temp       not used
solvent       cdcl3   gain             54
file            exp   spin       not used
   ACQUISITION         hst           0.008
sw          28258.6   pw90          9.200
at            1.300   alfa         10.000
np            73498         FLAGS
fb            16000   il                n
bs                2   in                n
d1            3.000   dp                y
nt            10000   hs               nn
ct               96        PROCESSING
   TRANSMITTER        lb             0.50
tn               C13   lsfid             2
sfrq        125.702   fn         not used
tof           865.4        DISPLAY
tpwr             56   sp            -337.7
pw           13.500   wp          21798.0
    DECOUPLER         rfl         11009.6
dn                H1   rfp          9678.0
dof                0   rp             26.1
dm               nny   lp            -902.4
decwave                    PLOT
dpwr              36   wc              250
dmf            11101   sc                0
                       vs              821
                       th                4
                       ai  cdc  ph
```

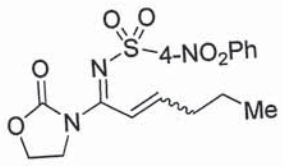


```
lcq2-242-H

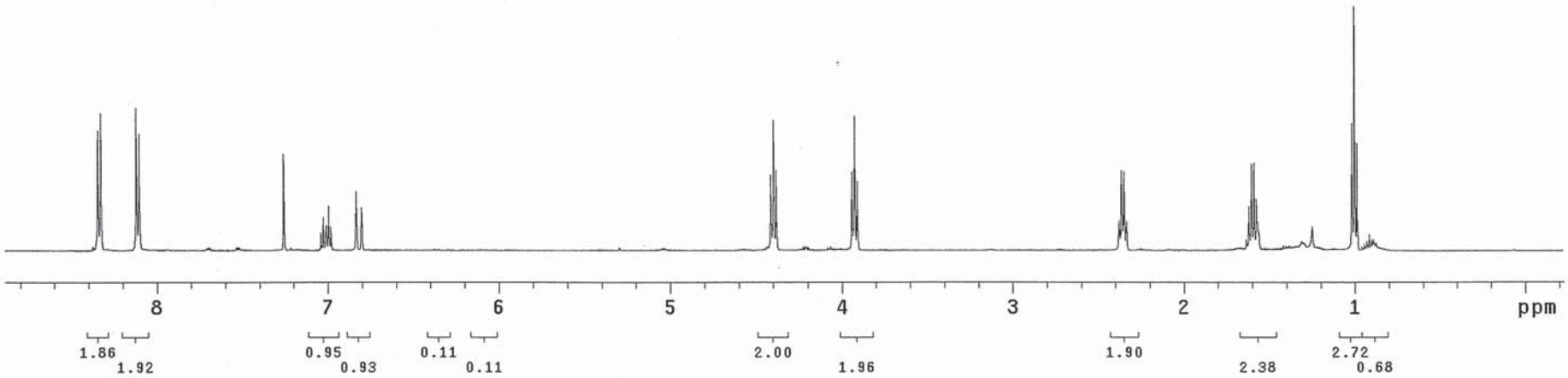
exp2  PROTON

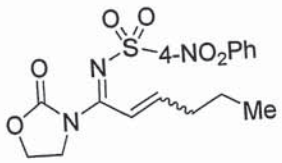
      SAMPLE
date    Dec 30 2010
solvent       CDCl3
file            exp
    ACQUISITION
sw           7997.6
at            2.049
np            32768
fb             4000
bs                2
d1            1.000
nt               16
ct               16
   TRANSMITTER
tn               H1
sfrq        499.859
tof           499.9
tpwr             53
pw            4.550
    DECOUPLER
dn              C13
dof               0
dm              nnn
decwave W40_5mm3Gi~
                dp
dpwr             47
dmf           32258

   PRESATURATION
satmode           n
wet               n
      SPECIAL
temp        not used
gain        not used
spin        not used
hst             0.008
pw90            9.100
alfa            6.600
       FLAGS
il                n
in                n
dp                y
hs               nn
    PROCESSING
fn          not used
     DISPLAY
sp             -113.1
wp             4556.3
rfl            4632.9
rfp            3629.0
rp              156.0
lp               -8.6
       PLOT
wc               250
sc                 0
vs                21
th                 2
ai  cdc  ph
```



14j



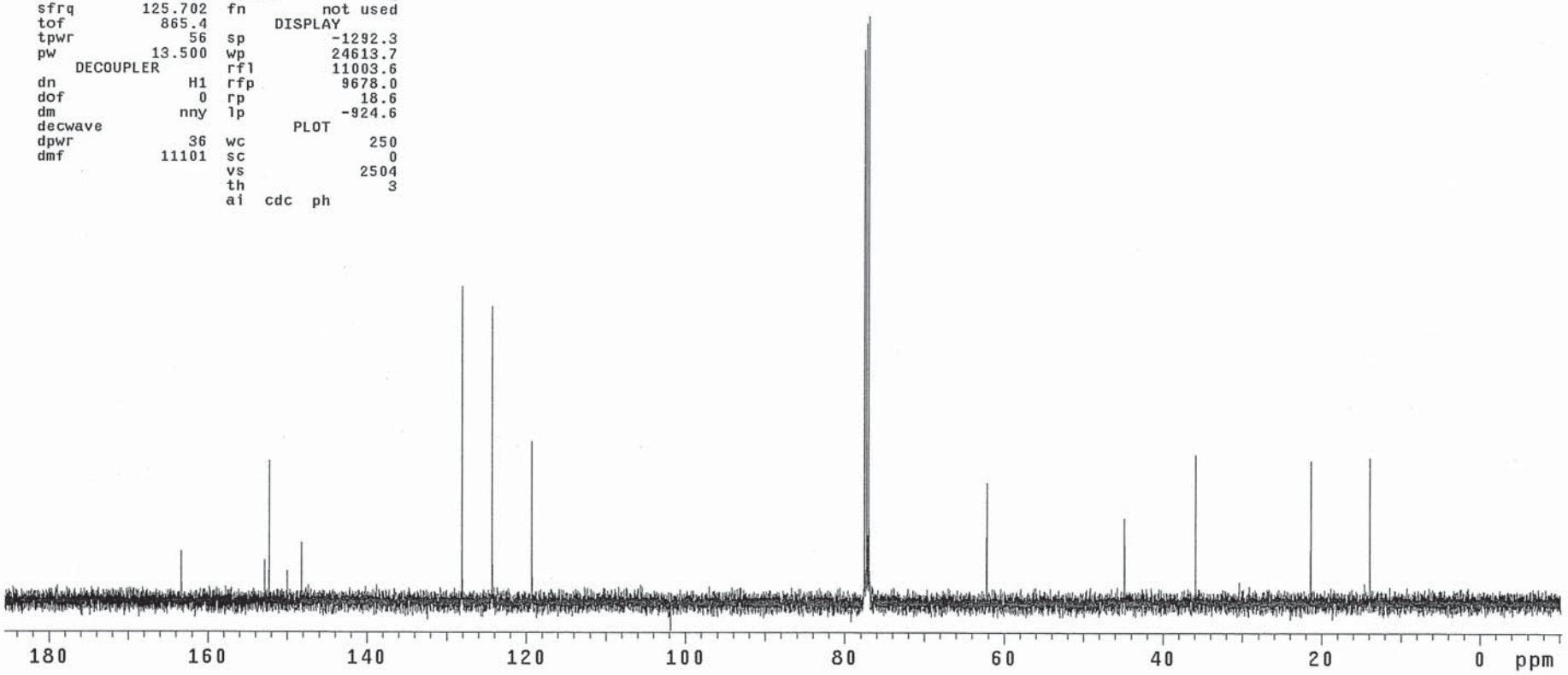


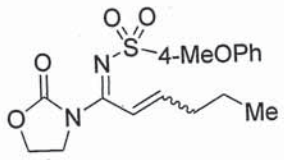
14j

lcq2-242-13C

exp25 CARBON

SAMPLE		SPECIAL	
date	Dec 27 2010	temp	not used
solvent	cdcl3	gain	54
file	exp	spin	not used
ACQUISITION		hst	0.008
sw	28258.6	pw90	9.200
at	1.300	alfa	10.000
np	73498	FLAGS	
fb	16000	il	n
bs	2	in	n
d1	3.000	dp	y
nt	10000	hs	nn
ct	524	PROCESSING	
TRANSMITTER		lb	0.50
tn	C13	lsfid	2
sfrq	125.702	fn	not used
tof	865.4	DISPLAY	
tpwr	56	sp	-1292.3
pw	13.500	wp	24613.7
DECOUPLER		rfl	11003.6
dn	H1	rfp	9678.0
dof	0	rp	18.6
dm	nny	lp	-924.6
decwave		PLOT	
dpwr	36	wc	250
dmf	11101	sc	0
		vs	2504
		th	3
		ai cdc ph	





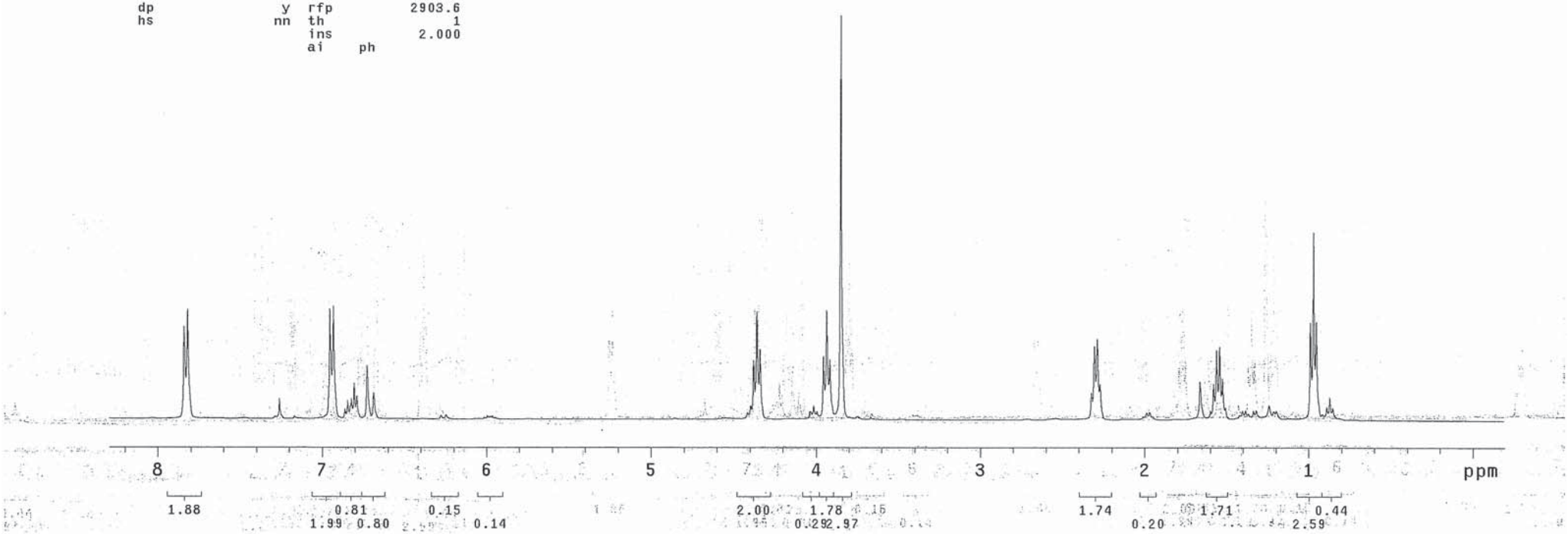
14i

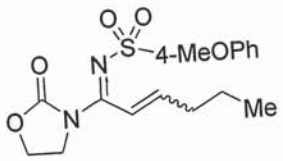
```
lcq3-121-H

exp25  s2pul

      SAMPLE
date    Dec 28 2010
solvent       cdcl3
file            exp
   ACQUISITION
sfrq        399.951
tn               H1
at           2.502
np           36008
sw          7196.8
fb        not used
bs                2
pw              8.0
pw              8.0
tpwr             57
d1            3.000
tof            -6.9
nt               16
ct               16
alock             n
gain      not used
      FLAGS
il                n
in                n
dp                y
hs               nn

      DEC. & VT
dn               H1
dof         -1425.0
dm              nnn
dmm               c
dmf             200
      PROCESSING
lb             0.10
fn            65536
math              f
werr
wexp
wbs
wnt
      DISPLAY
sp            -78.7
wp           3396.4
vs               72
sc                0
wc              250
hzmm          13.59
is           257.71
rfl          4504.2
rfp          2903.6
th                1
ins           2.000
ai    ph
```





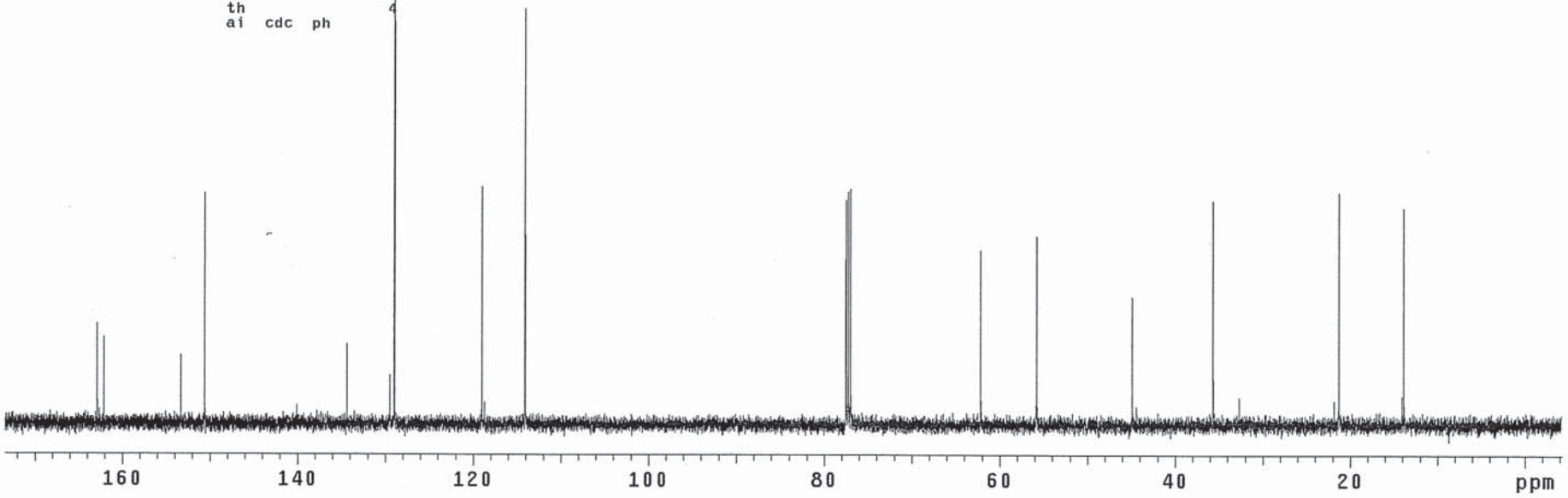
14i

```
lcq3-121-13C

exp2  CARBON

      SAMPLE
date    Dec 28 2010
solvent       cdcl3
file            exp
   ACQUISITION
sw          28258.6
at              1.300
np              73498
fb              16000
bs                  2
d1              3.000
nt              10000
ct                100
   TRANSMITTER
tn                C13
sfrq          125.702
tof             865.4
tpwr               56
pw             13.500
    DECOUPLER
dn                  H1
dof                  0
dm                 nny
decwave
dpwr               36
dmf             11101

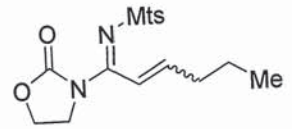
      SPECIAL
temp          not used
gain                54
spin          not used
hst                0.008
pw90               9.200
alfa              10.000
      FLAGS
il                    n
in                    n
dp                    y
hs                   nn
   PROCESSING
lb                 0.50
lsfid                 2
fn            not used
    DISPLAY
sp                -531.7
wp               22328.0
rfl              11004.9
rfp               9678.0
rp                  32.7
lp                -954.6
      PLOT
wc                   250
sc                     0
vs                   819
th                     4
ai  cdc  ph
```



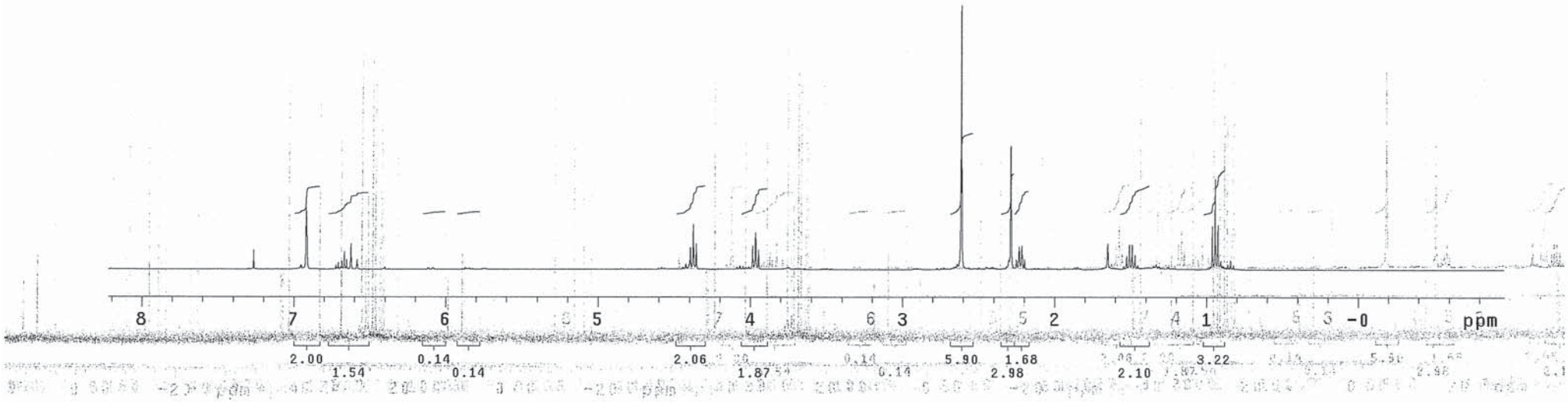
lcq3-170b

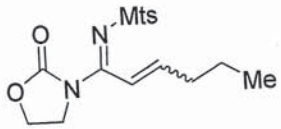
exp25 s2pul

SAMPLE		DEC. & VT	
date	Jan 18 2011	dn	C13
solvent	cdcl3	dof	-1425.0
file	exp	dm	nnn
ACQUISITION		dmm	c
sfrq	399.951	dmf	200
tn	H1	PROCESSING	
at	2.500	lb	0.20
np	40016	fn	65536
sw	8003.2	math	i
fb	not used		
bs	2	werr	
pw	11.7	wexp	
pw	11.7	wbs	
tpwr	60	wnt	
d1	4.800	DISPLAY	
tof	0	sp	-386.1
nt	16	wp	3674.1
ct	16	vs	17
alock	n	sc	0
gain	not used	wc	250
FLAGS		hzmm	14.70
il	n	is	211.16
in	n	rfl	1994.5
dp	y	rfp	0
hs	nn	th	5
		ins	2.000
		ai ph	



14k





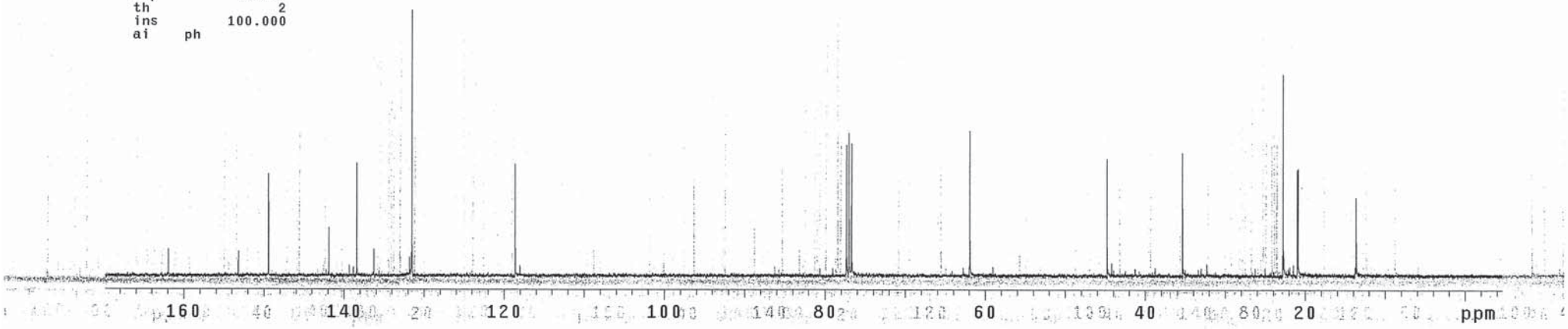
14k

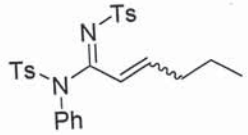
```
lcq3-170b-13C

exp25  std13c

      SAMPLE
date   Jan 18 2011
solvent      cdcl3
file           exp
   ACQUISITION
sfrq       100.577
tn              C13
at            0.701
np            39216
sw          27972.0
fb        not used
bs                2
ss                4
tpwr             58
pw              7.0
d1            1.000
tof           525.7
nt           100000
ct             1400
alock             n
gain             44
      FLAGS
il                n
in                n
dp                y
hs               nn
     DISPLAY
sp          -468.3
wp         17546.5
vs            3026
sc               0
wc             250
hzmm         70.19
is          500.00
rfl        11676.1
rfp         7743.7
th                2
ins         100.000
ai    ph

      DEC. & VT
dfrq       399.951
dn              H1
dpwr            40
dof              0
dm             yyy
dmm              w
dmf           6700
dseq
dres          90.0
homo             n
     PROCESSING
lb            1.00
wtfile
proc             ft
fn           65536
math             f
werr
wexp
wbs
wnt
```





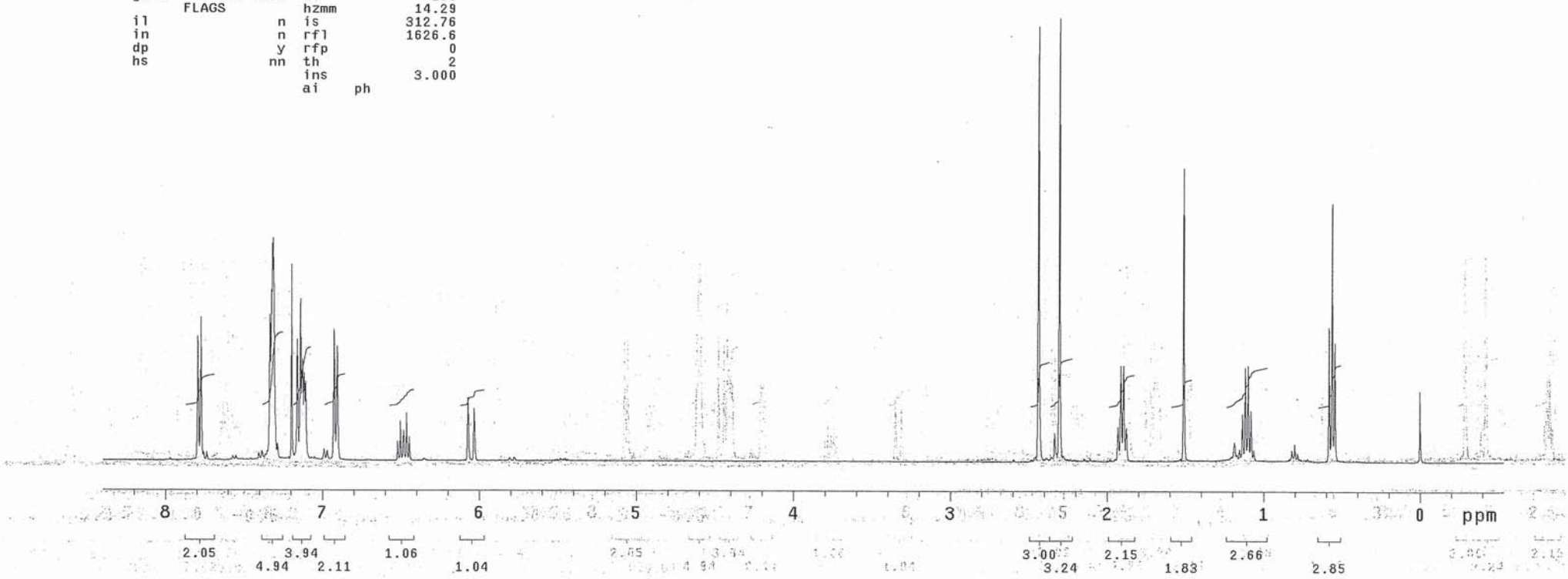
14l

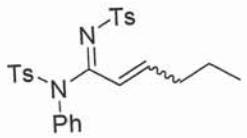
```
lcq3-65-4

exp25  s2pul

      SAMPLE
date    Dec  2 2010
solvent       cdcl3
file            exp
   ACQUISITION
sfrq        399.951
tn               H1
at             2.500
np             35984
sw            7196.8
fb         not used
bs                 2
pw               6.7
pw               6.7
tpwr              57
d1             4.800
tof              -6.9
nt                10
ct                10
alock              n
gain       not used
      FLAGS
il                 n
in                 n
dp                 y
hs                nn

      DEC. & VT
dn                H1
dof          -1425.0
dm               nnn
dmm                c
dmf              200
      PROCESSING
lb              0.20
fn             65536
math               f
werr
wexp
wbs
wnt
      DISPLAY
sp            -214.1
wp            3572.9
vs               101
sc                 0
wc               250
hzmm           14.29
is            312.76
rfl           1626.6
rfp                0
th                 2
ins            3.000
ai     ph
```





14l

```
lcq-3-65-4

exp1  CARBON

      SAMPLE                SPECIAL
date    Dec  2 2010  temp       not used
solvent       cdcl3  gain             54
file            exp  spin             20
   ACQUISITION        hst           0.008
sw          28258.6  pw90          9.200
at            1.300  alfa         10.000
np            73498        FLAGS
fb            16000  il                n
bs                4  in                n
d1            3.000  dp                y
nt            10000  hs               nn
ct              764       PROCESSING
   TRANSMITTER       lb            0.50
tn              C13  lsfid            2
sfrq        125.702  fn         not used
tof           865.4       DISPLAY
tpwr             56  sp           -403.6
pw           13.500  wp          23570.2
    DECOUPLER        rfl         11035.0
dn                H1  rfp          9707.0
dof                0  rp            -85.8
dm               nny  lp           -943.7
decwave                    PLOT
dpwr              36  wc              250
dmf            11101  sc                0
                      vs             3341
                      th                4
                      ai  cdc  ph
```