Supporting Information

Synthesis of spiro[isoquinolinone-4,2'-oxiranes] and isoindolinones via multicomponent reaction of 2-acetyl-oxirane-2-carboxamides, arylaldehydes and malononitrile

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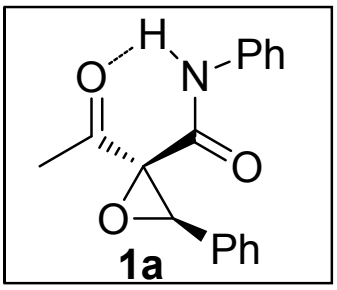
I. General

All reagents were purchased from commercial sources and used without treatment, unless otherwise indicated. The products were purified by column chromatography over silica gel. ^{1}H NMR and ^{13}C NMR spectra were recorded at 25 ºC on a Varian 500 MHz and 125 MHz, respectively, and TMS as internal standard. High resolution mass spectra (HRMS) were recorded on Bruck microTof by using ESI method. Data for ^{1}H NMR are reported as follows: chemical shift (ppm), and multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet), coupling constants (Hz) and integration; Data for ^{13}C NMR are reported as ppm. Melting points were measured on an X_4-type micro-melting point apparatus and were uncorrected.

II. Synthesis and analytical data of 1-5

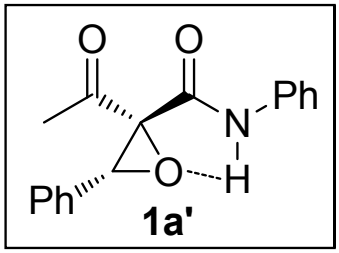
General procedure for substrate preparation (**1a** and **1a**' as an example): To a mixture of 2-benzylidene-3-oxo-*N*-phenylbutanamide (1 mmol, 0.265 g) in 2 mL of DCE added DBU (0.3 mmol, 0.045 mL) and TBHP (2.0 mmol, 0.2 mL). The reaction was stirred at room temperature for 15 min. After the reaction was completed (monitored by TLC), the resulting mixture was concentrated under reduced pressure and the residue was purified through column chromatography on silica gel (eluent, petroleum ether: ethyl acetate = 20: 1). Products **1a** and **1a'** were obtained as white solid in respective 48% and 49% yields.

(2*S*,3*R*)-2-Acetyl-*N*,3-diphenyloxirane-2-carboxamide (1a)



White solid. m.p. 123-125 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 2.53 (s, 3H), 4.48 (s, 1H), 7.08-7.11 (m, 1H), 7.25 (t, *J* = 5.5 Hz, 4H), 7.30-7.34 (m, 3H), 7.38-7.40 (m, 2H), 8.17 (s, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 27.4, 64.1, 67.7, 120.3, 125.0, 126.3, 128.5, 128.9, 129.2, 131.4, 136.2, 161.2, 201.2; HRMS (ESI) m/z calcd for $C_{17}H_{15}NO_3$ $[M+H]^+$: 282.1130; found: 282.1122.

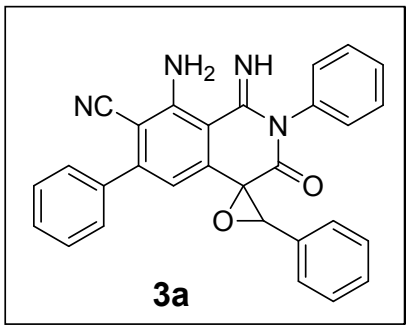
1-((2*R*,3*R*)-2-Benzoyl-3-phenyloxiran-2-yl)ethanone (1a')



White solid. m.p. 121-123 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 2.15 (s, 3H), 4.45 (s, 1H), 7.18 (d, *J* = 7.0 Hz, 1H), 7.33-7.35 (m, 3H), 7.38 (t, *J* = 3.5 Hz, 4H), 7.57 (d, *J* = 8.0 Hz, 2H), 8.61 (s, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 30.1, 63.9, 68.6, 119.9, 125.1, 126.2, 128.7, 129.1, 129.3, 131.3, 136.5, 162.5, 200.4; HRMS (ESI) m/z calcd for $C_{17}H_{15}NO_3$ $[M+H]^+$: 282.1130; found: 282.1125.

General procedure for the preparation of **3** (**3a** as an example): To a solution of (2*S*,3*R*)-2-acetyl-*N*,3-diphenyloxirane-2-carboxamide **1a** (1 mmol, 0.2813 g) and malononitrile (2.2 mmol, 0.1452 g) in CH_2Cl_2 (4.0 mL) was added benzaldehyde (1.1 mmol, 0.11 mL) and piperidine (2.2 mmol, 0.22 mL). The reaction mixture was stirred at room tempreture for about 1 h. After the starting material **1a** was consumed as indicated by TLC, the reaction mixture was poured into water and then extracted with CH_2Cl_2 (3 × 10 mL). The combined organic phase was washed with water (3 × 10 mL), dried over anhydrous $MgSO_4$, filtered and concentrated under reduced pressure. The crude product was purified by flash chromatography (silica gel, petroleum ether: ethyl acetate = 12: 1) to give **3a** (0.378 g, 83%) as yellow solid.

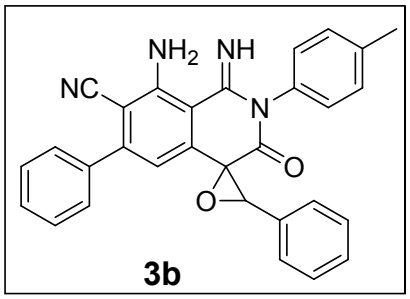
8-Amino-1-imino-3-oxo-2,3',6-triphenyl-2,3-dihydro-1*H*-spiro[isoquinoline-4,2'-oxirane]-7-carbonitrile (3a）



3a

Yellow solid. m.p. 195-197 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 4.26 (s, 1H), 6.89 (s, 1H), 7.36 (t, *J* = 3.5 Hz, 4H), 7.43 (s, 2H), 7.49-7.53 (m, 6H), 7.63-7.65 (m, 2H), 7.72 (s, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 62.3, 72.2, 96.3, 108.3, 110.1, 117.0, 127.2, 128.0, 128.5, 128.8, 129.0, 129.2, 129.4, 129.7, 130.4, 130.9, 133.3, 137.8, 140.2, 149.7, 152.0, 155.9, 162.3; HRMS (ESI) m/z calcd for $C_{29}H_{20}N_4O_2$ $[M+H]^+$: 457.1665; found: 457.1659.

8-Amino-1-imino-3-oxo-3',6-diphenyl-2-(*p*-tolyl)-2,3-dihydro-1*H*-spiro[isoquinoline-4,2'-oxirane]-7-carbonitrile (3b)

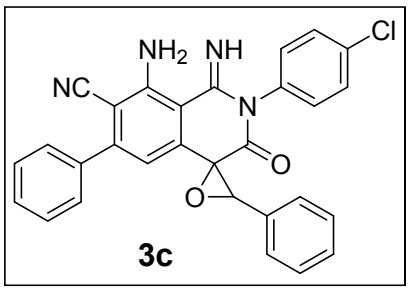


3b

White solid. m.p. 200-202 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 2.35 (s, 3H), 4.23 (s, 1H), 6.38 (s, 1H), 6.87 (s, 1H), 7.00 (s, 1H), 7.17 (s, 1H), 7.33-7.37 (m, 3H), 7.47-7.53 (m, 5H), 7.63 (d, *J* = 6.5 Hz, 2H) 7.74 (s, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 21.2, 62.4, 72.2, 96.4, 108.3, 110.1, 117.0, 127.3, 127.9,

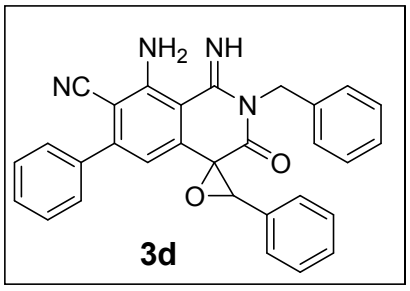
128.5, 128.8, 129.0, 129.4, 130.5, 131.0, 131.1, 137.8, 140.0, 140.3, 149.7, 152.1, 156.0, 162.4; HRMS (ESI) m/z calcd for $C_{30}H_{22}N_4O_2$ $[M+H]^+$: 471.1821; found: 471.1829.

8-Amino-2-(4-chlorophenyl)-1-imino-3-oxo-3',6-diphenyl-2,3-dihydro-1*H*-spiro[isoquinoline-4,2'-oxirane]-7-carbonitrile (3c)



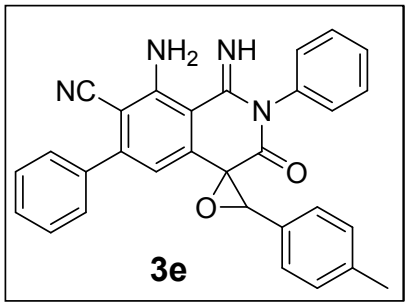
Yellow solid. m.p. 197-199 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 4.25 (s, 1H), 6.87 (s, 1H), 7.36 (d, *J* = 4.0 Hz,5H), 7.49-7.53 (m, 5H), 7.62 (d, *J* = 7.0 Hz, 2H), 7.70 (s, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 62.3, 72.3, 96.5, 108.1, 110.1, 116.9, 127.3, 128.0, 128.5, 128.8, 129.2, 129.5, 130.8, 130.9, 131.8, 135.9, 137.7, 140.1, 150.0, 152.1, 155.7, 162.4; HRMS (ESI) m/z calcd for $C_{29}H_{19}ClN_4O_2$ $[M+H]^+$: 491.1275; found: 491.1281.

8-Amino-2-benzyl-1-imino-3-oxo-3',6-diphenyl-2,3-dihydro-1*H*-spiro[isoquinoline-4,2'-oxirane]-7-carbonitrile (3d)



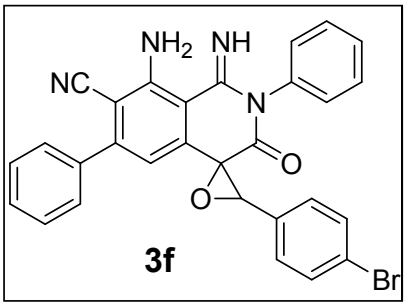
Yellow solid. m.p. 123-125 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 4.22 (s, 1H), 4.42 (d, *J* = 16.5 Hz, 1H), 5.52 (d, *J* = 16.5 Hz,1H), 6.67 (d, *J* = 4.0 Hz, 2H), 6.85 (s, 1H), 7.12 (t, *J* = 7.5 Hz, 2H), 7.18 (t, *J* = 7.0 Hz, 1H), 7.40-7.44 (m, 3H), 7.48-7.52 (m, 3H), 7.56-7.61 (m, 4H), 8.19 (s, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 44.7, 62.4, 72.1, 96.4, 108.7, 109.8, 117.0, 126.1, 127.5, 127.8, 128.0, 128.5, 128.8, 129.0, 129.2, 129.4, 130.9, 134.7, 137.8, 139.8, 149.6, 151.7, 155.4, 162.8; HRMS (ESI) m/z calcd for $C_{30}H_{22}N_4O_2$ $[M+H]^+$: 471.1821; found: 471.1825.

8-Amino-1-imino-3-oxo-2,6-diphenyl-3'-(*p*-tolyl)-2,3-dihydro-1*H*-spiro[isoquinoline-4,2'-oxirane]-7-carbonitrile (3e)



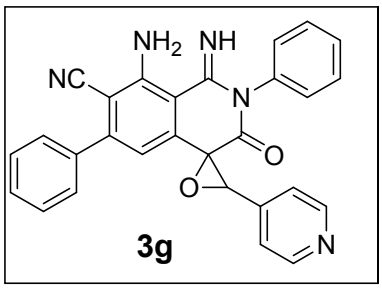
Yellow solid. m.p. 196-198 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 2.34 (s, 3H), 4.22 (s, 1H), 6.87 (s, 1H), 7.16 (d, *J* = 8.0 Hz,2H), 7.41 (t, *J* = 9.0 Hz,5H), 7.47-7.53 (m, 4H), 7.63 (d, *J* = 7.0 Hz, 2H), 7.70 (s, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 21.3, 62.3, 72.5, 96.3. 108.3, 110.1, 117.0, 127.2, 128.0, 128.5, 128.7, 128.8, 129.3, 129.4, 129.7, 130.4, 133.4, 137.8, 139.0, 140.4, 149.7, 152.1, 156.0, 162.5; HRMS (ESI) m/z calcd for $C_{30}H_{22}N_4O_2$ $[M+H]^+$: 471.1821; found: 471.1828.

8-Amino-3'-(4-bromophenyl)-1-imino-3-oxo-2,6-diphenyl-2,3-dihydro-1*H*-spiro[isoquinoline-4,2'-oxirane]-7-carbonitrile (3f)



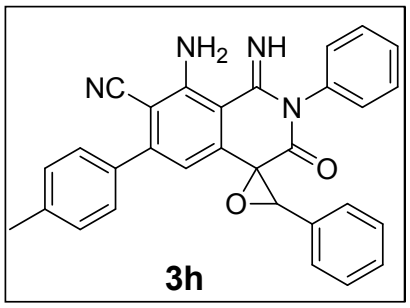
Yellow solid. m.p. 172-174 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 4.20 (d, *J* = 4.5 Hz, 1H), 6.60 (s, 1H), 6.82 (d, *J* = 23.5 Hz,1H), 7.14 (s, 1H), 7.40-7.42 (m, 2H), 7.47-7.54 (m, 7H), 7.62-7.66 (m, 2H), 7.75 (d, *J* = 10.5 Hz, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 62.3, 72.2, 96.1, 108.6, 109.7, 116.8, 124.0, 127.2, 128.0, 129.1, 129.2, 129.8, 130.0, 130.4, 130.8, 132.0, 133.2, 136.6, 140.5, 148.4, 152.1, 155.8, 162.2; HRMS (ESI) m/z calcd for $C_{29}H_{19}BrN_4O_2$ $[M+H]^+$: 535.0770; found: 535.0764.

8-Amino-1-imino-3-oxo-2,6-diphenyl-3'-(pyridin-4-yl)-2,3-dihydro-1H-spiro[isoquinoline-4,2'-oxirane]-7-carbonitrile (3g)



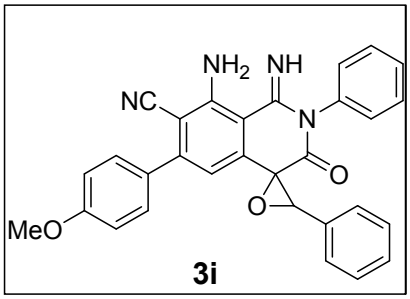
Yellow solid. m.p. 193-195 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 4.23 (s, 1H), 6.57 (s, 1H), 6.87 (s, 1H), 7.14 (s, 1H), 7.46-7.64 (m, 10H), 7.80 (s, 1H), 8.64 (s, 2H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 61.9, 70.3, 96.9, 108.3, 110.2, 116.8, 122.0, 128.4, 128.9, 129.2, 129.6, 130.0, 130.6, 133.0, 137.6, 139.3, 139.6, 149.6, 149.9, 152.1, 155.6, 161.8; HRMS (ESI) m/z calcd for $C_{28}H_{19}N_5O_2$ $[M+H]^+$: 458.1617; found: 458.1609.

8-Amino-1-imino-3-oxo-2,3'-diphenyl-6-(*p*-tolyl)-2,3-dihydro-1*H*-spiro[isoquinoline-4,2'-oxirane]-7-carbonitrile (3h）



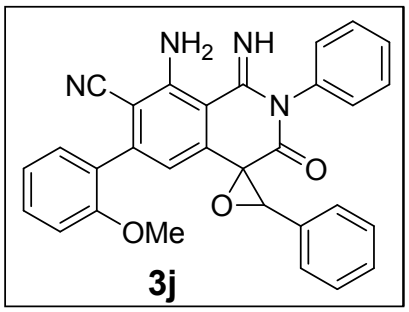
Yellow solid. m.p. 210-212 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 2.44 (s, 3H), 4.24 (s, 1H), 6.87 (s, 1H), 7.32-7.36 (m, 6H), 7.42 (d, *J* = 2.0 Hz, 2H), 7.50-7.54 (m, 4H), 7.70 (s, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 21.3, 62.4, 72.2, 96.4, 108.1, 110.0, 117.1, 127.3, 128.0, 128.4, 129.0, 129.3, 129.5, 129.7, 130.4, 131.0, 133.4, 135.0, 139.6, 140.2, 149.9, 152.1, 156.0, 162.4; HRMS (ESI) m/z calcd for $C_{30}H_{22}N_4O_2$ $[M+H]^+$: 471.1821; found: 471.1827.

8-Amino-1-imino-6-(4-methoxyphenyl)-3-oxo-2,3'-diphenyl-2,3-dihydro-1*H*-spiro[isoquinoline-4,2'-oxirane]-7-carbonitrile (3i）



Yellow solid. m.p. 187-189 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 3.88 (s, 3H), 4.24 (s, 1H), 6.86 (s, 1H), 7.03-7.04 (m, 2H), 7.34-7.37 (m, 3H), 7.42 (d, *J* = 2.0 Hz, 2H), 7.50-7.52 (m, 2H), 7.59-7.60 (m, 2H), 7.68 (s, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 55.4, 62.4, 72.2, 96.1, 107.8, 109.8, 114.2, 117.2, 127.3, 127.9, 129.0, 129.3, 129.7, 129.8, 130.1, 130.4, 131.0, 133.4, 140.1, 149.4, 152.1, 155.9, 160.6, 162.4; HRMS (ESI) m/z calcd for $C_{30}H_{22}N_4O_3$ $[M+H]^+$: 487.1770; found: 487.1761.

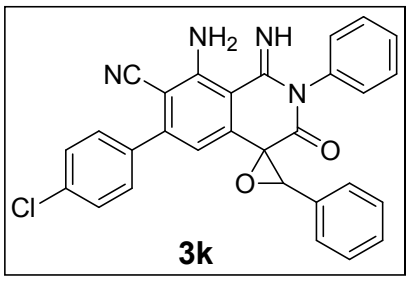
8-Amino-1-imino-6-(2-methoxyphenyl)-3-oxo-2,3'-diphenyl-2,3-dihydro-1*H*-spiro[isoquinoline-4,2'-oxirane]-7-carbonitrile (3j)



Yellow solid. m.p. 189-191 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 3.89 (s, 3H), 4.26 (s, 1H), 6.85 (s, 1H), 7.05-7.10 (m, 3H), 7.32-7.36 (m, 4H), 7.42-7.47 (m, 3H), 7.52 (d, *J* = 6 Hz, 3H), 7.71 (s, 1H); ^{13}C NMR

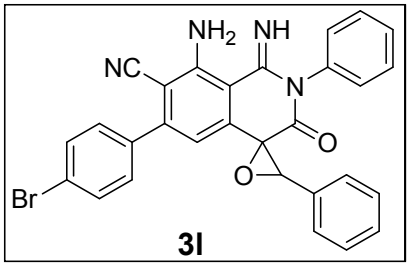
($CDCl_3$, 125 MHz): δ = 55.5, 62.3, 72.1, 98.7, 108.3, 111.2, 111.3, 116.7, 120.8, 126.8, 127.2, 127.9, 129.0, 129.3, 129.7, 130.4, 130.4, 130.8, 131.1, 133.4, 139.8, 147.1, 151.3, 156.0, 156.3, 162.5; HRMS (ESI) m/z calcd for $C_{30}H_{22}N_4O_3$ $[M+H]^+$: 487.1770; found: 487.1763.

8-Amino-6-(4-chlorophenyl)-1-imino-3-oxo-2,3'-diphenyl-2,3-dihydro-1*H*-spiro[isoquinoline-4,2'-oxirane]-7-carbonitrile (3k）



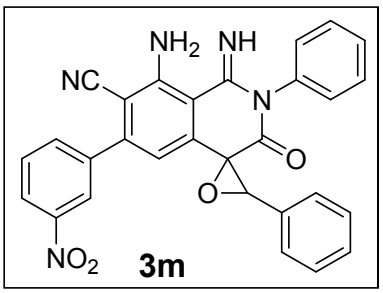
Yellow solid. m.p. 155-157 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 4.25 (s, 1H), 6.84 (s, 1H), 7.36 (d, *J* = 5 Hz, 4H), 7.43 (s, 2H), 7.49 (d, *J* = 8.5 Hz, 5H), 7.57 (d, *J* = 8.0 Hz, 2H),7.74 (s, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ =62.3, 72.2, 96.2, 108.6, 109.8, 116.8, 127.2, 128.0, 128.5, 128.8, 129.1, 129.1, 129.8, 130.4, 130.8, 133.2, 135.7, 136.2, 140.5, 148.4, 152.1, 155.8, 162.2; HRMS (ESI) m/z calcd for $C_{29}H_{19}ClN_4O_2$ $[M+H]^+$: 491.1275; found: 491.1263.

8-Amino-6-(4-bromophenyl)-1-imino-3-oxo-2,3'-diphenyl-2,3-dihydro-1*H*-spiro[isoquinoline-4,2'-oxirane]-7-carbonitrile (3l)



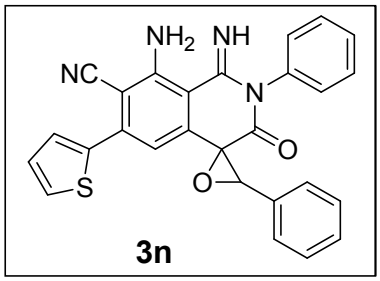
Yellow solid. m.p. 185-187 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 4.24 (s, 1H), 6.84 (s, 1H), 7.35 (t, *J* = 3.8 Hz, 4H), 7.43 (s, 2H), 7.49-7.52 (m, 4H), 7.65 (d, *J* = 8.5 Hz, 2H),7.74 (s, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 62.2, 72.2, 96.0, 108.5, 109.7, 116.7, 123.9, 127.2, 127.9, 129.0, 129.2, 129.7, 130.0, 130.4, 130.8, 131.9, 133.2, 136.6, 140.4, 148.3, 152.0, 155.8, 162.2; HRMS (ESI) m/z calcd for $C_{29}H_{19}BrN_4O_2$ $[M+H]^+$: 535.0770; found: 535.0781.

8-Amino-1-imino-6-(3-nitrophenyl)-3-oxo-2,3'-diphenyl-2,3-dihydro-1*H*-spiro[isoquinoline-4,2'-oxirane]-7-carbonitrile (3m)



Yellow solid. m.p. 207-209 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 4.30 (s, 1H), 6.52 (s, 1H), 6.88 (s, 1H), 7.14 (s, 1H), 7.36-7.52 (m, 8H), 7.71 (t, *J* = 8.0 Hz, 1H), 7.97 (d, *J* = 7.5 Hz, 1H), 8.34 (d, *J* = 7.5 Hz, 4H), 8.46 (s, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 62.2, 72.3, 96.1, 109.3, 109.8, 116.3, 123.5, 124.0, 127.2, 127.9, 129.1, 129.8, 129.9, 130.4, 130.6, 133.1, 134.5, 139.3, 140.9, 146.8, 148.2, 152.1, 155.6, 162.0; HRMS (ESI) m/z calcd for $C_{29}H_{19}N_5O_4$ $[M+H]^+$: 502.1515; found: 502.1503.

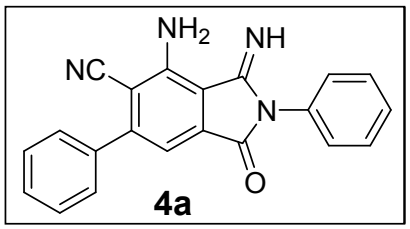
8-Amino-1-imino-3-oxo-2,3'-diphenyl-6-(4-(thiophen-2-yl)phenyl)-2,3-dihydro-1*H*-spiro[isoquinoline-4,2'-oxirane]-7-carbonitrile (3n)



3n

Brown solid. m.p. 193-195 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 4.26 (s, 1H), 6.98 (s, 1H), 7.18-7.20 (m, 1H), 7.34-7.37 (m, 4H), 7.42 (t, *J* = 3.5 Hz, 2H), 7.50-7.53 (m, 4H), 7.70 (s, 1H), 7.77-7.78 (m, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 62.3, 72.2, 94.6, 108.2, 109.4, 117.2, 127.3, 128.0, 128.3, 128.4, 128.5, 129.1, 129.3, 129.7, 130.4, 130.9, 133.4, 139.2, 140.5, 141.5, 152.5, 155.8, 162.2; HRMS (ESI) m/z calcd for $C_{27}H_{18}N_4O_2S$ $[M+H]^+$: 463.1229; found: 463.1235.

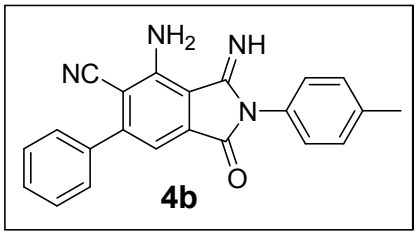
4-Amino-3-imino-1-oxo-2,6-diphenylisoindoline-5-carbonitrile (4a)



4a

Yellow solid. m.p. 229-231 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 6.48 (s, 2H), 7.32 (t, *J* = 5.0 Hz, 3H), 7.47-7.53 (m, 4H), 7.57-7.61 (m, 4H), 8.23 (s, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 99.4, 112.6, 113.8, 116.1, 127.8, 128.5, 128.8, 129.2, 129.5, 130.1,130.8, 134.8, 137.7, 147.9, 151.1, 157.1, 165.8; HRMS (ESI) m/z calcd for $C_{21}H_{14}N_4O$ $[M+H]^+$: 339.1246; found: 339.1251.

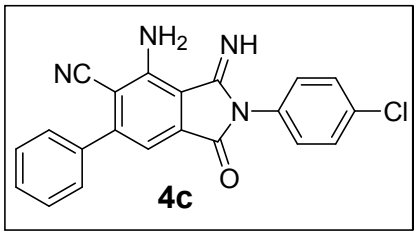
4-Amino-3-imino-1-oxo-6-phenyl-2-(*p*-tolyl)isoindoline-5-carbonitrile (4b)



4b

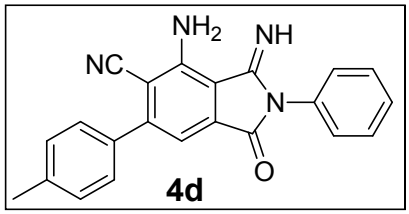
Yellow solid. m.p. 225-227 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 2.45 (s, 3H), 7.19 (d, *J* = 8.5 Hz, 2H), 7.30 (s, 1H), 7.38 (d, *J* = 8.0 Hz, 2H), 7.49-7.53 (m, 4H), 7.60 (t, *J* = 3.5 Hz), 8.19 (s, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 21.2, 99.2, 112.5, 113.8, 116.1, 127.6, 127.9, 128.5, 128.8, 129.4, 130.6, 134.8, 137.7, 139.3, 147.8, 151.0, 157.2, 165.9; HRMS (ESI) m/z calcd for $C_{22}H_{16}N_4O$ $[M+H]^+$: 353.1402; found: 353.1408.

4-Amino-2-(4-chlorophenyl)-3-imino-1-oxo-6-phenylisoindoline-5-carbonitrile (4c)



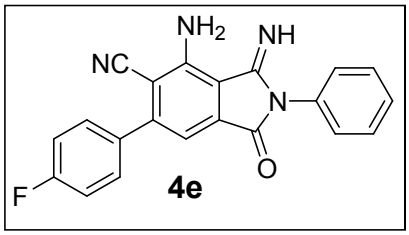
Yellow solid. m.p. 242-244 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.29 (d, *J* = 10.0 Hz, 4H), 7.51-7.61 (m, 8H), 8.21 (s, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 99.5, 112.7, 113.7, 116.0, 128.5, 128.9, 129.1, 129.3, 129.5, 130.4, 134.5, 135.2, 137.7, 148.0, 151.3, 156.7, 165.7; HRMS (ESI) m/z calcd for $C_{21}H_{13}ClN_4O$ $[M+H]^+$: 373.0856; found: 373.0848.

4-Amino-3-imino-1-oxo-2-phenyl-6-(*p*-tolyl)isoindoline-5-carbonitrile (4d)



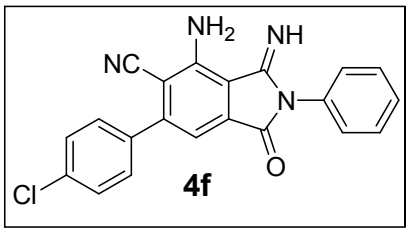
Yellow solid. m.p. 204-206 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 2.44 (s, 3H), 7.31 (t, *J* = 17.0 Hz, 5H), 7.51 (d, *J* = 8.0 Hz, 4H), 7.59 (t, *J* = 15.0 Hz, 3H), 8.21 (s, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 21.4, 99.2, 112.5, 113.5, 116.3, 127.8, 128.5, 129.1, 129.6, 130.1, 130.8, 134.8, 134.9, 139.7, 148.0, 151.2, 157.1, 165.9; HRMS (ESI) m/z calcd for $C_{22}H_{16}N_4O$ $[M+H]^+$: 353.1402; found: 353.1396.

4-Amino-6-(4-fluorophenyl)-3-imino-1-oxo-2-phenylisoindoline-5-carbonitrile (4e)



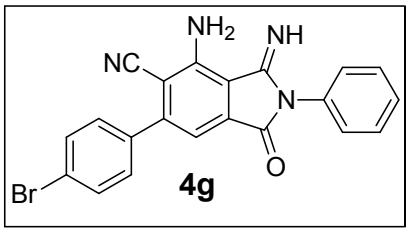
Yellow solid. m.p. 192-194 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.22, (t, *J* = 16.5 Hz, 2H), 7.27 (s, 2H), 7.32 (d, *J* = 7.5 Hz, 2H), 7.52 (d, *J* = 7.5 Hz,1H), 7.60 (t, *J* = 5.5 Hz, 4H), 8.25 (s, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 99.2, 112.4, 113.9, 115.9, 116.0, 116.1, 127.7, 129.2, 130.1, 130.4, 130.5, 130.7, 133.8, 134.9, 147.9, 149.9, 157.0, 162.4, 164.4, 165.7; HRMS (ESI) m/z calcd for $C_{21}H_{13}FN_4O$ $[M+H]^+$: 357.1152; found: 357.1159.

4-Amino-6-(4-chlorophenyl)-3-imino-1-oxo-2-phenylisoindoline-5-carbonitrile (4f)



Yellow solid. m.p. 219-221 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.27 (s, 2H), 7.32 (d, *J* = 5.0 Hz, 2H), 7.49-7.54 (m, 6H), 7.55-7.61 (m, 2H), 8.26 (s, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 99.1, 112.4, 114.2, 115.9, 127.7, 129.1, 129.2, 129.9, 130.1, 130.7, 134.9, 135.8, 136.1,148.0, 149.7, 157.0, 165.7; HRMS (ESI) m/z calcd for $C_{21}H_{13}ClN_4O$ $[M+H]^+$: 373.0856; found: 373.0854.

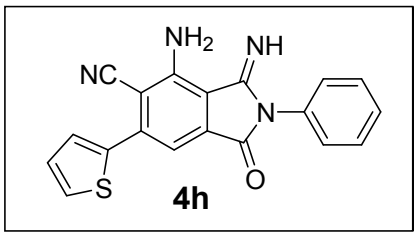
4-Amino-6-(4-bromophenyl)-3-imino-1-oxo-2-phenylisoindoline-5-carbonitrile (4g)



4g

Yellow solid. m.p. 246-248 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 6.50 (s, 2H), 7.27 (s, 2H), 7.32 (d, *J* = 5.0 Hz, 2H), 7.41-7.52 (m, 3H), 7.60 (t, *J* = 7.0 Hz,2H), 7.66 (d, *J* = 5.0 Hz, 2H), 8.26 (s, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 99.1, 112.3, 114.2, 115.9, 124.1, 127.8, 129.3, 130.1, 130.7, 132.1, 135.0, 136.6, 148.0, 149.7, 157.0, 165.7; HRMS (ESI) m/z calcd for $C_{21}H_{13}BrN_4O$ $[M+H]^+$: 417.0351; found: 417.0360.

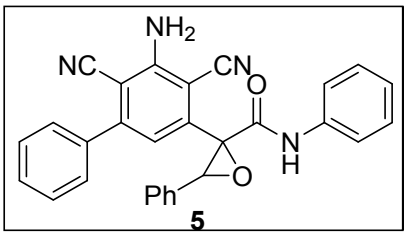
4-Amino-3-imino-1-oxo-2-phenyl-6-(thiophen-2-yl)isoindoline-5-carbonitrile (4h)



4h

Yellow solid. m.p. 246-248 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 6.52 (s, 2H), 7.20 (t, *J* = 4.5 Hz,1H), 7.34 (t, *J* = 12.3 Hz, 2H), 7.43 (s, 1H), 7.51 (t, *J* = 7.0 Hz, 2H), 7.60 (t, *J* = 6.5 Hz, 2H), 7.75 (d, *J* = 5.0 Hz, 1H), 8.22 (s, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 97.5, 112.1, 113.6, 116.4, 127.8, 128.3, 128.4,128.5, 129.2, 130.1, 130.8, 135.0, 139.3, 142.7, 148.3, 156.9, 165.6; HRMS (ESI) m/z calcd for $C_{19}H_{12}N_4OS$ $[M+H]^+$: 345.0810; found: 345.0803.

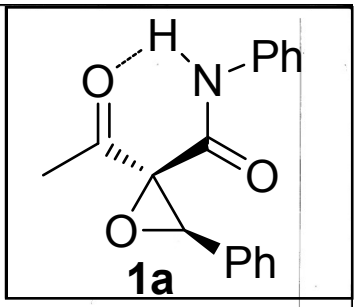
2-(5-Amino-4,6-dicyano-[1,1'-biphenyl]-3-yl)-*N*,3-diphenyloxirane-2-carboxamide



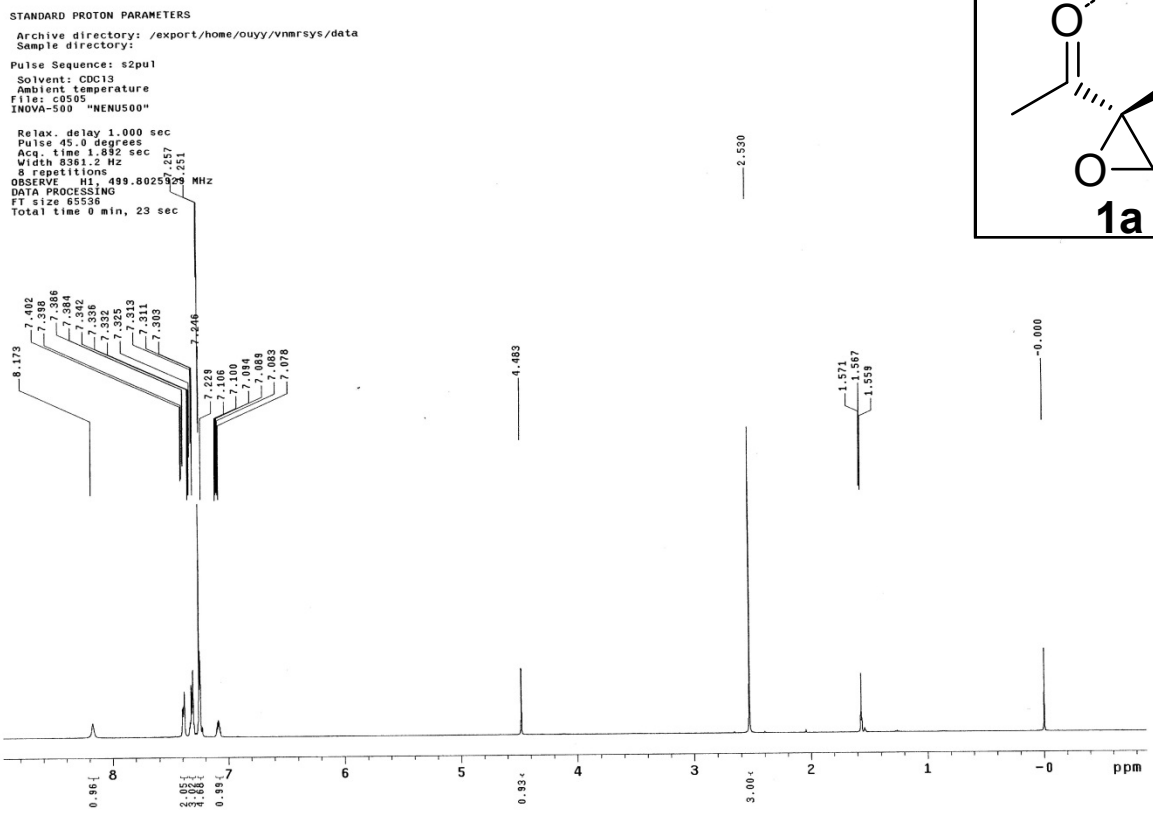
5

White solid. m.p. 143-145 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 4.81 (s, 1H), 6.32 (s, 1H), 7.05 (d, *J* = 10.0 Hz, 2H), 7.35-7.42 (m, 9H), 7.59 (t, *J* = 7.5 Hz,1H), 7.65 (t, *J* = 6.0 Hz, 2H), 7.90 (s, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 59.8, 69.8, 96.3, 108.3, 114.4, 116.9, 127.7, 128.3, 128.4, 128.5, 128.9, 129.1, 129.4, 130.1, 130.6, 131.5, 133.3, 136.1, 137.7, 147.8, 151.9, 155.7, 165.6; HRMS (ESI) m/z calcd for $C_{29}H_{20}N_4O_2$ $[M+H]^+$: 457.1665; found: 457.1664.

III. Copies of ^{1}H and ^{13}C NMR spectra for compounds 1-5


H
Ph
O
N
O
O
Ph

1a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Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: c0505
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.882 sec
Width 8361.2 Hz
8 repetitions
OBSERVE H1, 499.8025929 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
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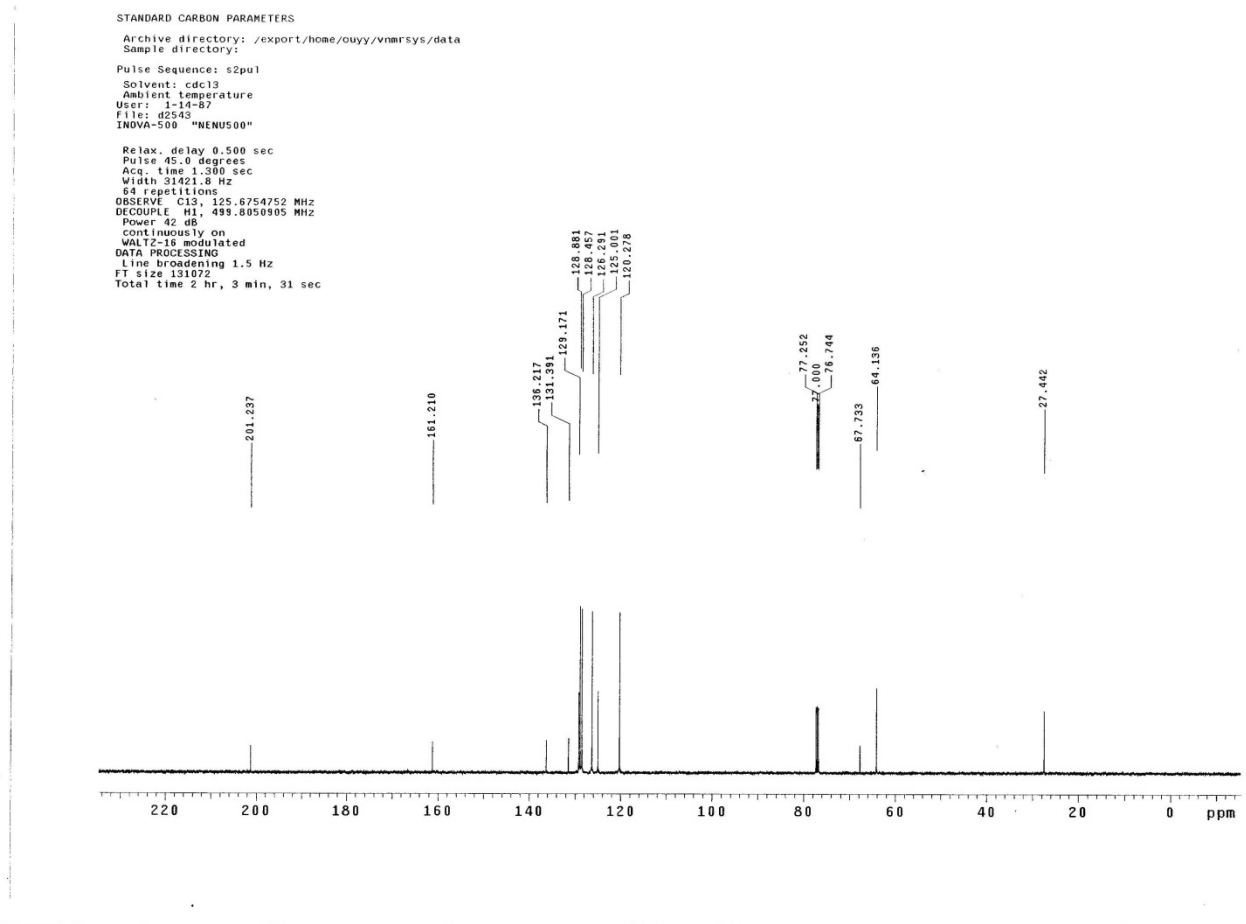
7.402
7.398
7.386
7.384
7.342
7.338
7.332
7.325
7.313
7.311
7.303
7.257
7.251
7.246
7.228
7.106
7.100
7.094
7.089
7.083
7.078
4.483
2.530
1.571
1.567
1.559
-0.000
ppm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Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: d2543
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
64 repetitions
OBSERVE C13, 125.6754752 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec
201.237
161.210
136.217
131.391
129.171
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128.291
126.201
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77.252
77.000
76.744
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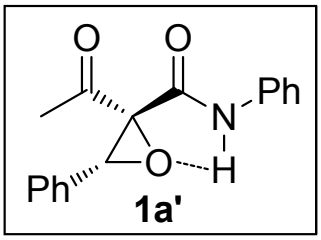
64.136
27.442
ppm



1a'

```
STANDARD PROTON PARAMETERS

 Archive directory: /export/home/ouyy/vnmrsys/data
 Sample directory:

Pulse Sequence: s2pul

 Solvent: CDCl3
 Ambient temperature
File: c0407
INOVA-500  "NENU500"

 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 1.882 sec
 Width 8291.0 Hz
 8 repetitions
OBSERVE    H1, 499.8025907 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
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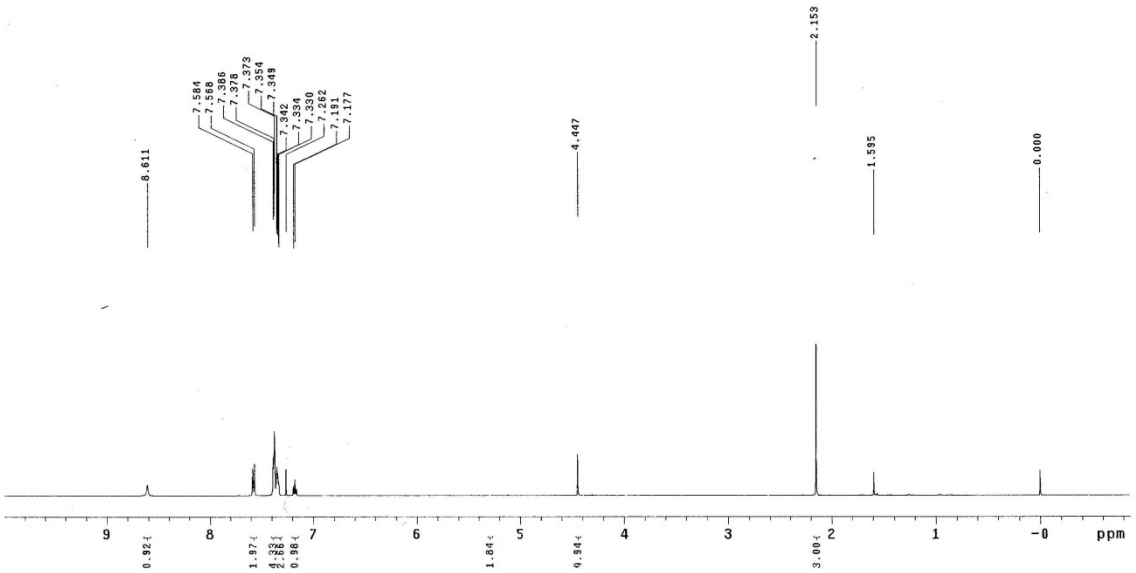


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STANDARD CARBON PARAMETERS

 Archive directory: /export/home/ouyy/vnmrsys/data
 Sample directory:

Pulse Sequence: s2pul

 Solvent: cdcl3
 Ambient temperature
User:  1-14-87
File: d2542
INOVA-500  "NENU500"

 Relax. delay 0.500 sec
 Pulse 45.0 degrees
 Acq. time 1.300 sec
 Width 31421.8 Hz
 64 repetitions
OBSERVE  C13, 125.6754699 MHz
DECOUPLE  H1, 499.8050905 MHz
 Power 42 dB
 continuously on
 WALTZ-16 modulated
DATA PROCESSING
 Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec
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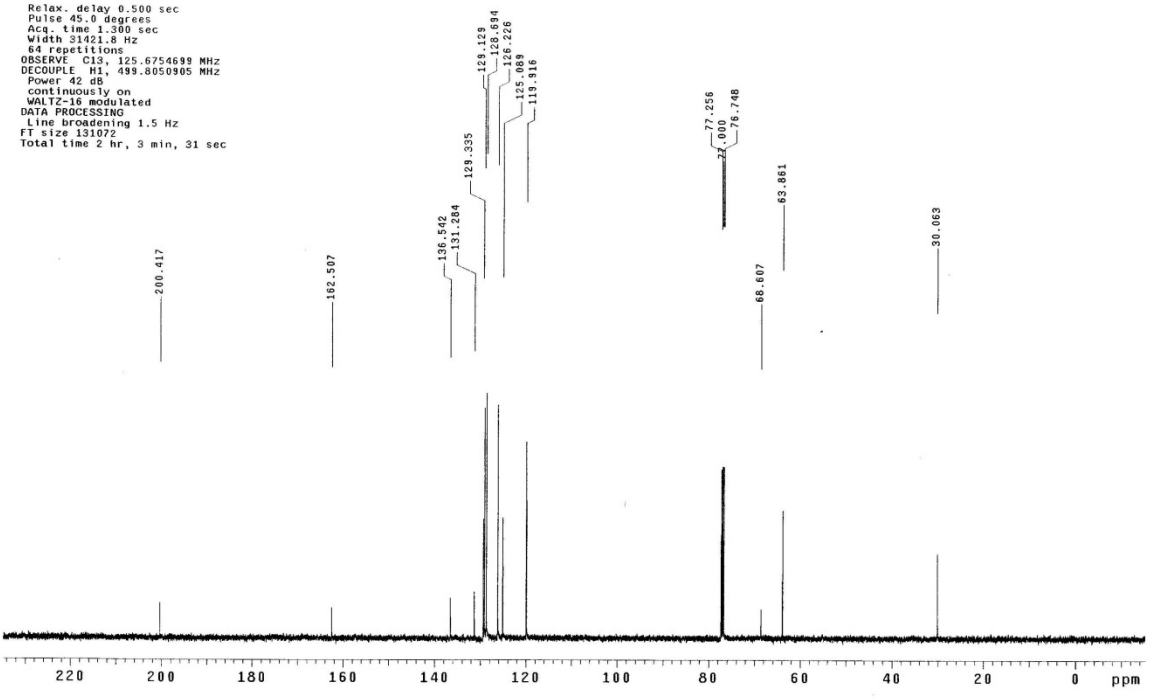

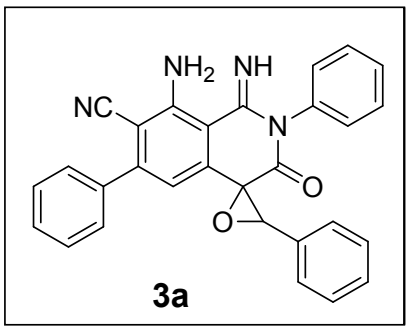

3a

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STANDARD PROTON PARAMETERS

 Archive directory: /export/home/ouyy/vnmrsys/data
 Sample directory:

Pulse Sequence: s2pul

 Solvent: CDCl3
 Ambient temperature
File: d0912
INOVA-500  "NENU500"

 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 1.882 sec
 Width 8500.7 Hz
 8 repetitions
OBSERVE   H1, 499.8025894 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
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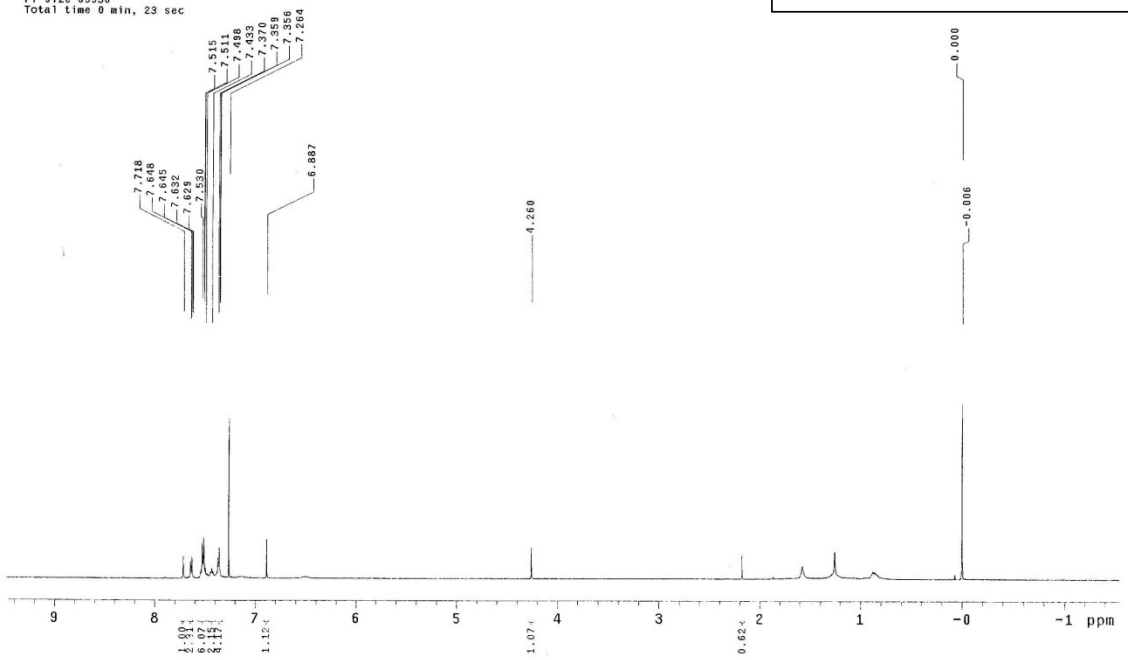


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STANDARD CARBON PARAMETERS

 Archive directory: /export/home/ouyy/vnmrsys/data
 Sample directory:

Pulse Sequence: s2pul

 Solvent: cdcl3
 Ambient temperature
User:  1-14-87
File: d2387
INOVA-500  "NENU500"

 Relax. delay 0.500 sec
 Pulse 45.0 degrees
 Acq. time 1.300 sec
 Width 31421.8 Hz
 128 repetitions
OBSERVE  C13, 125.6754714 MHz
DECOUPLE  H1, 499.8050905 MHz
 Power 42 dB
 continuously on
 WALTZ-16 modulated
DATA PROCESSING
 Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec
```
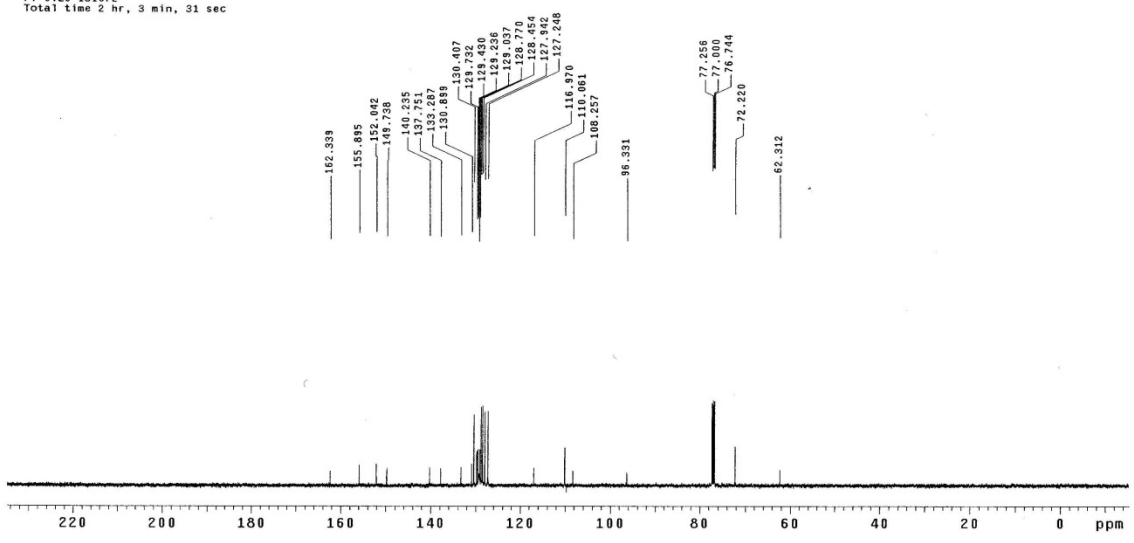
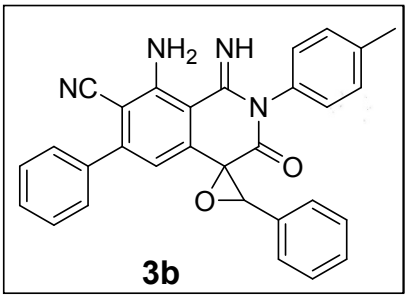
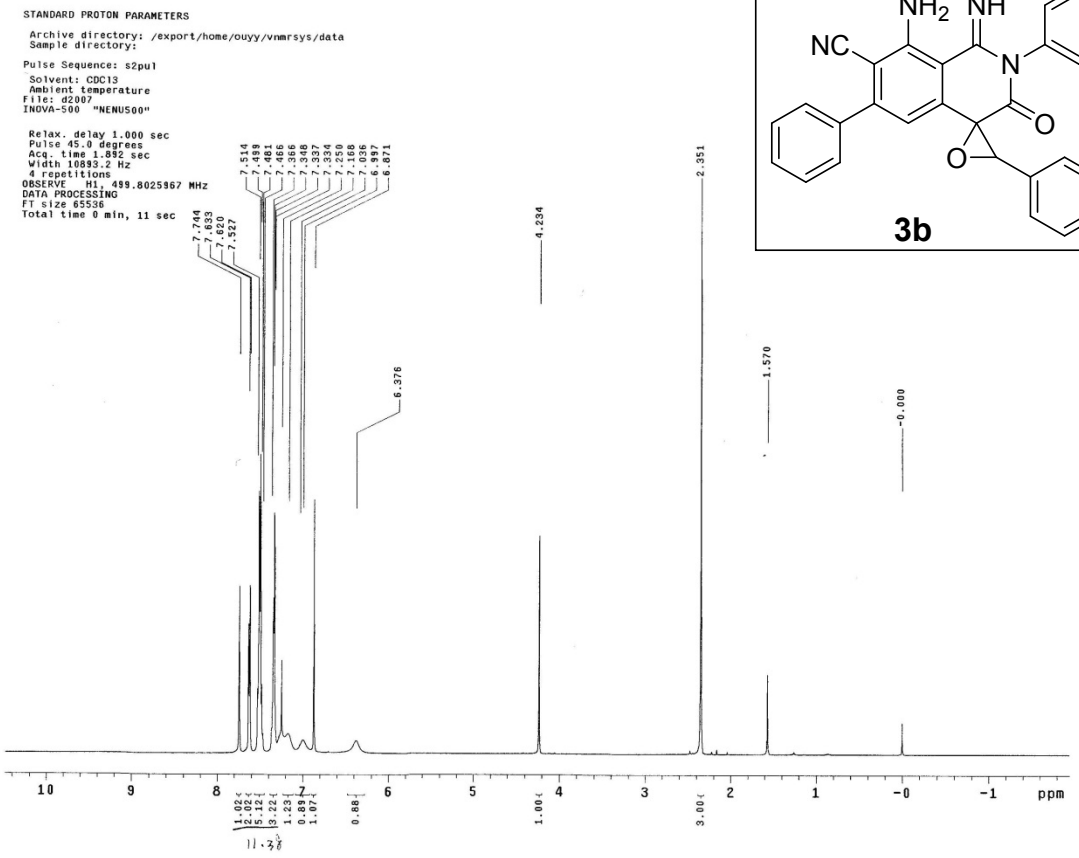




NH2
NH
NC
N
O
O

3b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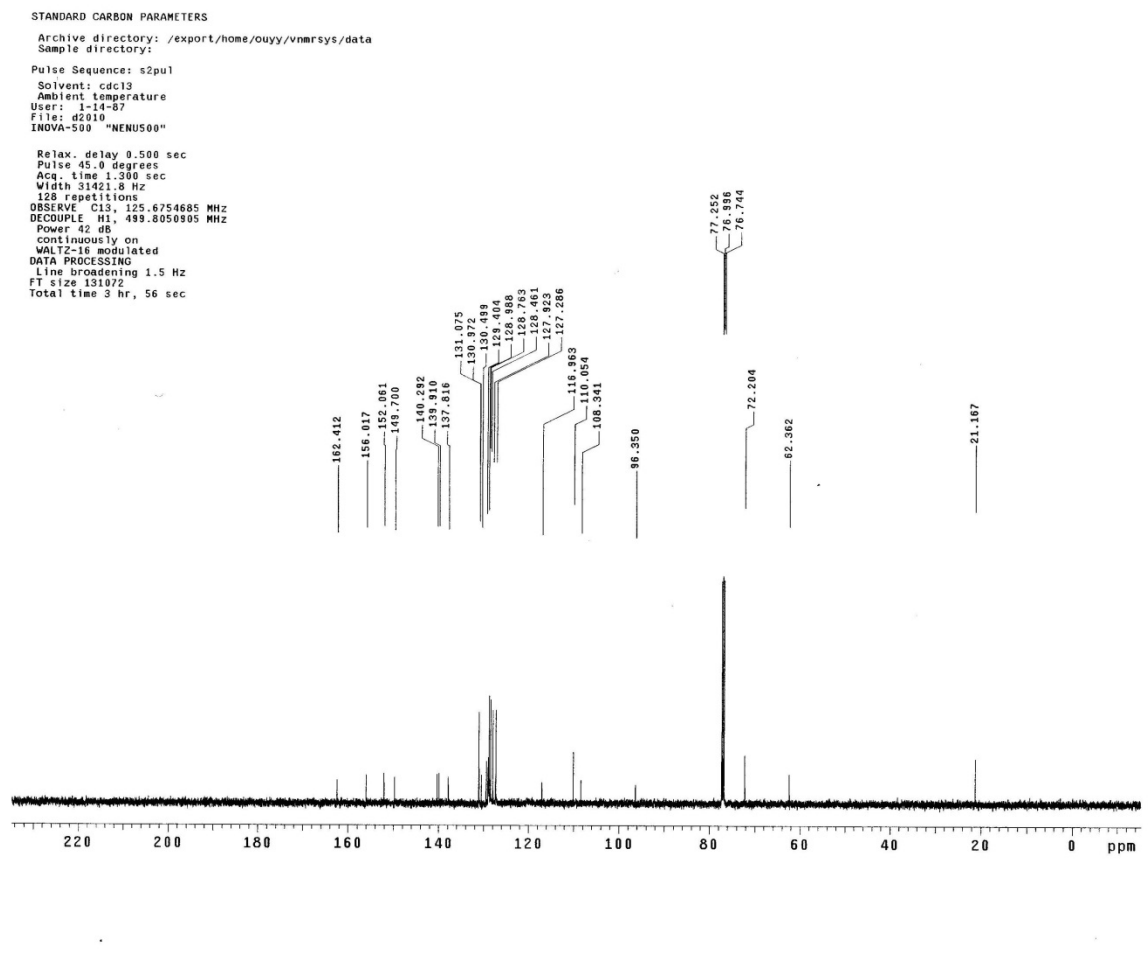
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: d2007
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 10893.2 Hz
4 repetitions
OBSERVE H1, 499.8025967 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 11 sec
7.744
7.683
7.620
7.527
7.514
7.499
7.481
7.466
7.366
7.349
7.333
7.334
7.250
7.168
7.036
6.997
6.871
6.376
4.234
2.351
1.570
-0.000
ppm


STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: d2010
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
128 repetitions
OBSERVE C13, 125.6754685 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
77.252
76.996
76.744
162.412
156.017
152.061
149.700
140.282
139.910
137.816
131.075
130.972
130.499
129.404
128.988
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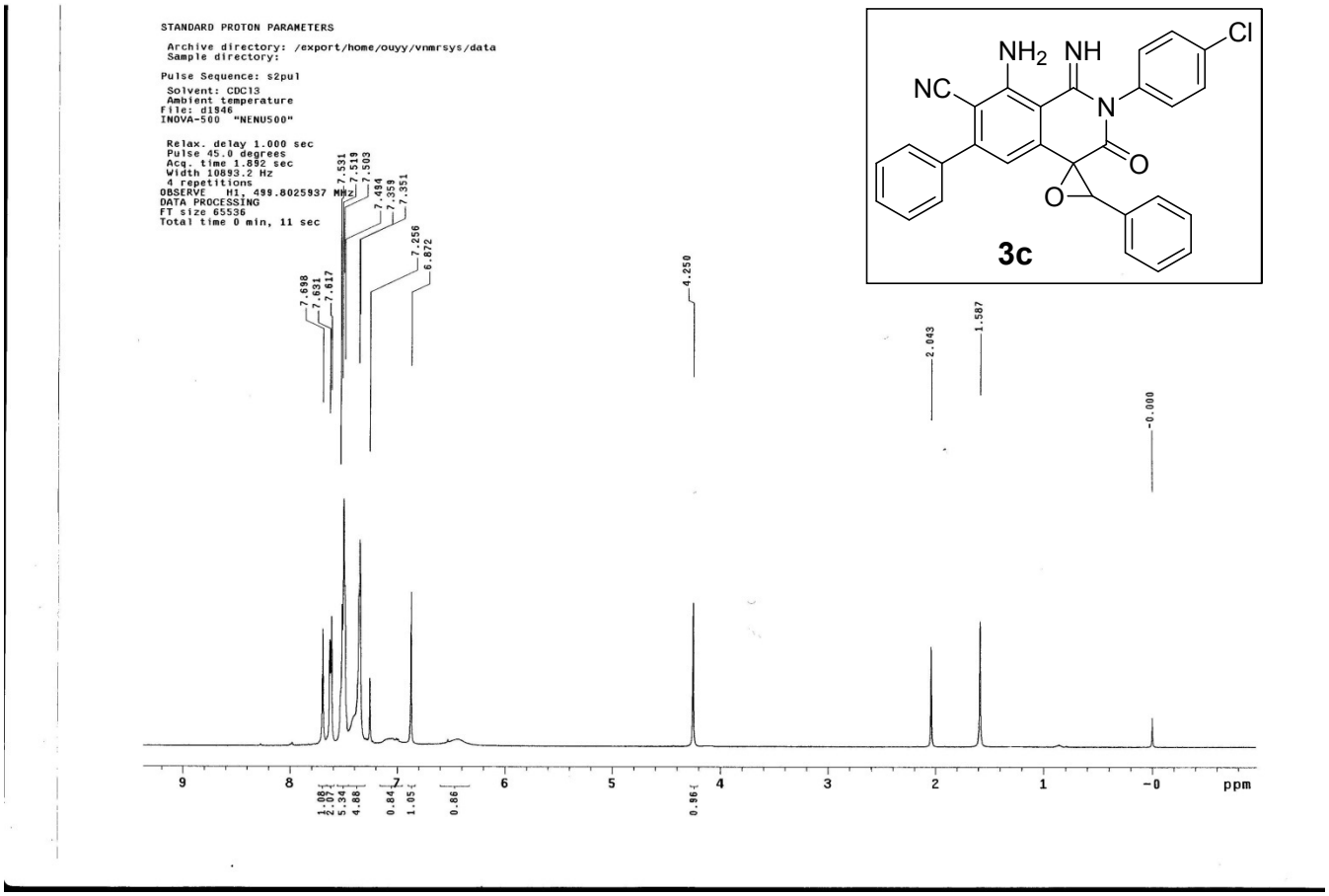
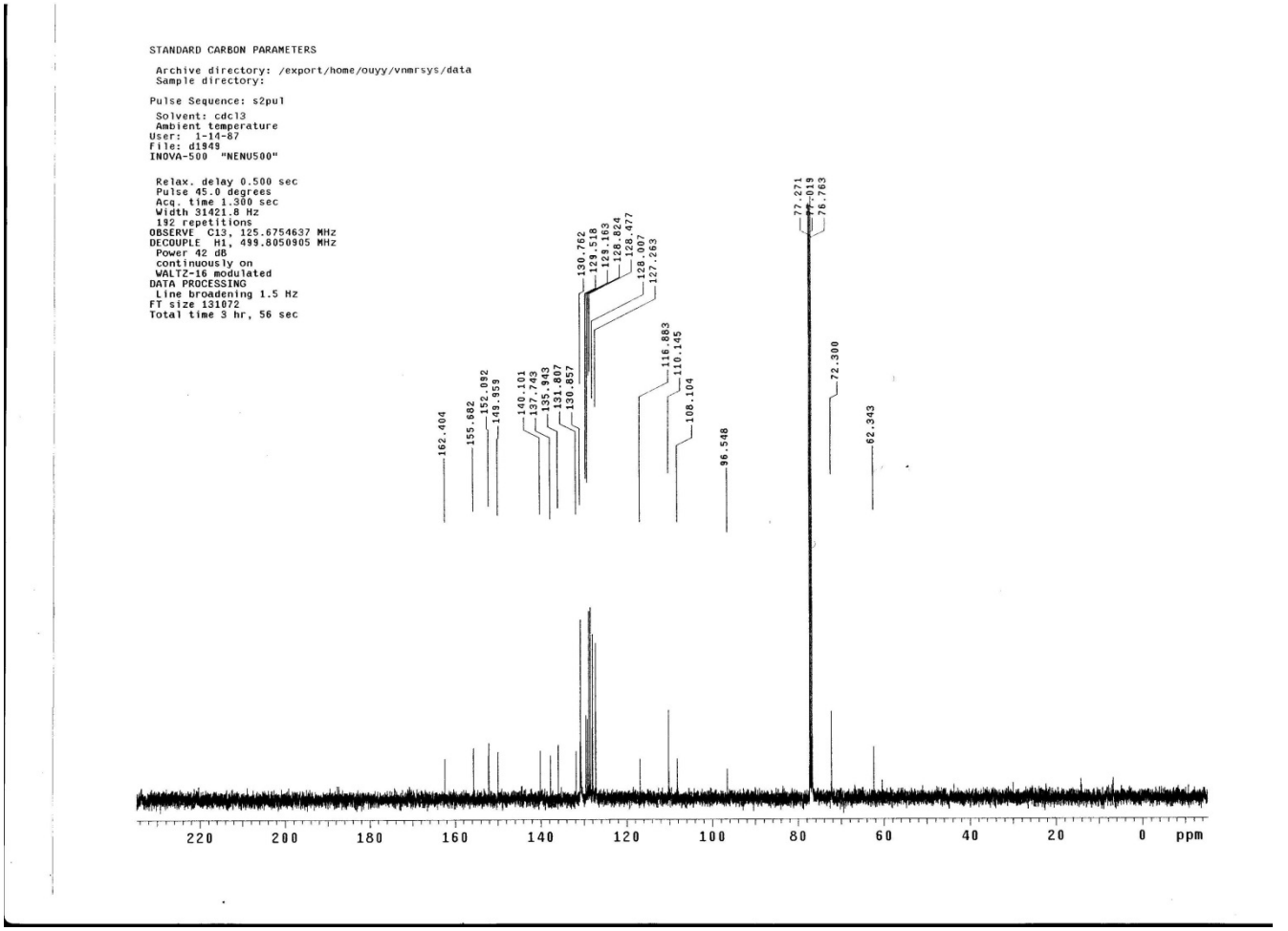
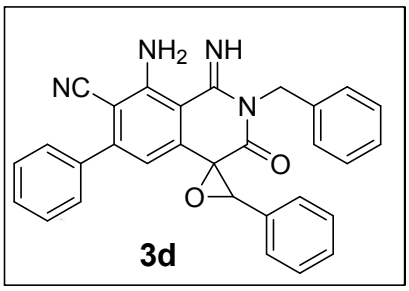
72.204
62.362
21.167
ppm

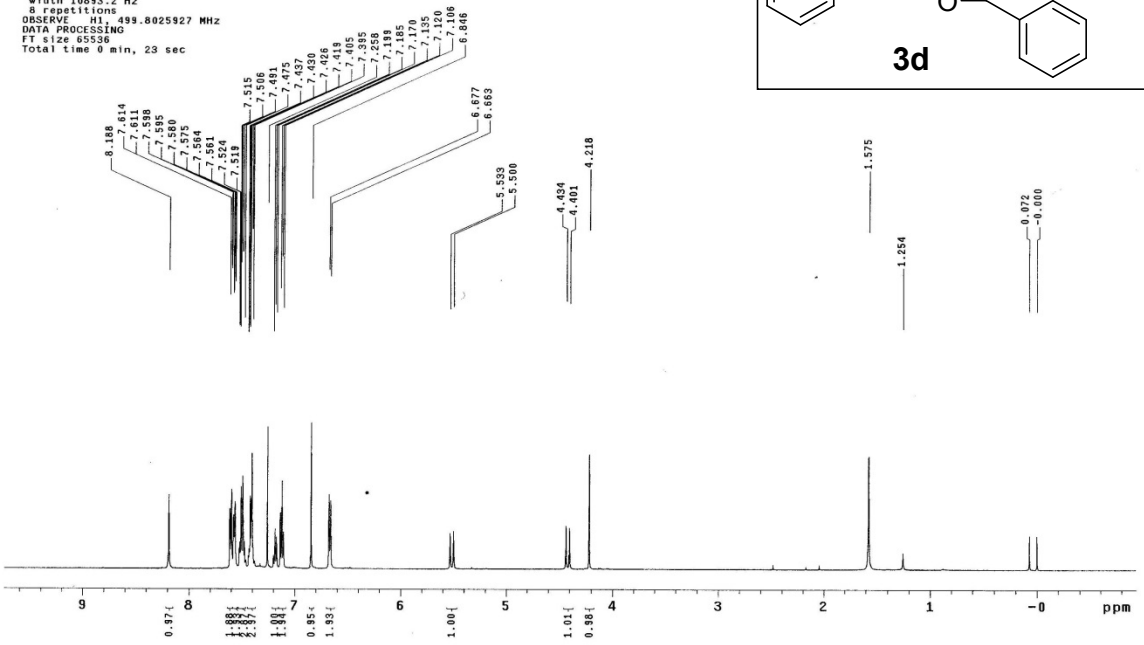

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: d1846
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 10893.2 Hz
4 repetitions
OBSERVE H1, 499.8025937 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 11 sec
7.698
7.631
7.617
7.531
7.519
7.503
7.494
7.358
7.351
7.256
6.872
4.250
2.043
1.587
0.000
ppm
NH2
NH
NC
Cl
N
O
O
3c


STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: d1949
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
192 repetitions
OBSERVE C13, 125.6754637 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
162.404
155.682
152.082
149.959
140.101
137.743
135.943
131.807
130.857
130.762
129.518
128.824
128.477
128.007
127.263
116.883
110.145
108.104
96.548
77.271
77.019
76.763
72.390
62.343
ppm

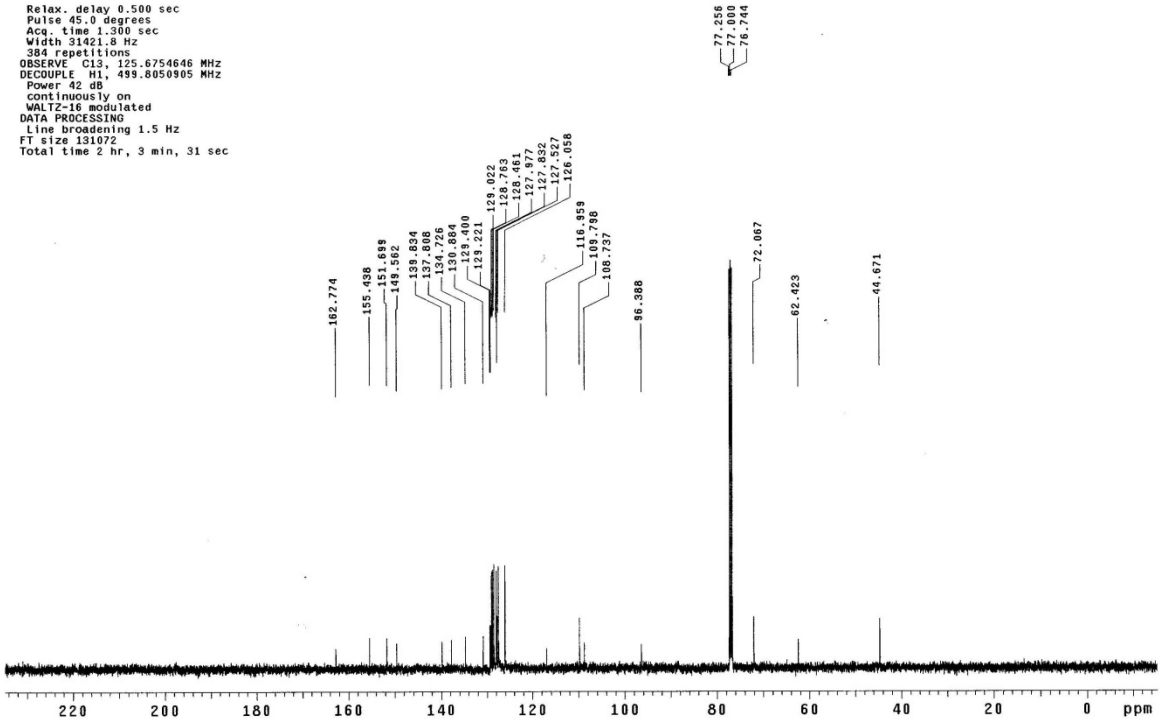


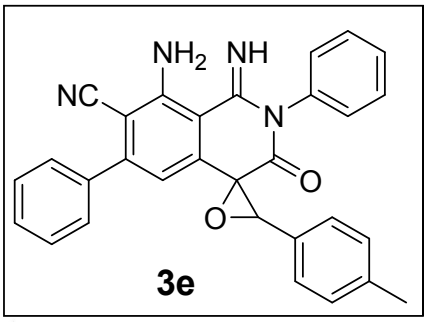
3d

```
STANDARD PROTON PARAMETERS

 Archive directory: /export/home/ouyy/vnmrsys/data
 Sample directory:

Pulse Sequence: s2pul

 Solvent: CDCl3
 Ambient temperature
File: d1851
INOVA-500  "NENU500"

 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 1.892 sec
 Width 10893.2 Hz
 8 repetitions
OBSERVE   H1, 499.8025927 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
```



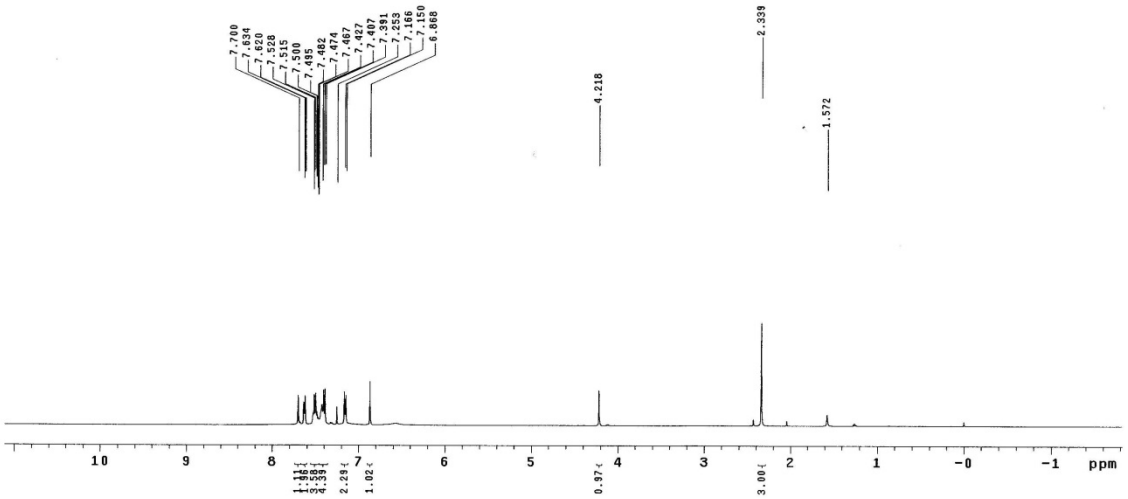

```
STANDARD CARBON PARAMETERS

 Archive directory: /export/home/ouyy/vnmrsys/data
 Sample directory:

Pulse Sequence: s2pul

 Solvent: cdcl3
 Ambient temperature
User:  1-14-87
File: d1969
INOVA-500  "NENU500"

 Relax. delay 0.500 sec
 Pulse 45.0 degrees
 Acq. time 1.300 sec
 Width 31421.8 Hz
 384 repetitions
OBSERVE   C13, 125.6754646 MHz
DECOUPLE  H1, 499.8050905 MHz
 Power 42 dB
 continuously on
 WALTZ-16 modulated
DATA PROCESSING
 Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec
```



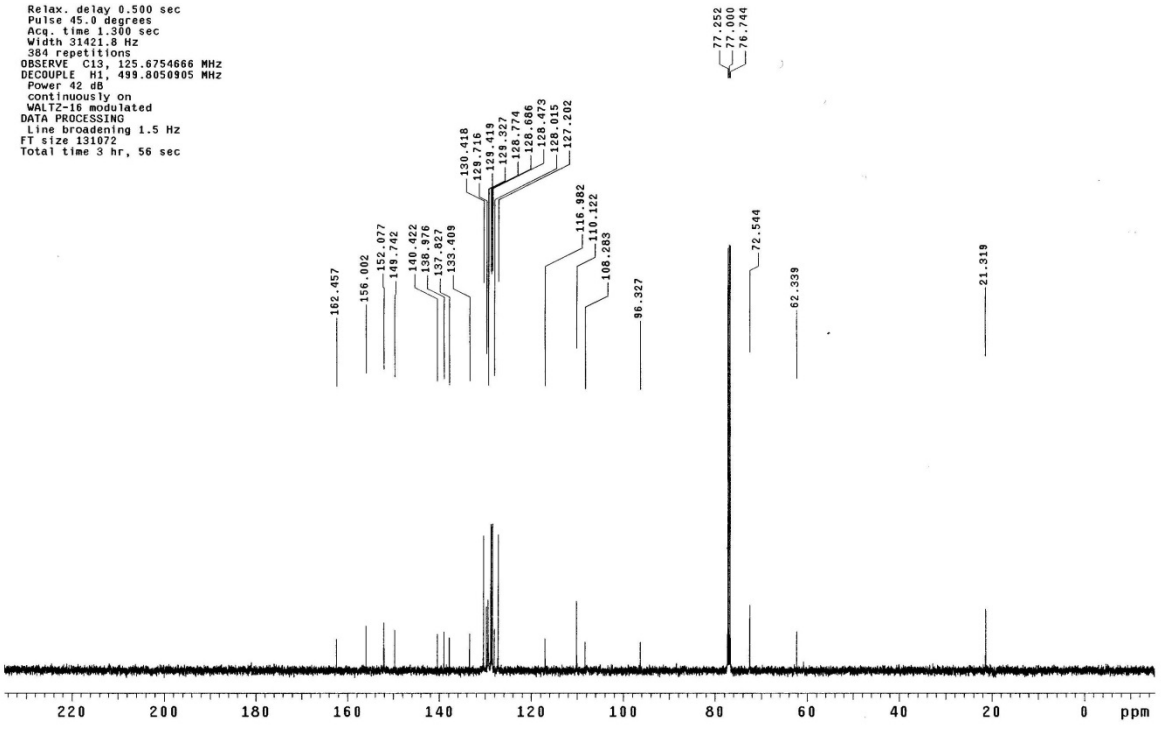


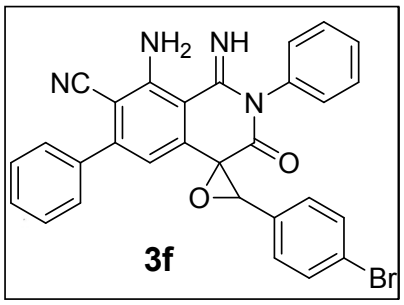
3e

```
STANDARD PROTON PARAMETERS

 Archive directory: /export/home/ouyy/vnmrsys/data
 Sample directory:

Pulse Sequence: s2pul
 Solvent: CDCl3
 Ambient temperature
File: d1921
INOVA-500  "NENU500"

 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 1.892 sec
 Width 10893.2 Hz
 8 repetitions
OBSERVE    H1, 499.8025950 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
```

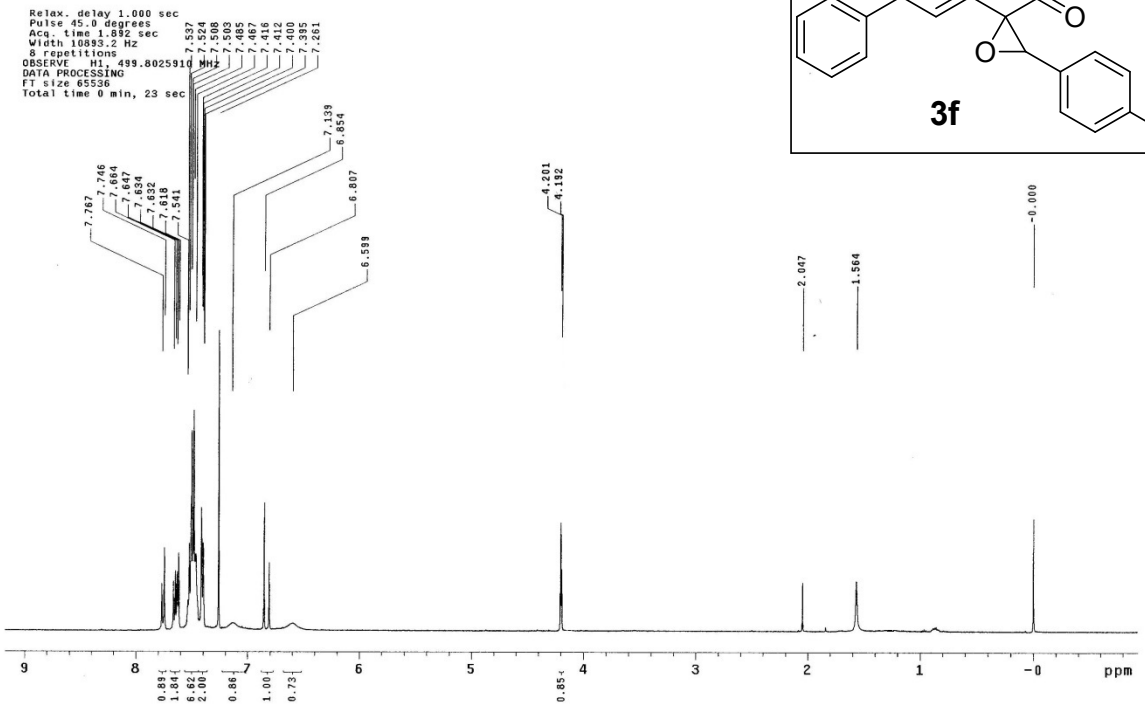


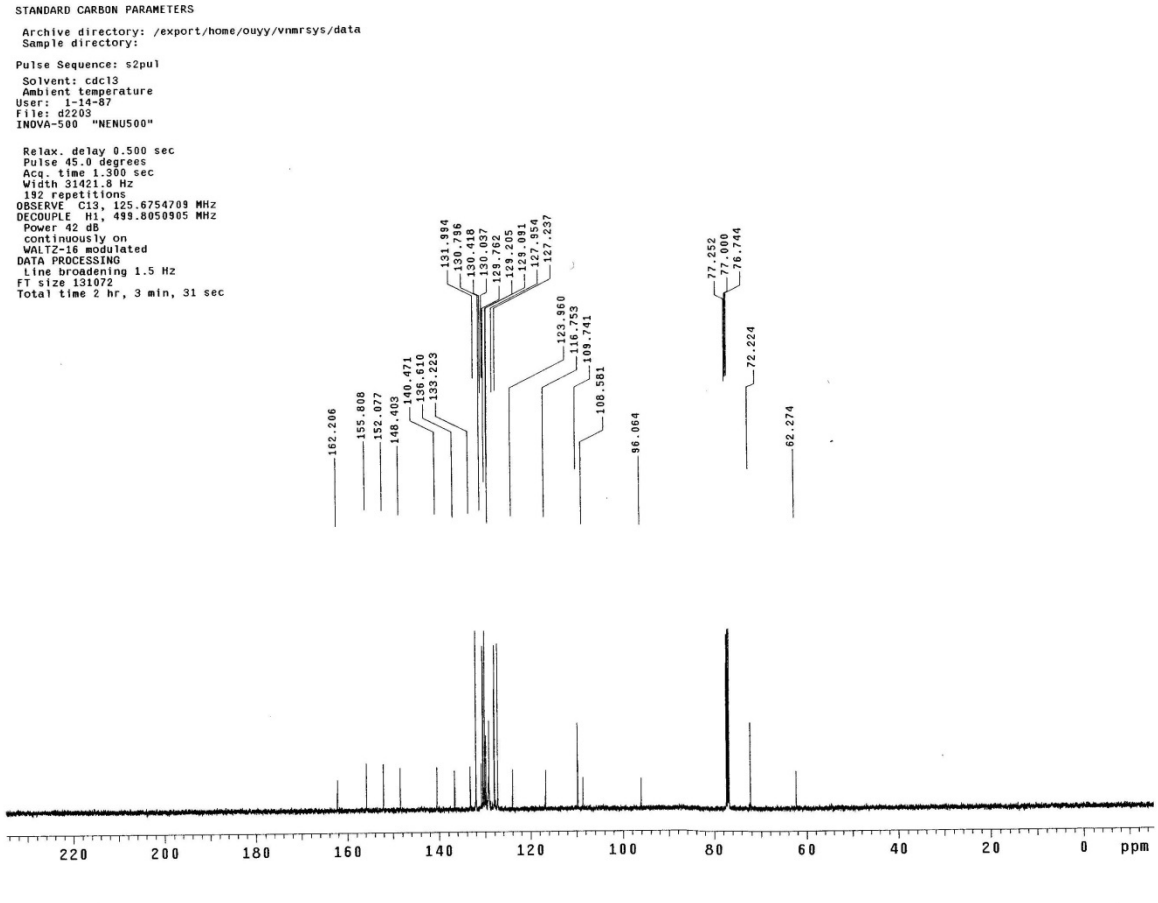

```
STANDARD CARBON PARAMETERS

 Archive directory: /export/home/ouyy/vnmrsys/data
 Sample directory:

Pulse Sequence: s2pul
 Solvent: cdcl3
 Ambient temperature
User:  l-14-87
File: d1922
INOVA-500  "NENU500"

 Relax. delay 0.500 sec
 Pulse 45.0 degrees
 Acq. time 1.300 sec
 Width 31421.8 Hz
 384 repetitions
OBSERVE  C13, 125.6754666 MHz
DECOUPLE  H1, 499.8050905 MHz
 Power 42 dB
 continuously on
 WALTZ-16 modulated
DATA PROCESSING
 Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
```

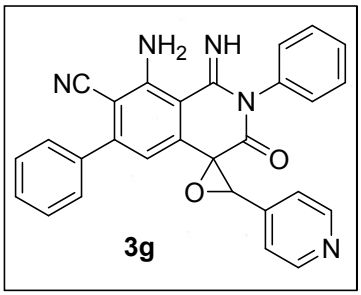



NH2
NH
NC
N
O
O
Br

3f

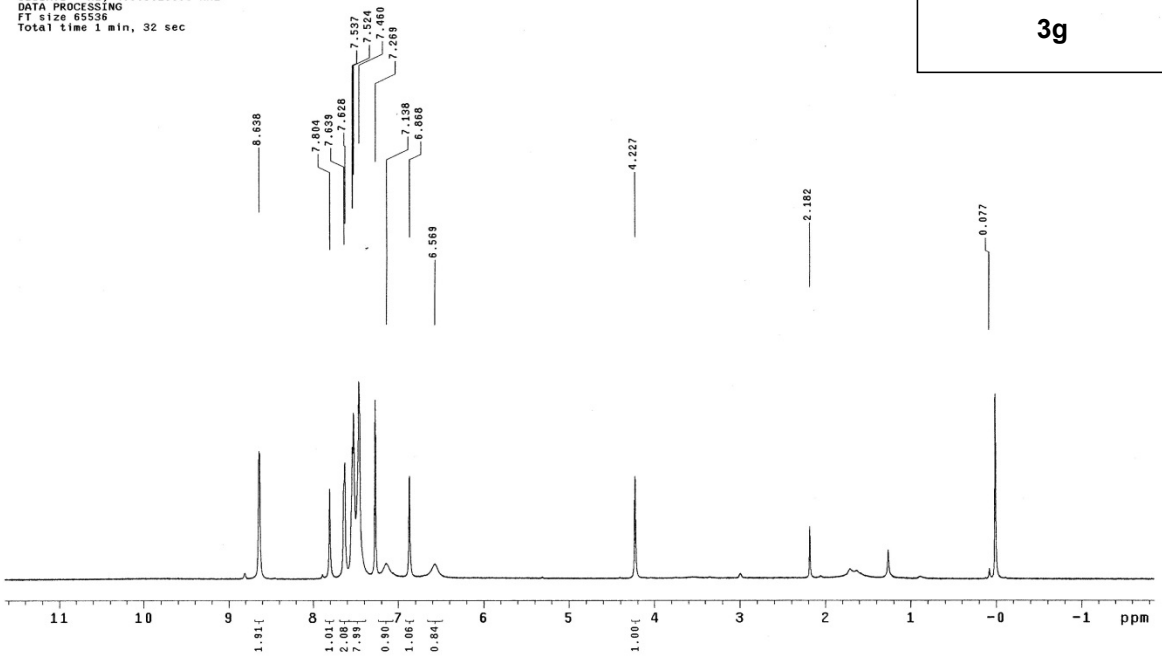

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: d2032
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 10893.2 Hz
8 repetitions
OBSERVE H1, 499.8025910 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
7.767
7.746
7.664
7.647
7.634
7.632
7.618
7.541
7.537
7.524
7.508
7.503
7.485
7.467
7.416
7.412
7.400
7.395
7.261
7.139
6.854
6.807
6.589
4.201
4.192
2.047
1.564
-0.000
ppm


STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: d2203
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
192 repetitions
OBSERVE C13, 125.6754709 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec
162.206
155.808
152.077
148.403
140.471
136.610
133.223
131.994
130.796
130.418
130.037
128.762
129.205
129.081
127.554
127.297
123.960
116.753
109.741
108.581
96.064
77.252
77.000
76.744
72.224
62.274
ppm

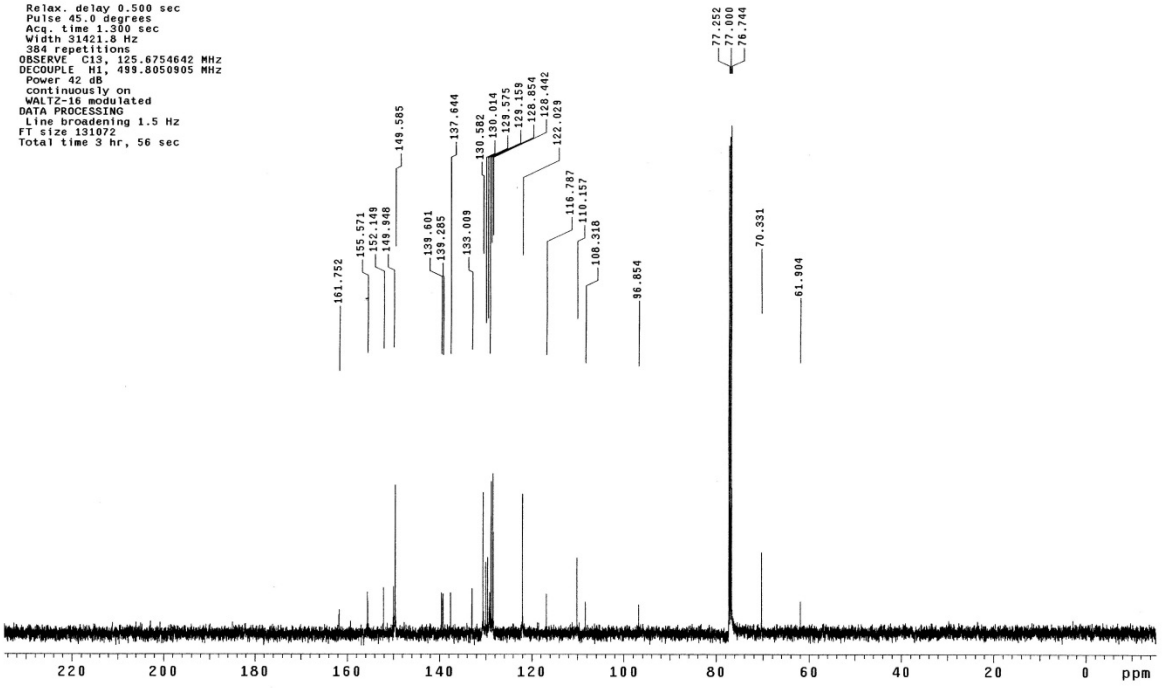


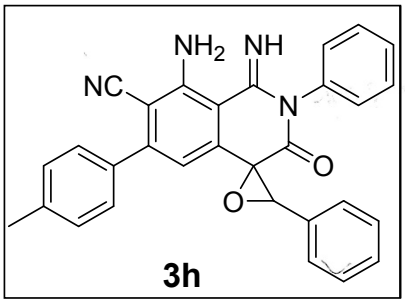
3g

```
STANDARD PROTON PARAMETERS

 Archive directory: /export/home/ouyy/vnmrsys/data
 Sample directory:

Pulse Sequence: s2pul

 Solvent: CDCl3
 Ambient temperature
File: d3096
INOVA-500  "NENU500"

 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 1.892 sec
 Width 9949.0 Hz
 32 repetitions
OBSERVE   H1, 499.8025866 MHz
DATA PROCESSING
FT size 65536
Total time 1 min, 32 sec
```



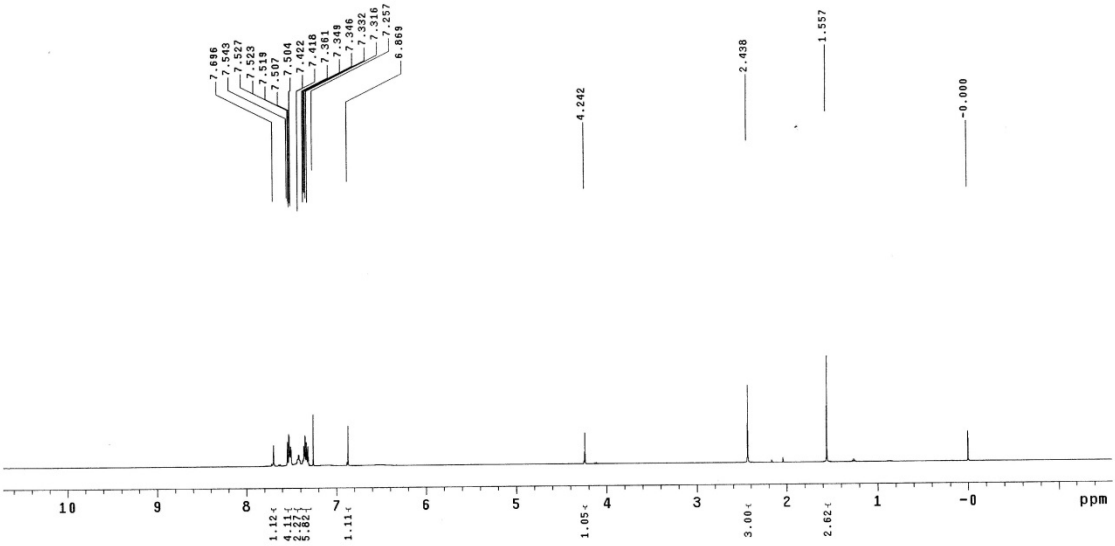

```
STANDARD CARBON PARAMETERS

 Archive directory: /export/home/ouyy/vnmrsys/data
 Sample directory:

Pulse Sequence: s2pul

 Solvent: cdcl3
 Ambient temperature
User:  l-14-87
File: d3098
INOVA-500  "NENU500"

 Relax. delay 0.500 sec
 Pulse 45.0 degrees
 Acq. time 1.300 sec
 Width 31421.8 Hz
 384 repetitions
OBSERVE   C13, 125.6754642 MHz
DECOUPLE  H1, 499.8050905 MHz
 Power 42 dB
 continuously on
 WALTZ-16 modulated
DATA PROCESSING
 Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
```



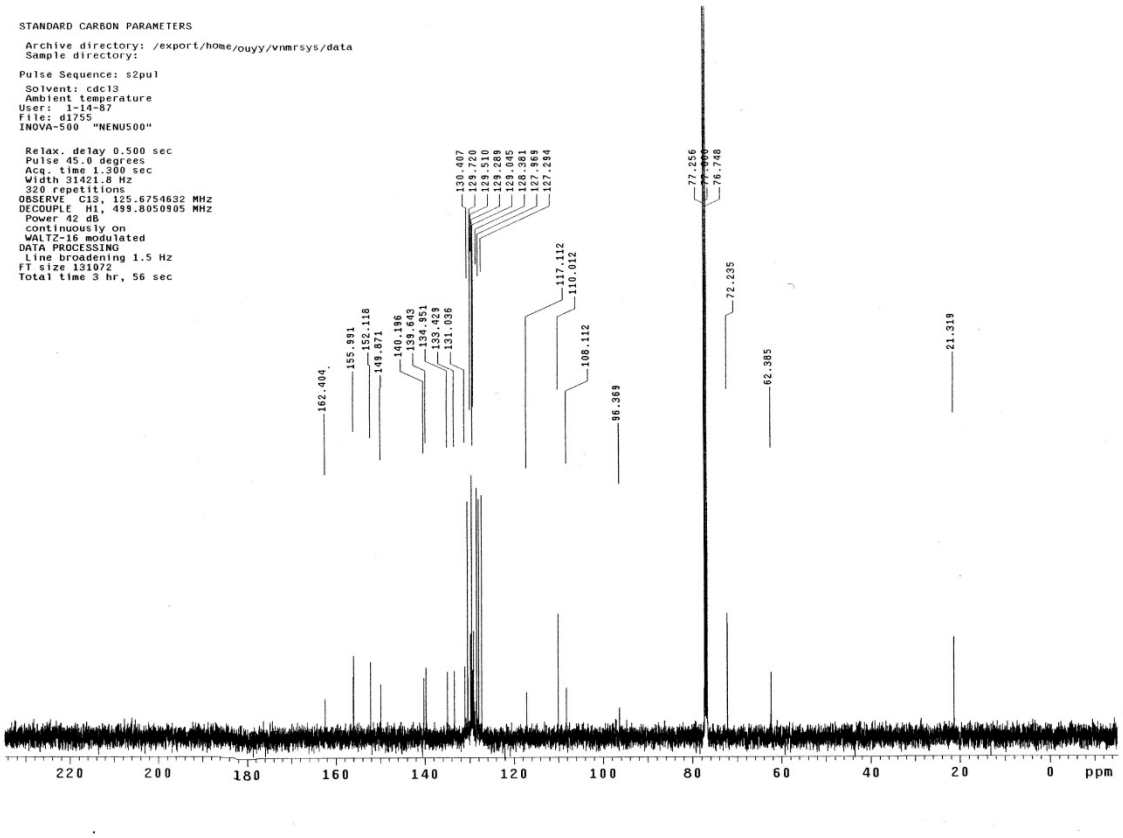


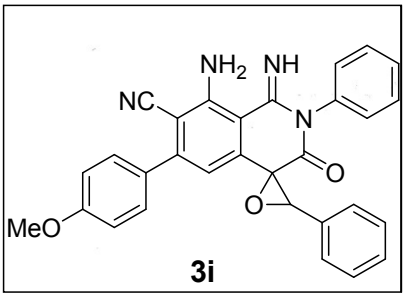
3h

```
STANDARD PROTON PARAMETERS

 Archive directory: /export/home/ouyy/vnmrsys/data
 Sample directory:

Pulse Sequence: s2pul

 Solvent: CDCl3
 Ambient temperature
File: d1750
INOVA-500  "NENU500"

 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 1.892 sec
 Width 10893.2 Hz
 8 repetitions
OBSERVE   H1, 499.8025934 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
```



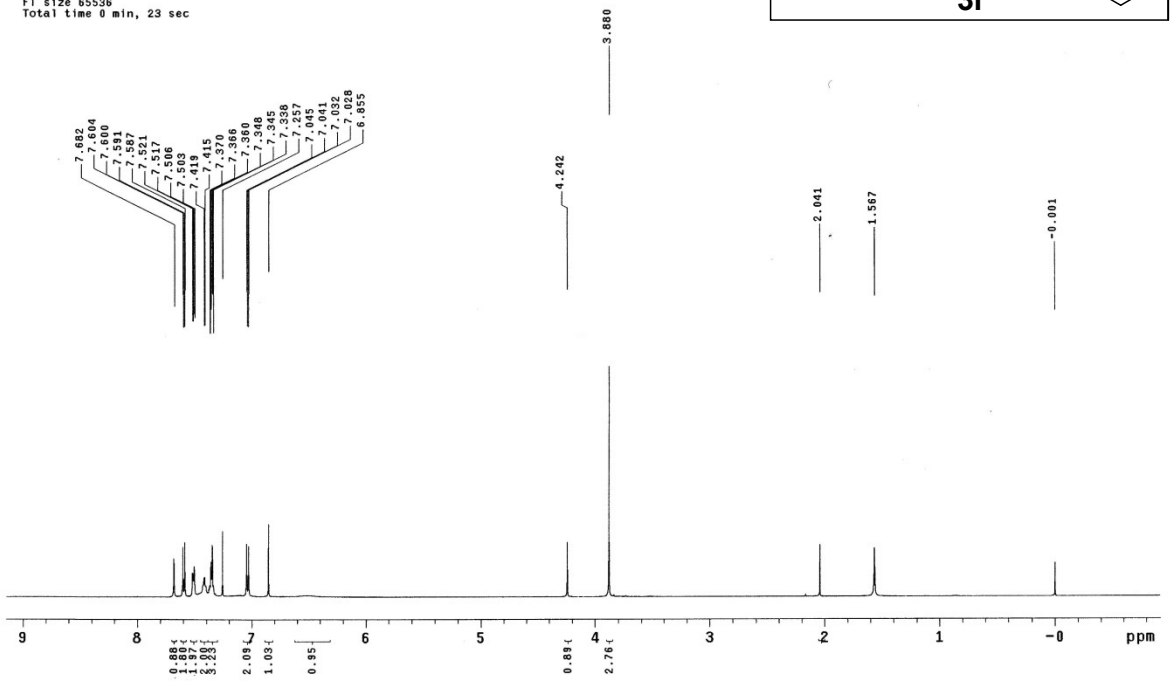

```
STANDARD CARBON PARAMETERS

 Archive directory: /export/home/ouyy/vnmrsys/data
 Sample directory:

Pulse Sequence: s2pul

 Solvent: cdcl3
 Ambient temperature
User:  1-14-87
File: d1755
INOVA-500  "NENU500"

 Relax. delay 0.500 sec
 Pulse 45.0 degrees
 Acq. time 1.300 sec
 Width 31421.8 Hz
 320 repetitions
OBSERVE  C13, 125.6754632 MHz
DECOUPLE  H1, 499.8050905 MHz
 Power 42 dB
 continuously on
 WALTZ-16 modulated
DATA PROCESSING
 Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
```



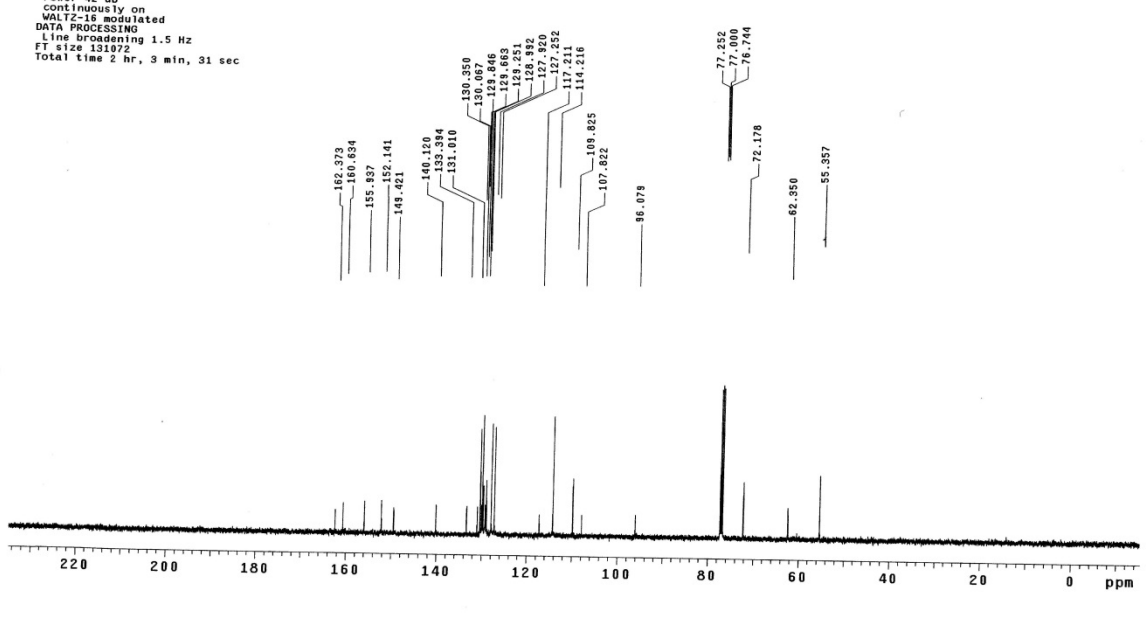


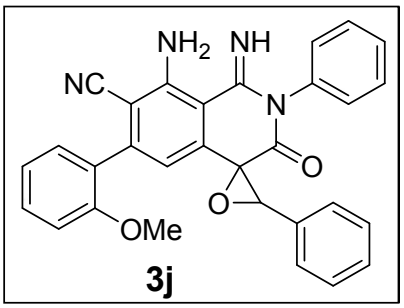
3i

```
STANDARD PROTON PARAMETERS

 Archive directory: /export/home/ouyy/vnmrsys/data
 Sample directory:

Pulse Sequence: s2pul

 Solvent: CDCl3
 Ambient temperature
File: d1767
INOVA-500  "NENU500"

 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 1.892 sec
 Width 10893.2 Hz
 8 repetitions
OBSERVE    H1, 499.8025937 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
```



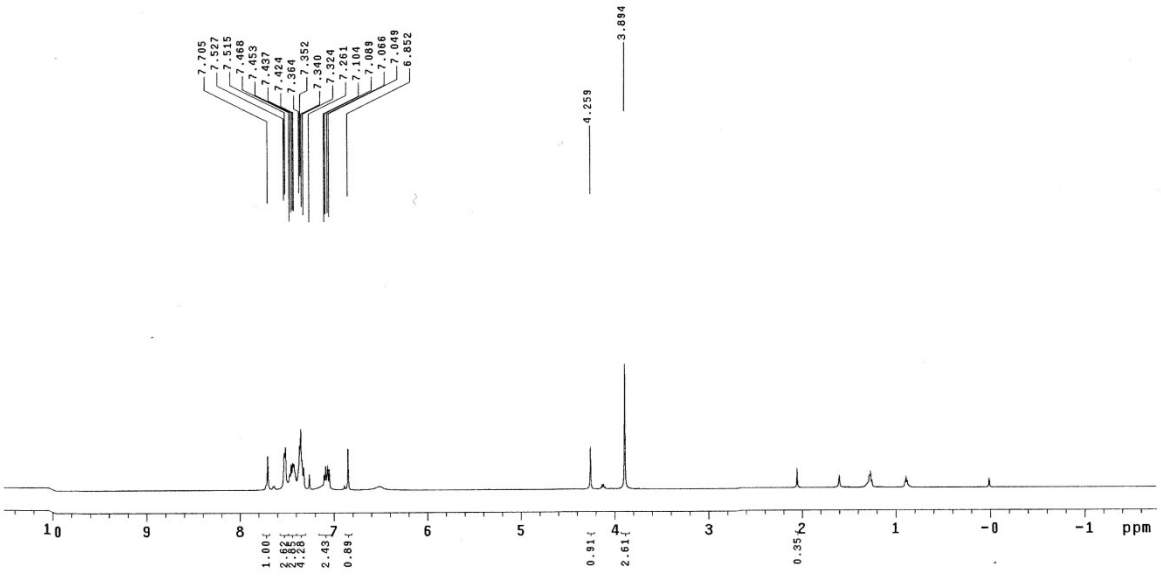

```
STANDARD CARBON PARAMETERS

 Archive directory: /export/home/ouyy/vnmrsys/data
 Sample directory:

Pulse Sequence: s2pul

 Solvent: cdcl3
 Ambient temperature
User:  1-14-87
File: d1768
INOVA-500  "NENU500"

 Relax. delay 0.500 sec
 Pulse 45.0 degrees
 Acq. time 1.300 sec
 Width 31421.8 Hz
 192 repetitions
OBSERVE  C13, 125.6754694 MHz
DECOUPLE  H1, 499.8050905 MHz
 Power 42 dB
 continuously on
 WALTZ-16 modulated
DATA PROCESSING
 Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec
```



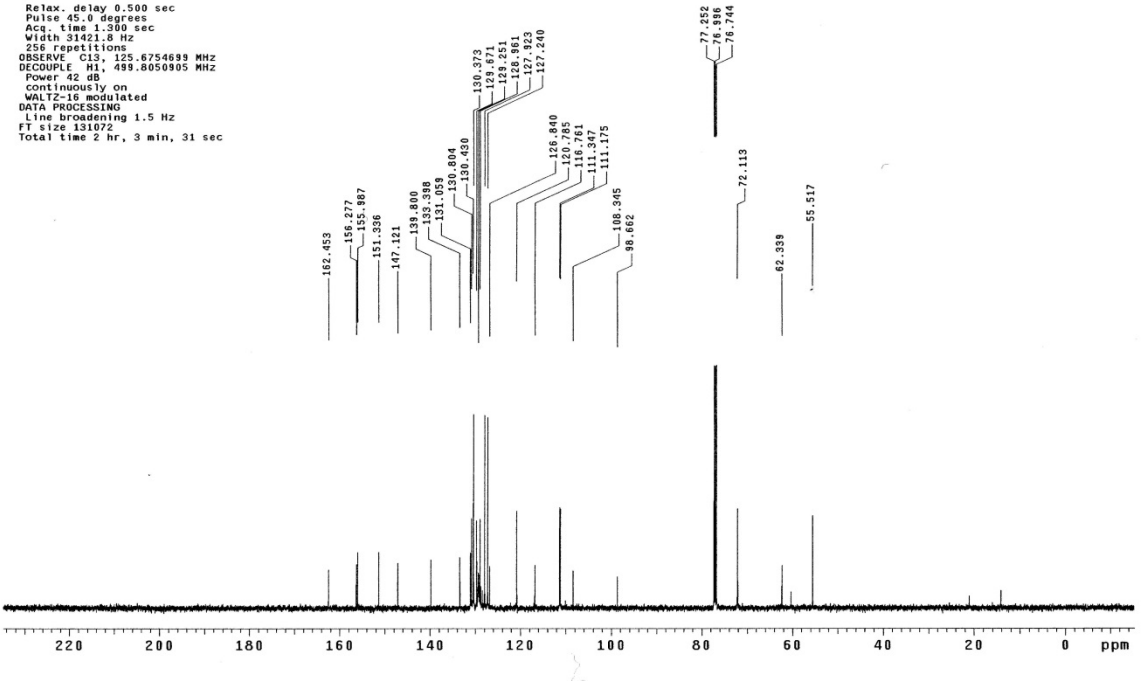


3j

```
STANDARD PROTON PARAMETERS

 Archive directory: /export/home/ouyy/vnmrsys/data
 Sample directory:

Pulse Sequence: s2pul
 Solvent: CDCl3
 Ambient temperature
File: d2185
INOVA-500  "NENU500"

 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 1.892 sec
 Width 10893.2 Hz
 4 repetitions
OBSERVE   H1, 499.8025904 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 11 sec
```




```
STANDARD CARBON PARAMETERS

 Archive directory: /export/home/ouyy/vnmrsys/data
 Sample directory:

Pulse Sequence: s2pul
 Solvent: cdcl3
 Ambient temperature
User:  1-14-87
File: d2225
INOVA-500  "NENU500"

 Relax. delay 0.500 sec
 Pulse 45.0 degrees
 Acq. time 1.300 sec
 Width 31421.8 Hz
 256 repetitions
OBSERVE  C13, 125.6754699 MHz
DECOUPLE  H1, 499.8050905 MHz
 Power 42 dB
 continuously on
 WALTZ-16 modulated
DATA PROCESSING
 Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec
```



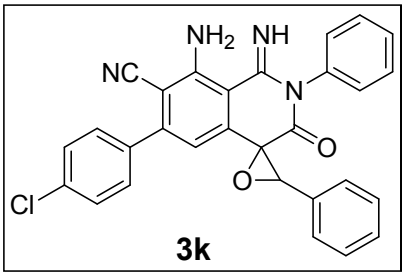
STANDARD PROTON PARAMETERS

Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:

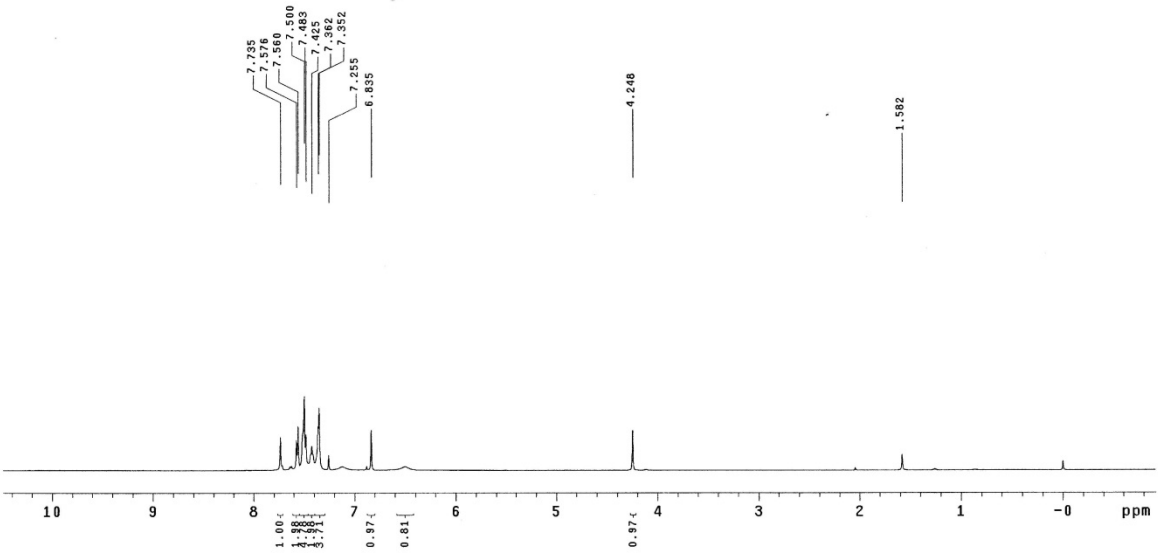
Pulse Sequence: s2pul

Solvent: CDCl3
Ambient temperature
File: d2187
INOVA-500 "NENU500"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 10893.2 Hz
4 repetitions
OBSERVE H1, 499.8025934 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 11 sec



3k



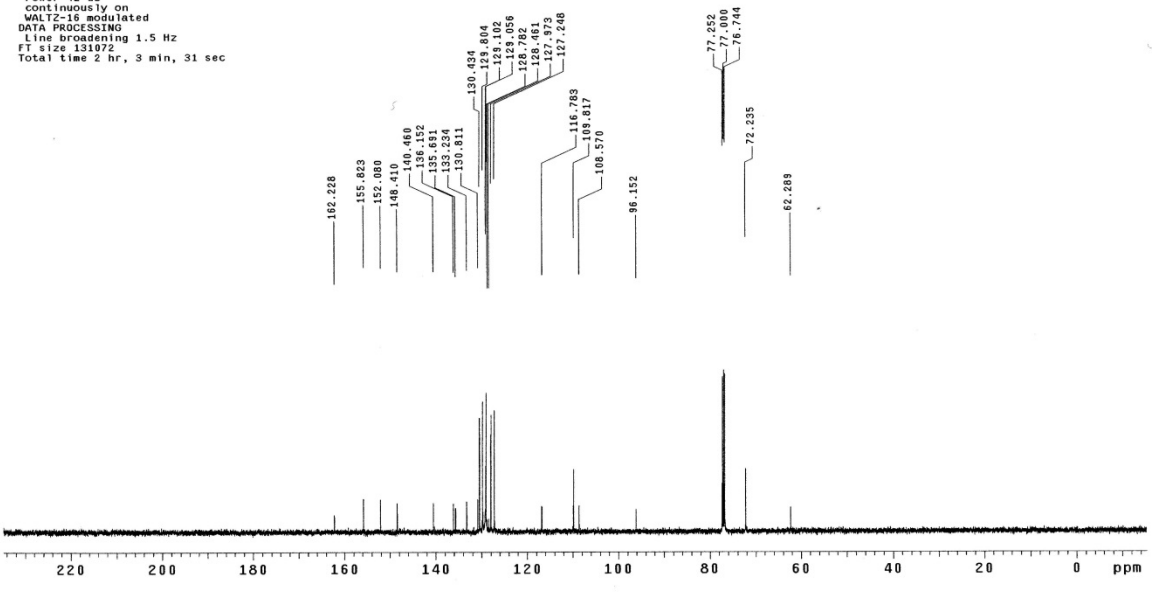
STANDARD CARBON PARAMETERS

Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:

Pulse Sequence: s2pul

Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: d2188
INOVA-500 "NENU500"

Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
128 repetitions
OBSERVE C13, 125.6754690 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec



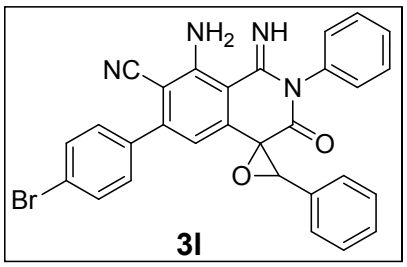
STANDARD PROTON PARAMETERS

Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:

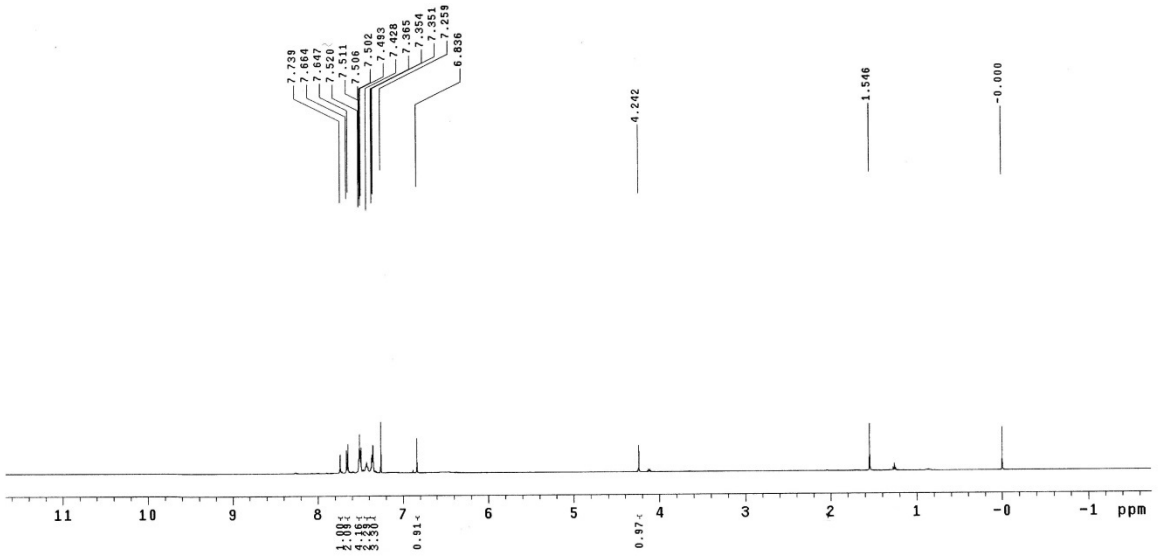
Pulse Sequence: s2pul

Solvent: CDCl3
Ambient temperature
File: d1749
INOVA-500 "NENU500"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 10893.2 Hz
8 repetitions
OBSERVE H1, 499.8025930 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec



3l



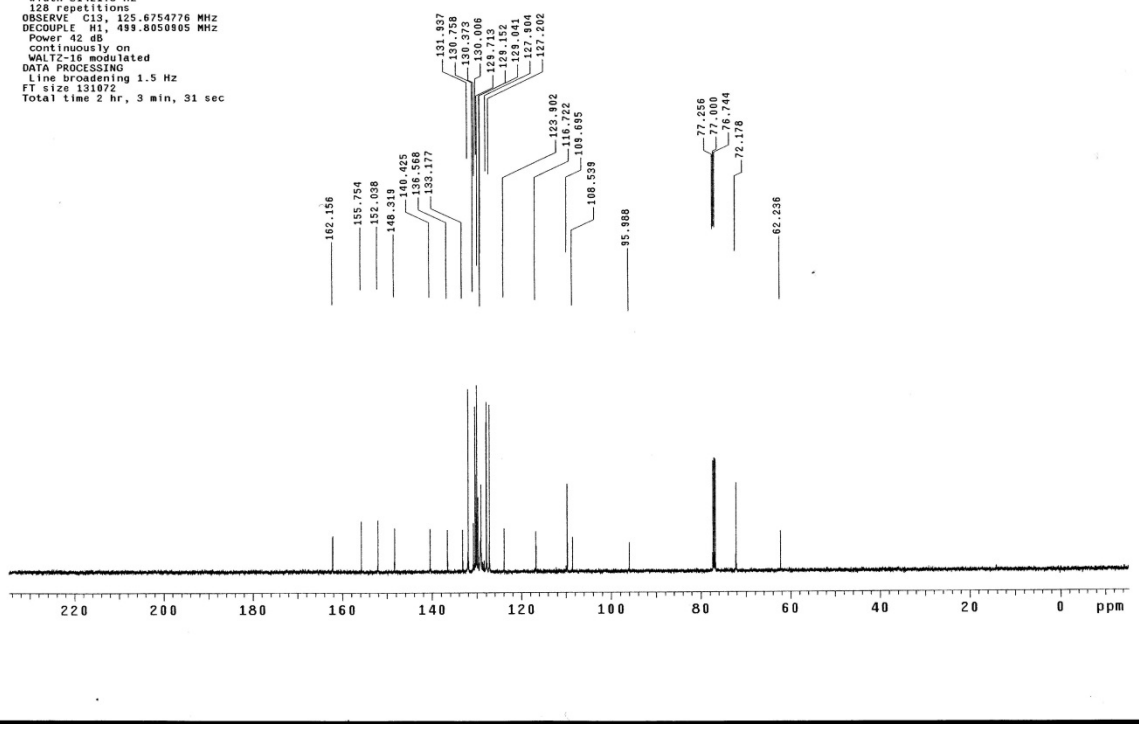
STANDARD CARBON PARAMETERS

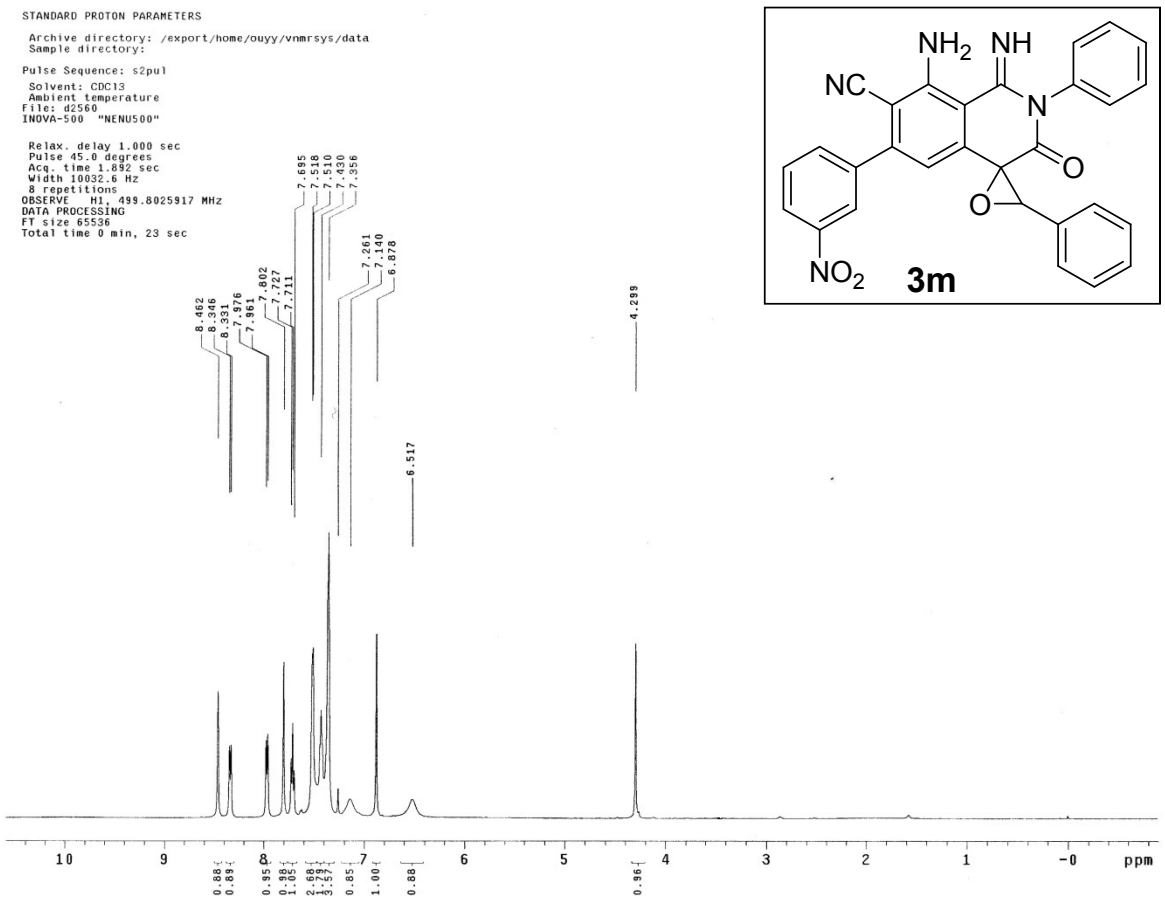
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:

Pulse Sequence: s2pul

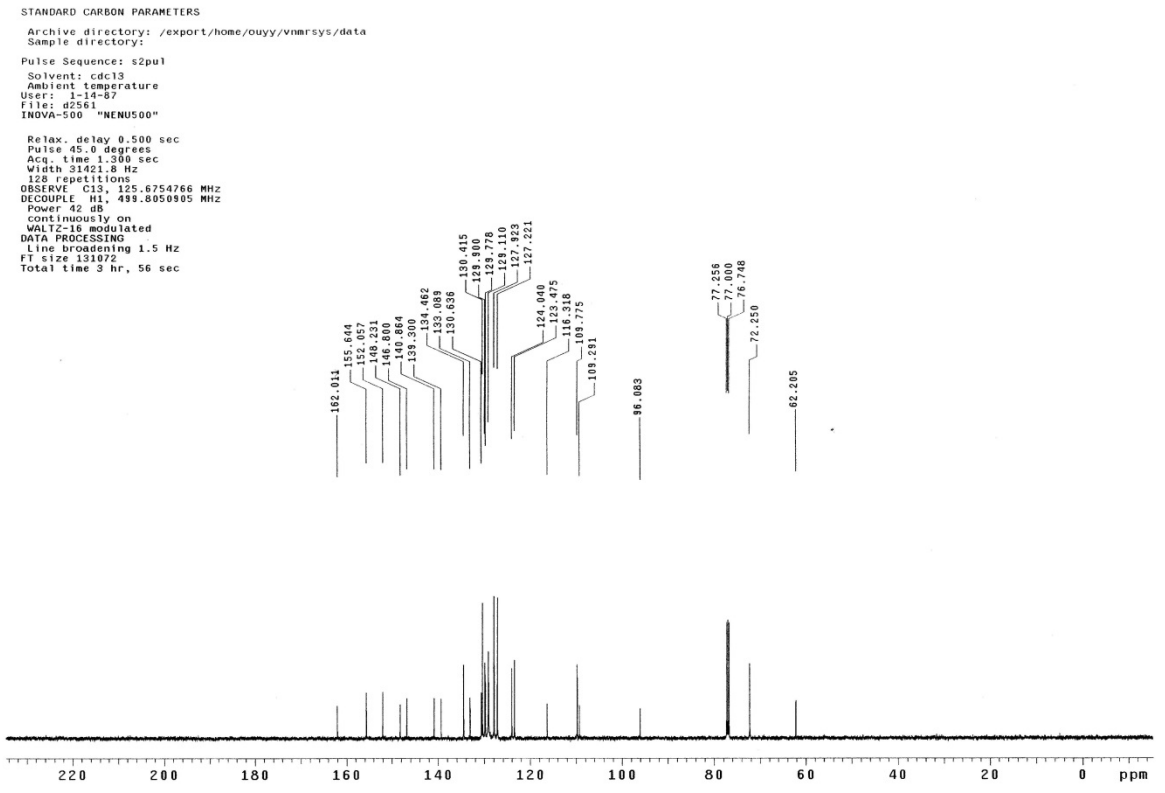
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: d2163
INOVA-500 "NENU500"

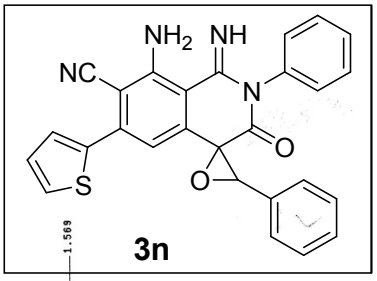
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
128 repetitions
OBSERVE C13, 125.6754776 MHz
DECOUPLE H1, 499.8050805 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec




STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: d2560
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 10032.6 Hz
8 repetitions
OBSERVE H1, 499.8025917 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
8.462
8.446
8.331
7.976
7.961
7.802
7.727
7.711
7.685
7.518
7.510
7.430
7.356
7.261
7.140
6.878
6.517
4.299
ppm

NH2
NH
NC
N
O
O
NO2
3m


STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: d2561
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
128 repetitions
OBSERVE C13, 125.6754766 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
162.011
155.644
152.057
148.231
146.800
140.864
139.300
134.462
133.089
130.636
130.415
129.900
129.778
129.110
127.923
127.221
124.040
123.475
116.318
109.775
109.281
96.083
77.256
77.000
76.748
72.250
62.205
ppm



3n

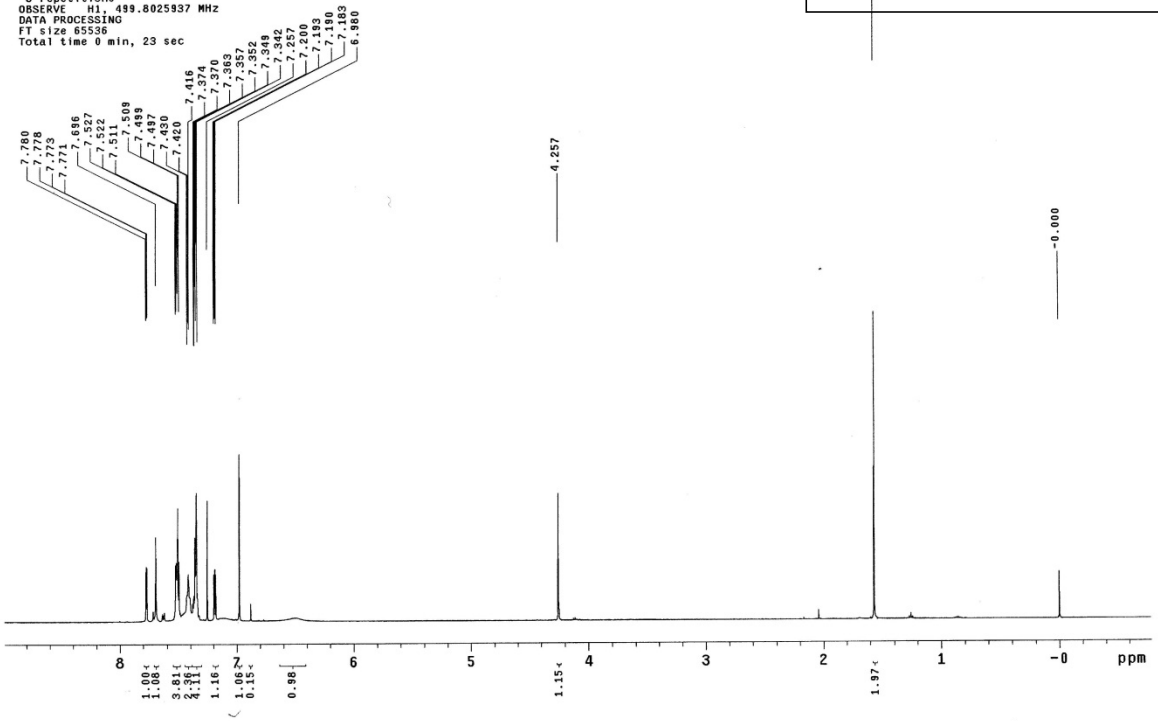
STANDARD PROTON PARAMETERS

Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:

Pulse Sequence: s2pul

Solvent: CDCl3
Ambient temperature
File: d1765
INOVA-500 "NENU500"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 10893.2 Hz
8 repetitions
OBSERVE H1, 499.8025937 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec



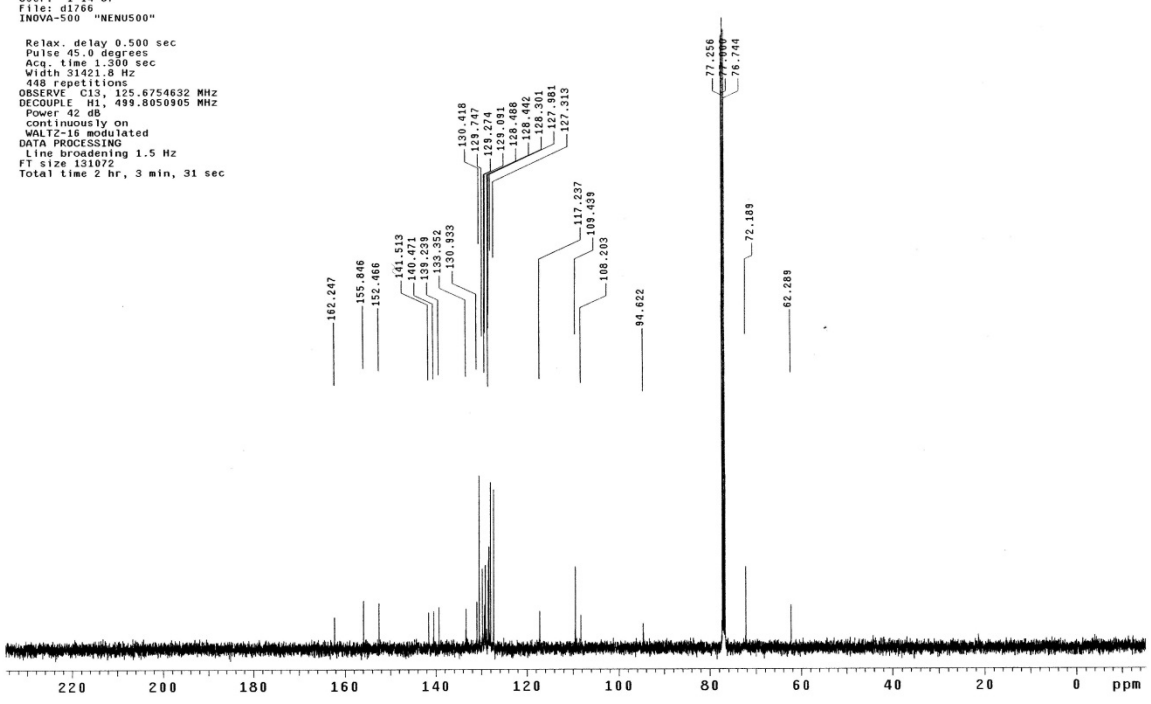
STANDARD CARBON PARAMETERS

Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:

Pulse Sequence: s2pul

Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: d1766
INOVA-500 "NENU500"

Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
448 repetitions
OBSERVE C13, 125.6754632 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec



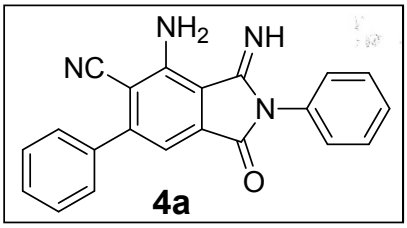
STANDARD PROTON PARAMETERS

Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:

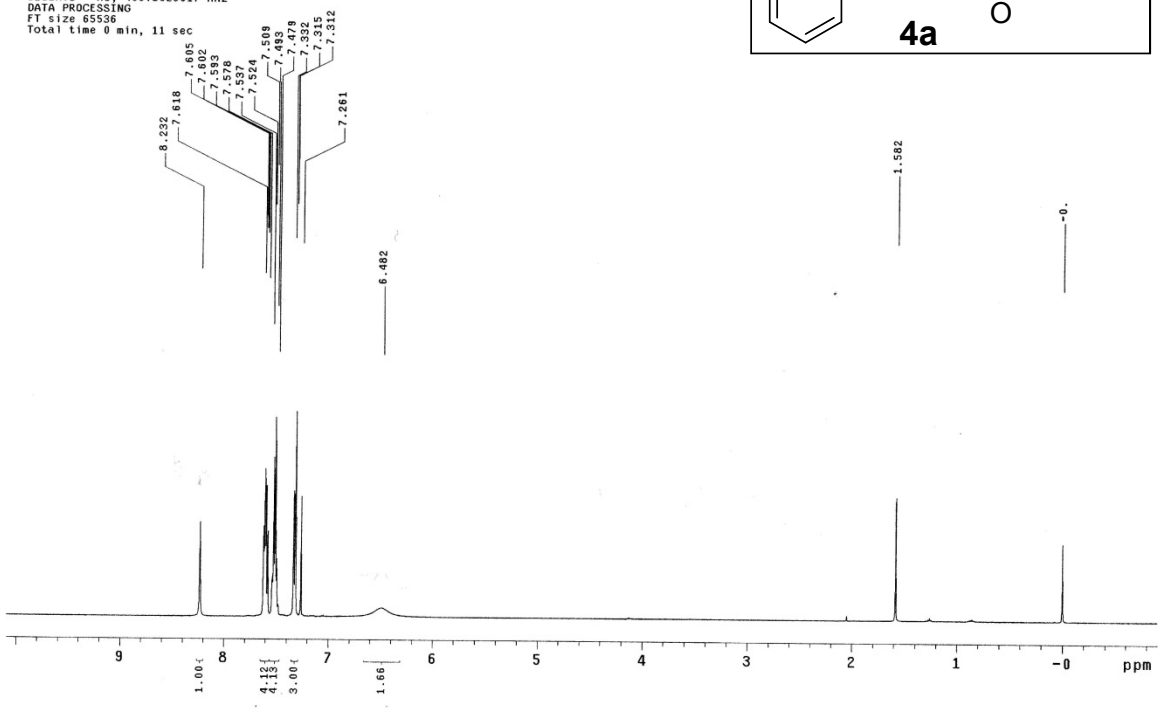
Pulse Sequence: s2pul

Solvent: CDCl3
Ambient temperature
File: d2052
INOVA-500 "NENU500"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 10893.2 Hz
4 repetitions
OBSERVE H1, 499.8025917 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 11 sec



4a



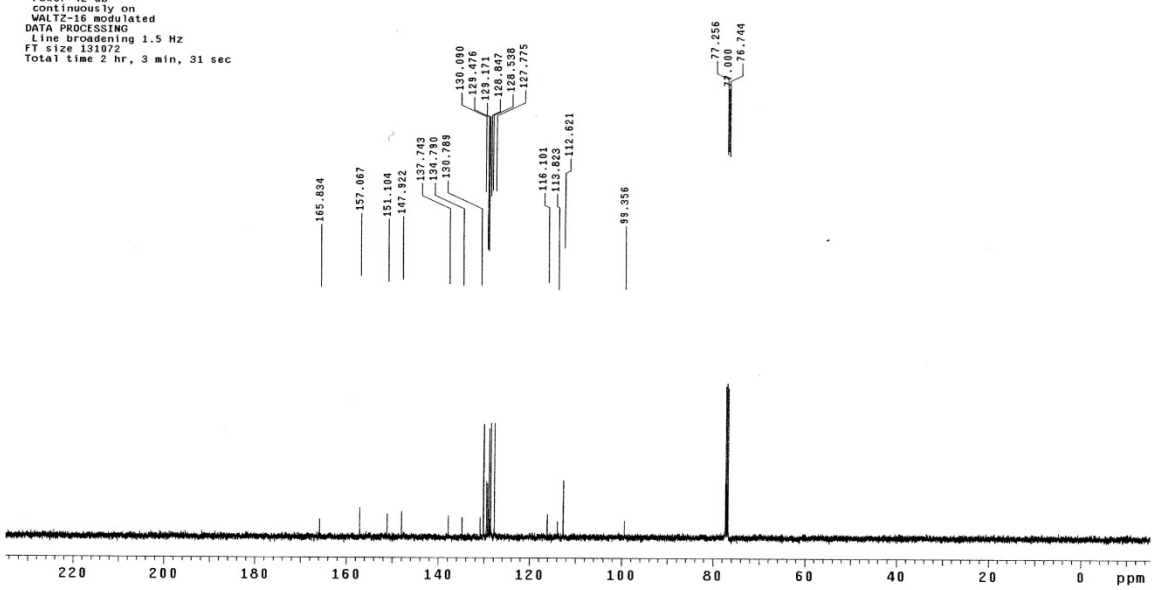
STANDARD CARBON PARAMETERS

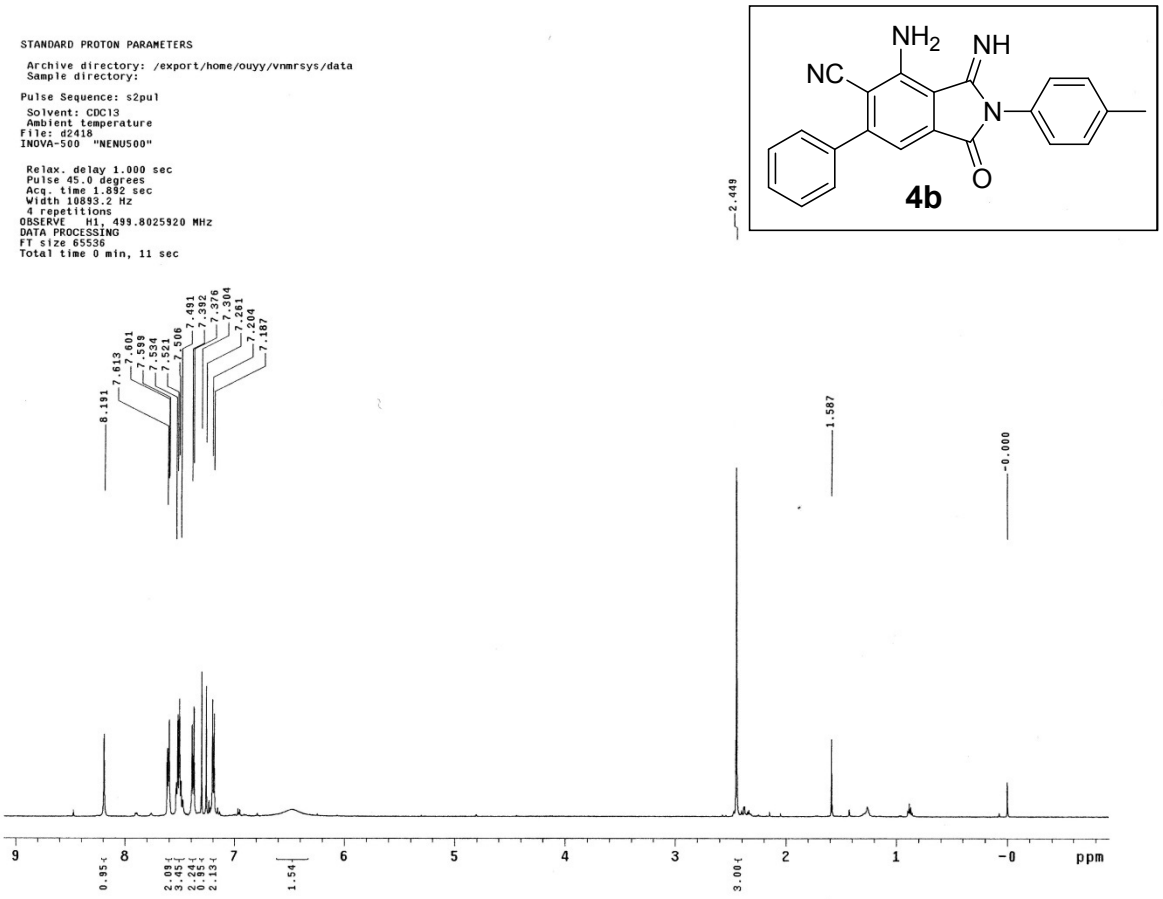
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:

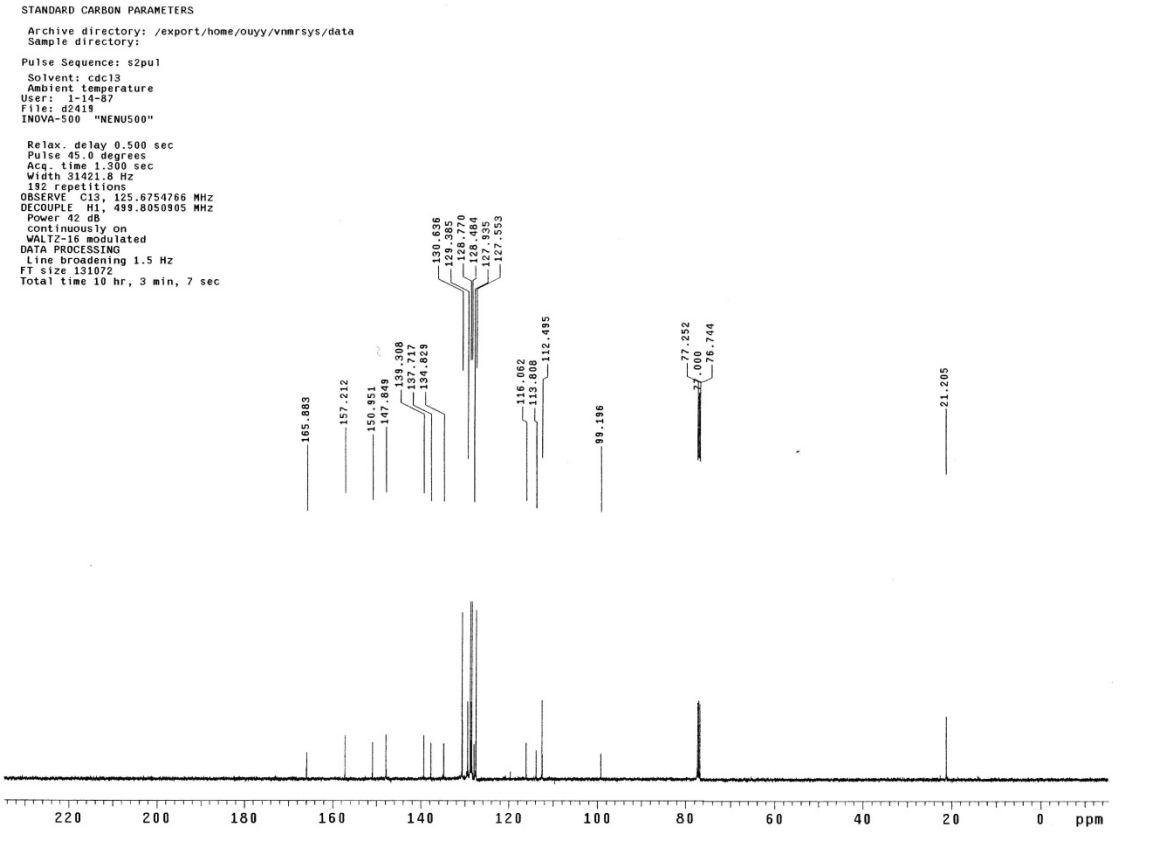
Pulse Sequence: s2pul

Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: d2308
INOVA-500 "NENU500"

Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
128 repetitions
OBSERVE C13, 125.6754690 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec




STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: d2418
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 10893.2 Hz
4 repetitions
OBSERVE H1, 499.8025920 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 11 sec
NH2
NH
NC
N
O
4b
2.449
8.191
7.613
7.601
7.599
7.534
7.521
7.506
7.491
7.480
7.376
7.304
7.261
7.204
7.187
1.587
-0.000
0.95
2.09
3.45
2.24
2.25
2.13
1.54
3.00
9
8
7
6
5
4
3
2
1
-0
ppm


STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: d2419
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
192 repetitions
OBSERVE C13, 125.6754766 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 10 hr, 3 min, 7 sec
165.883
157.212
150.451
147.849
139.308
137.717
134.829
130.636
129.385
128.770
128.484
127.935
127.553
116.062
113.808
112.495
99.196
77.252
77.000
76.744
21.205
220
200
180
160
140
120
100
80
60
40
20
0
ppm

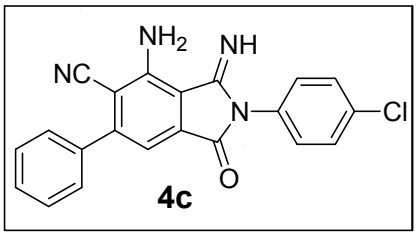
STANDARD PROTON PARAMETERS

Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:

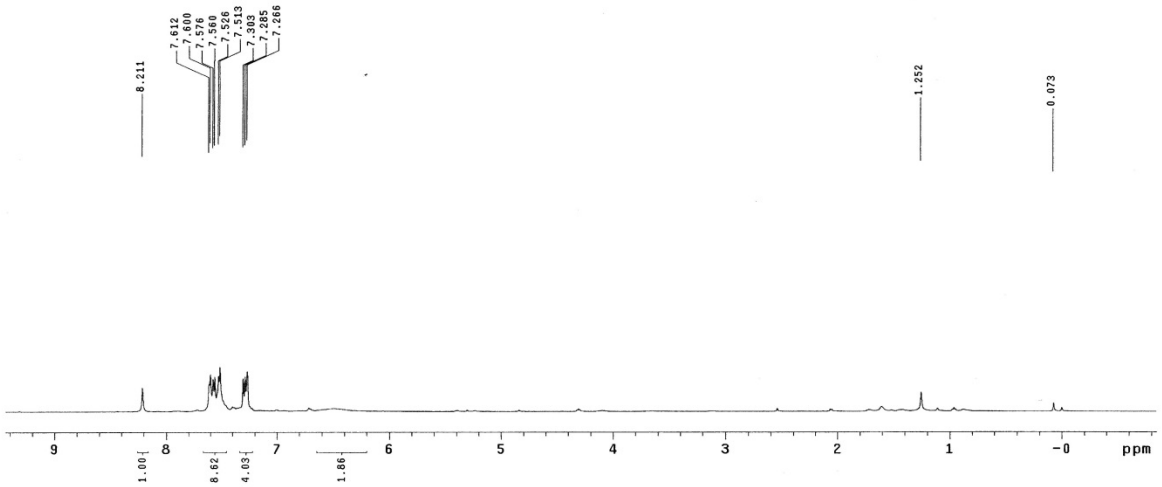
Pulse Sequence: s2pul

Solvent: CDCl3
Ambient temperature
File: d2488
INOVA-500 "NENU500"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 9605.0 Hz
16 repetitions
OBSERVE H1, 499.8025909 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 46 sec



4c



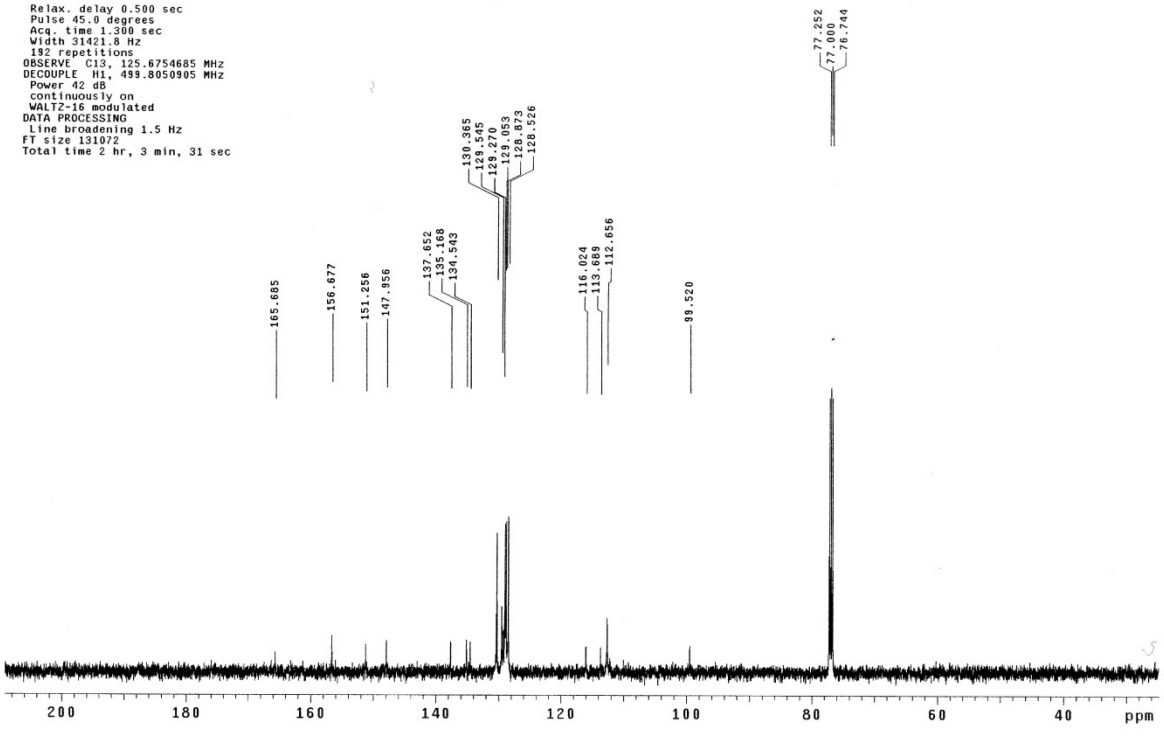
STANDARD CARBON PARAMETERS

Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:

Pulse Sequence: s2pul

Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: d2521
INOVA-500 "NENU500"

Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
192 repetitions
OBSERVE C13, 125.6754685 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec

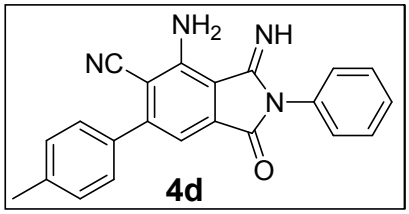


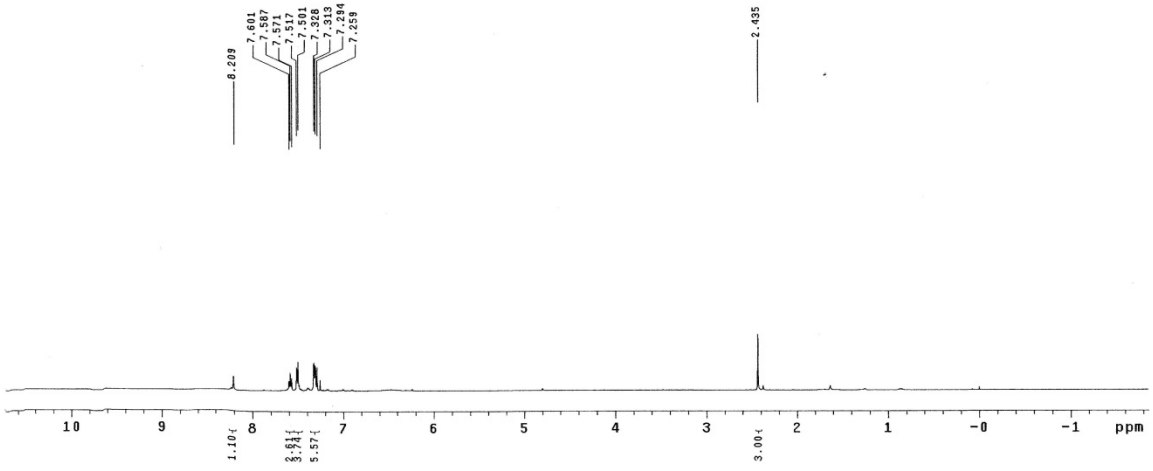
STANDARD PROTON PARAMETERS

Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:

Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: d2354
INOVA-500 "NENU500"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 10893.2 Hz
4 repetitions
OBSERVE H1, 499.8025920 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 11 sec



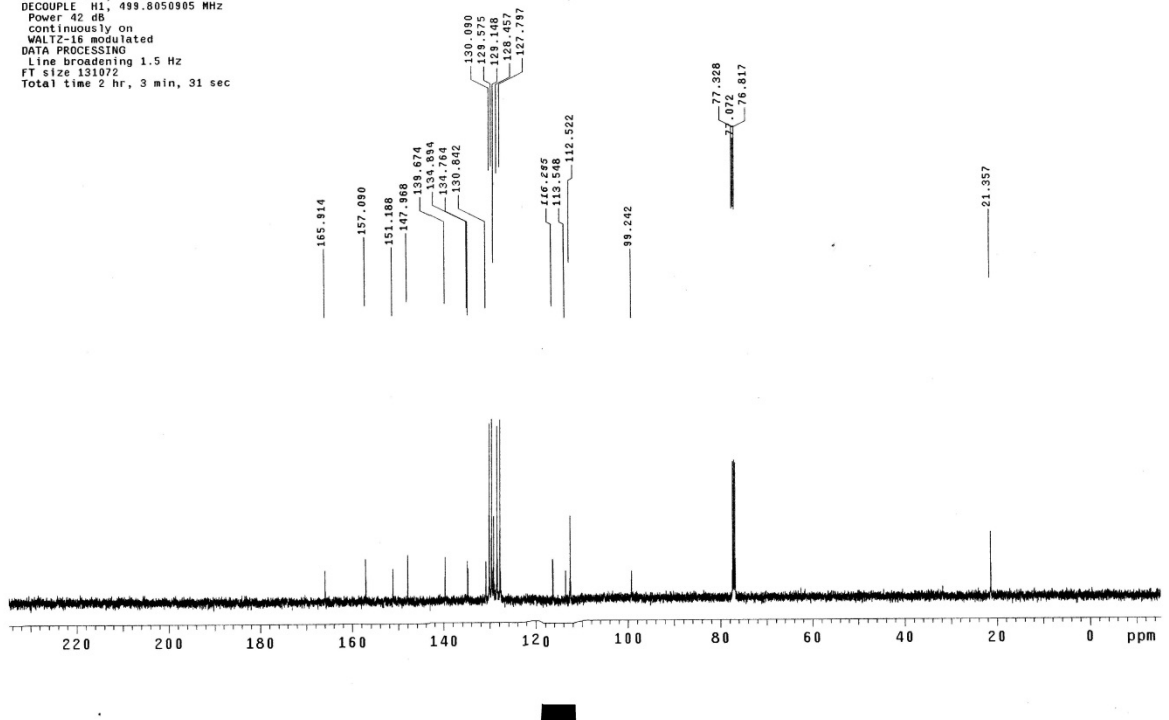


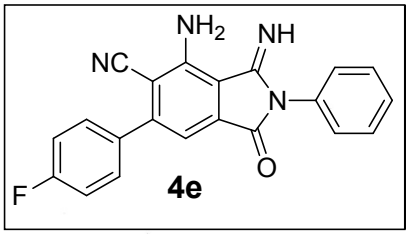
STANDARD CARBON PARAMETERS

Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:

Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: d2517
INOVA-500 "NENU500"

Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
64 repetitions
OBSERVE C13, 125.6754666 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec





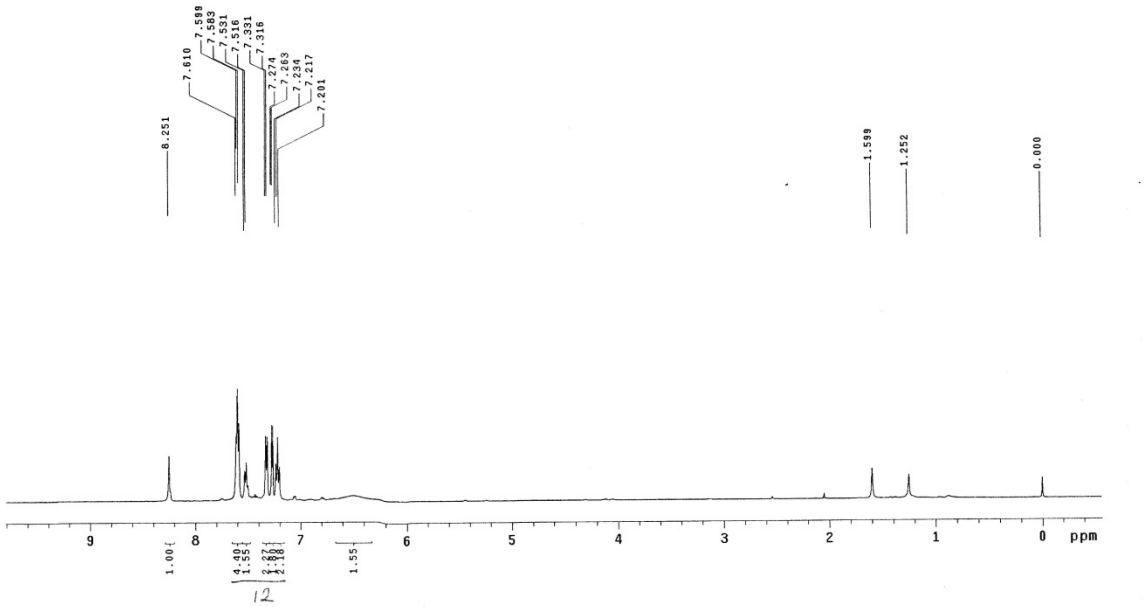
STANDARD PROTON PARAMETERS

Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:

Pulse Sequence: s2pul

Solvent: CDCl3
Ambient temperature
File: d2498
INOVA-500 "NENU500"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 9605.0 Hz
4 repetitions
OBSERVE H1, 499.8025915 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 11 sec



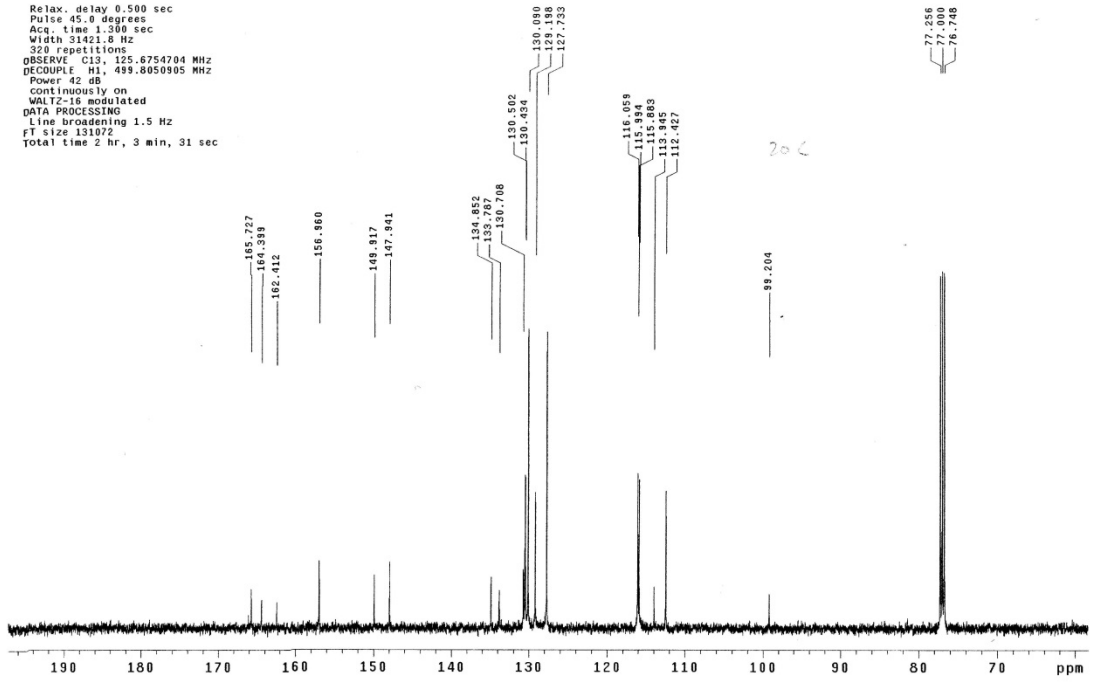
STANDARD CARBON PARAMETERS

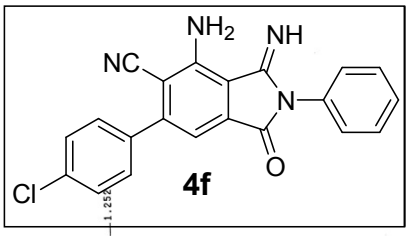
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:

Pulse Sequence: s2pul

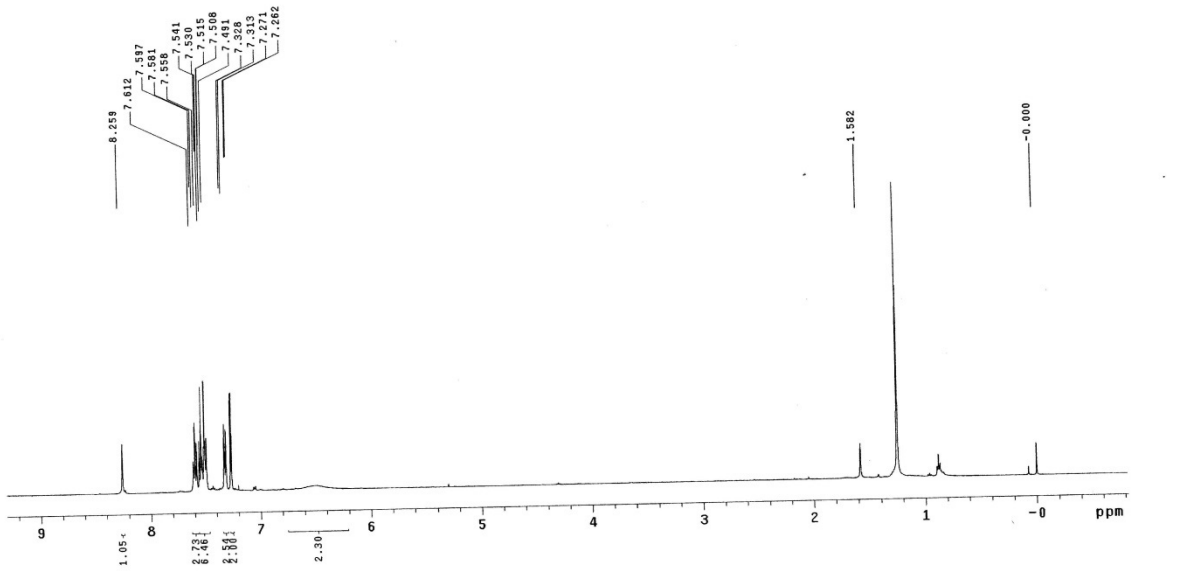
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: d2520
INOVA-500 "NENU500"

Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
320 repetitions
OBSERVE C13, 125.6754704 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec

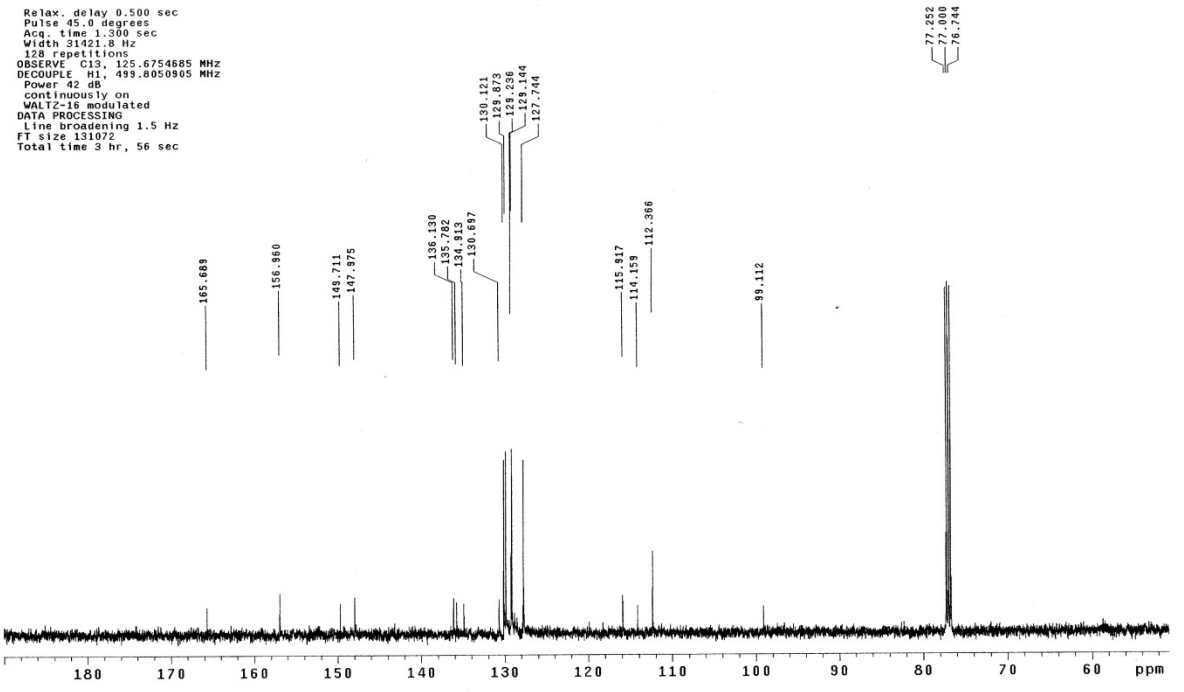


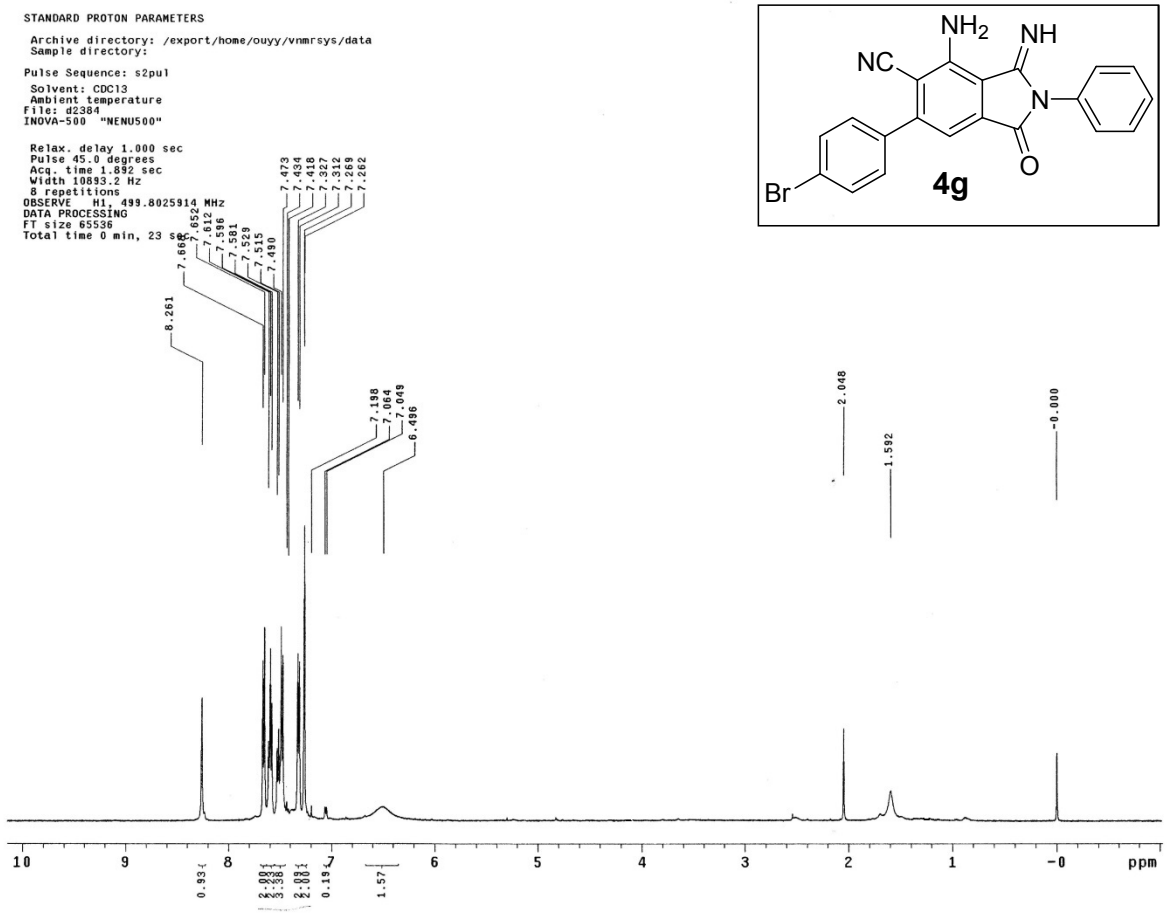


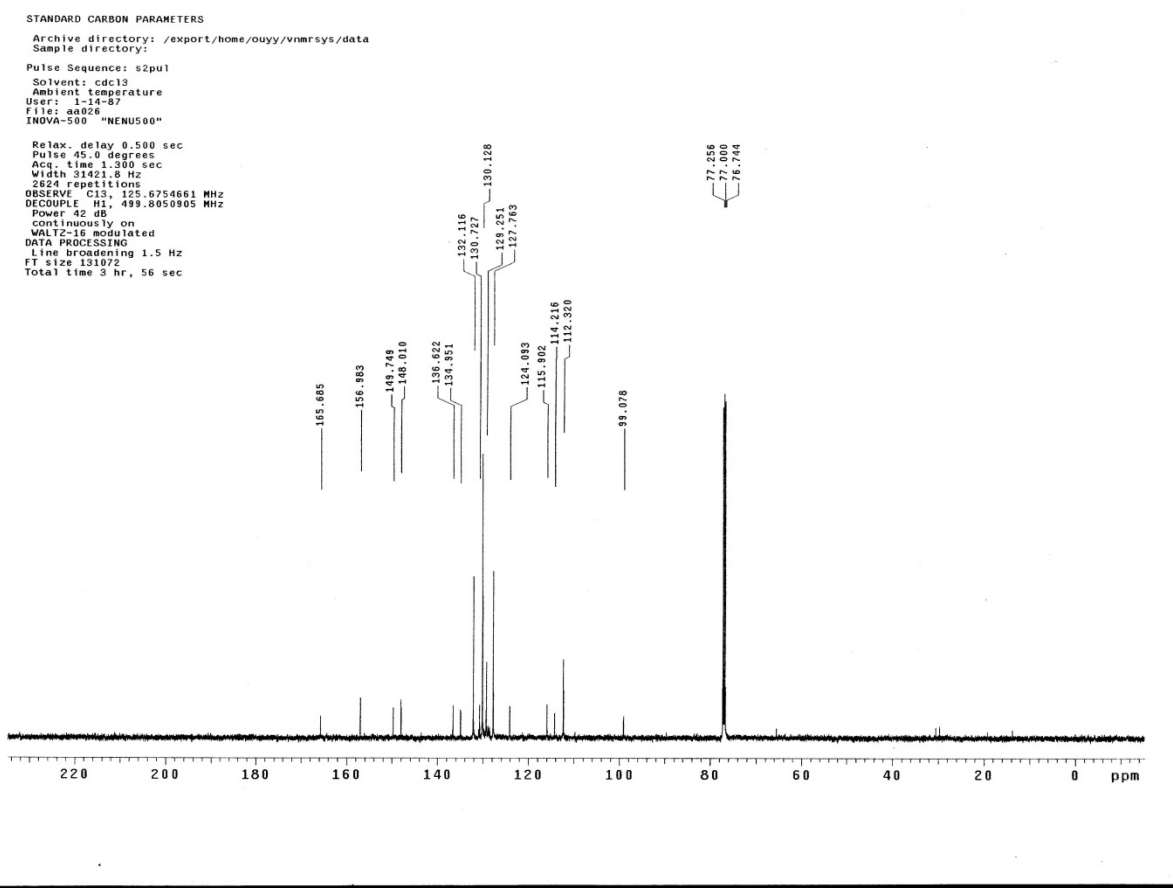

```
STANDARD PROTON PARAMETERS

 Archive directory: /export/home/ouyy/vnmrsys/data
 Sample directory:

Pulse Sequence: s2pul

 Solvent: CDCl3
 Ambient temperature
File: d2429
INOVA-500  "NENU500"

 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 1.892 sec
 Width 9947.8 Hz
 8 repetitions
OBSERVE   H1, 499.8025915 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
```

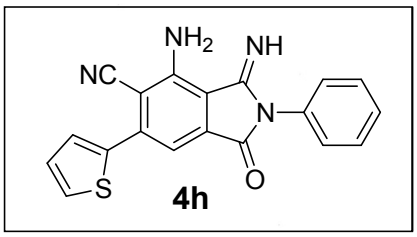



```
STANDARD CARBON PARAMETERS

 Archive directory: /export/home/ouyy/vnmrsys/data
 Sample directory:

Pulse Sequence: s2pul

 Solvent: cdcl3
 Ambient temperature
User:  1-14-87
File: d2470
INOVA-500  "NENU500"

 Relax. delay 0.500 sec
 Pulse 45.0 degrees
 Acq. time 1.300 sec
 Width 31421.8 Hz
 128 repetitions
OBSERVE  C13, 125.6754685 MHz
DECOUPLE  H1, 499.8050905 MHz
 Power 42 dB
 continuously on
 WALTZ-16 modulated
DATA PROCESSING
 Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
```



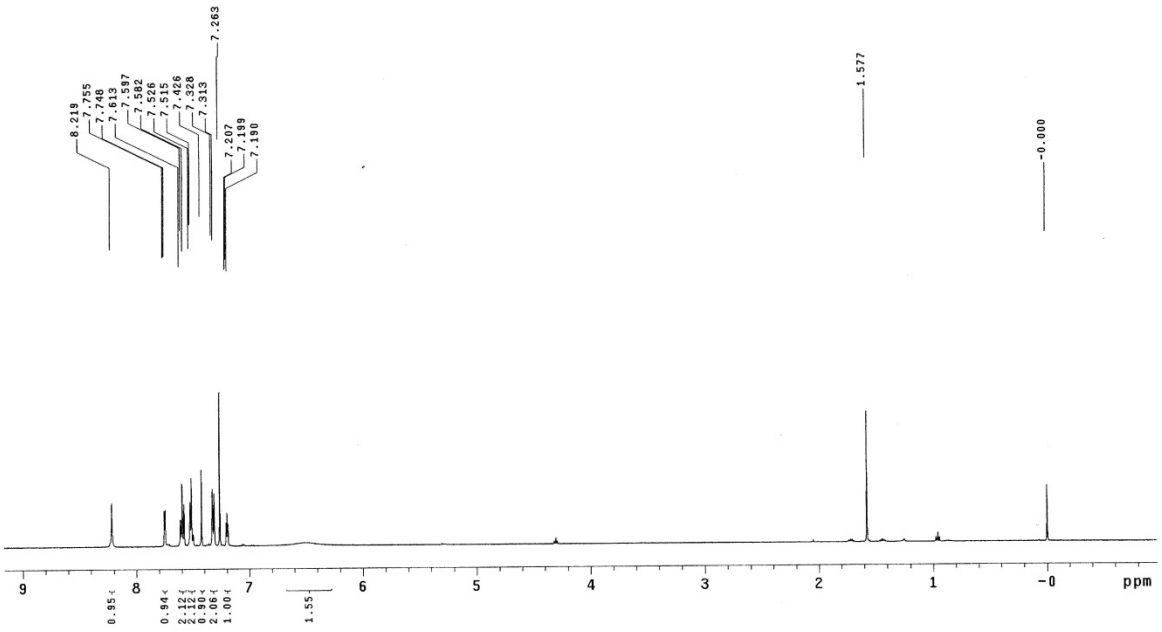

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: d2384
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 10893.2 Hz
8 repetitions
OBSERVE H1, 499.8025914 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
NH2
NH
NC
N
O
Br
4g
ppm


STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: aa026
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
2624 repetitions
OBSERVE C13, 125.6754661 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
ppm

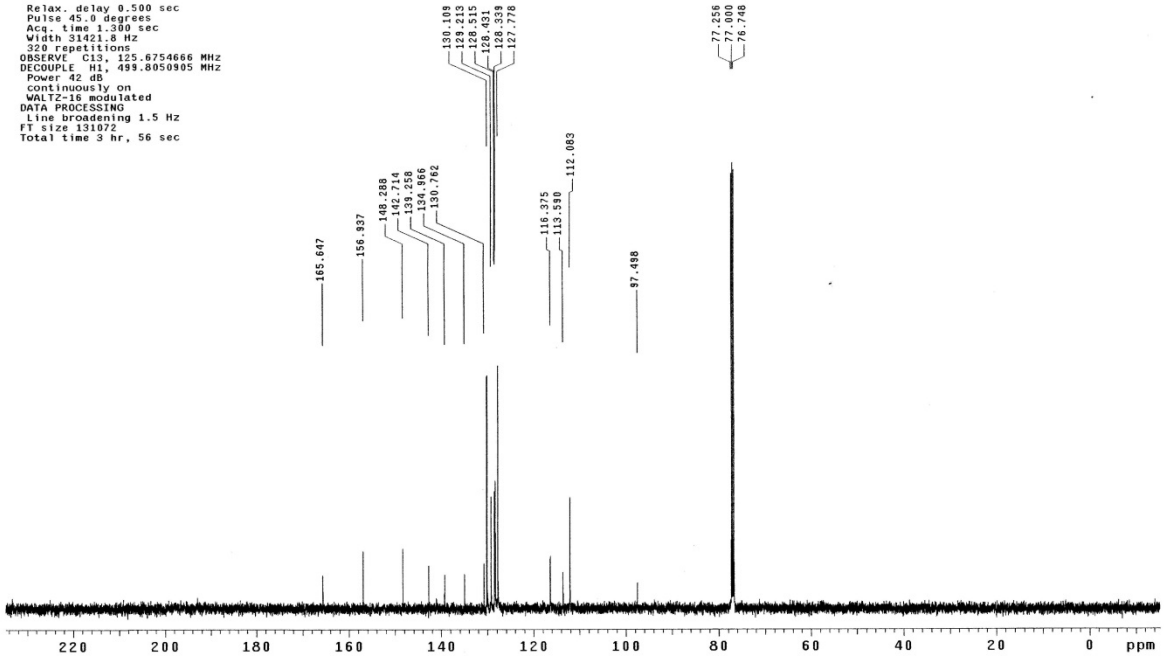


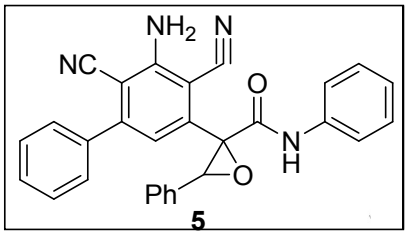
4h

```
STANDARD PROTON PARAMETERS

 Archive directory: /export/home/ouyy/vnmrsys/data
 Sample directory:

Pulse Sequence: s2pul

 Solvent: CDCl3
 Ambient temperature
File: d2431
INOVA-500  "NENU500"

 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 1.892 sec
 Width 9947.8 Hz
 4 repetitions
OBSERVE    H1, 499.8025906 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 11 sec
```




```
STANDARD CARBON PARAMETERS

 Archive directory: /export/home/ouyy/vnmrsys/data
 Sample directory:

Pulse Sequence: s2pul

 Solvent: cdcl3
 Ambient temperature
User:  1-14-87
File: d2516
INOVA-500  "NENU500"

 Relax. delay 0.500 sec
 Pulse 45.0 degrees
 Acq. time 1.300 sec
 Width 31421.8 Hz
 320 repetitions
OBSERVE  C13, 125.6754666 MHz
DECOUPLE  H1, 499.8050905 MHz
 Power 42 dB
 continuously on
 WALTZ-16 modulated
DATA PROCESSING
 Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
```





5

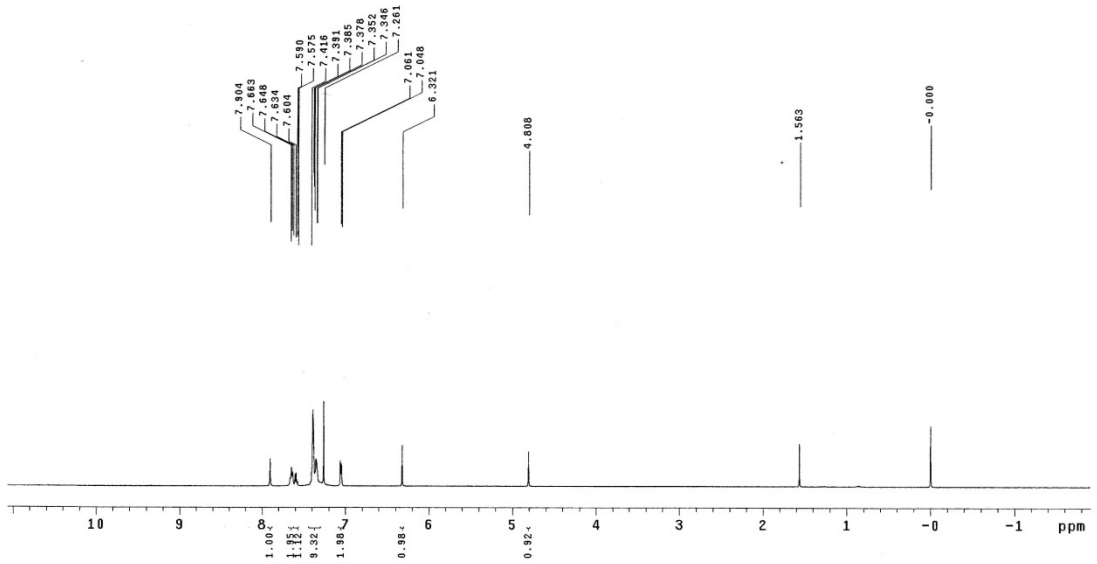
STANDARD PROTON PARAMETERS

Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:

Pulse Sequence: s2pul

Solvent: CDCl3
Ambient temperature
File: d2256
INOVA-500 "NENU500"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 10893.2 Hz
4 repetitions
OBSERVE H1, 499.8025907 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 11 sec



STANDARD CARBON PARAMETERS

Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:

Pulse Sequence: s2pul

Solvent: cdcl3
Ambient temperature
User: 1-14-87
File: d2513
INOVA-500 "NENU500"

Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
256 repetitions
OBSERVE C13, 125.6754680 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec