Supporting Information

A novel protocol for the facile construction of tetrahydro quinoline fused tricyclic frame works via an intramolecular 1, 3 - dipolar nitrile oxide cycloaddition reaction

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EXPERIMENTAL SECTION

Typical experimental procedure for the synthesis of compound (3a):

A solution of N-(2-formylphenyl)-4-methylbenzene-1-sulfonamide (**1**) (1 mmol, 0.28 g) and potassium carbonate (2 mmol, 0.28 g) in acetonitrile solvent was stirred for 15 minutes at room temperature. To this solution, (Z)-methyl 2-(bromomethyl)-3-phenylacrylate (**2a**) (1.2 mmol, 0.31 g) was added drop wise till the addition is complete. After the completion of the reaction as indicated by TLC, the reaction mixture was concentrated and extracted with ethylacetate (2x15 mL). The organic layer thus obtained was washed with water (2x10 mL), followed by brine solution (2x 10 mL) and dried over anhydrous sodium sulphate. The crude product obtained was purified by a pad of silica gel (100-200 mesh) column chromatography using ethylacetate and Hexane (1:9) to afford the compound (**3a**) as a colourless solid (0.44 g, 98% yield).

Methyl (2E)-2-{[N-(2-formylphenyl)(4-methylbenzene) sulfo namido]methyl}-3-phenylprop-2-enoate (3a):

Colourless solid; Yield: 98% mp: 98-100 ºC; ^{1}H NMR ($CDCl_3$, 300 MHz) :δ 2.43 (s, 3H), 3.68 (s, 3H), 4.53 (d, 1H, J = 13.5 Hz), 5.06 (d, 1H, J = 13.5 Hz), 6.42 - 7.91 (m, 14H), 9.89 (s, 1H); ^{13}C NMR ($CDCl_3$, 75 MHz): δ 21.6, 46.4, 52.3, 126.3, 127.6, 127.9, 128.3, 128.3, 128.7, 129.5, 129.5, 129.63, 132.9, 133.4, 133.9, 136.1, 141.4, 144.3, 167.5, 189.9; MS (m/z): 451 (M^++1).

Methyl (2E)-2-{[N-(2-formylphenyl)(2-methylbenzene) sulfo namido]methyl}-3-(4-methylphenyl)prop-2-enoate (3b):

Colourless solid; Yield: 87%; mp: 100-102ºC;^{1}H NMR ($CDCl_3$, 300 MHz) : δ 1.96 (s, 3H), 2.39 (s, 3H), 3.76 (s, 3H), 4.35 (d, 1H, J = 13.8Hz), 4.91 (d, 1H, J = 13.5 Hz), 6.25-7.94 (m, 13H), 10.01 (s, 1H); ^{13}C NMR ($CDCl_3$, 75 MHz): δ 19.6, 21.6, 46.8, 52.3, 125.6, 127, 127.6, 127.8, 128.1, 128.2, 128.9, 129.1, 129.5, 130.2, 132.9, 133.5, 133.6, 135.9, 137.5, 142.2, 143.6, 144.2, 167.1, 190.1; MS (m/z): 465 (M^++1).

Methyl (2E)-2-{[N-(2-formylphenyl)(4-methylbenzene) sulfo namido]methyl}-3-(4-methylphenyl)prop-2-enoate (3c):

Colourless solid; Yield: 87%; mp: 103-105 ºC; ^{1}H NMR ($CDCl_3$, 300 MHz): δ 2.42 (s, 3H), 2.44 (s, 3H), 3.64 (s, 3H), 4.57 (d, 1H, J = 13.5 Hz), 5.08 (d, 1H, J = 13.5 Hz), 6.48-7.90 (m, 13H), 9.87 (s, 1H); ^{13}C NMR ($CDCl_3$, 75 MHz): δ 21.5, 21.6, 46.4, 52.2, 124.9,

127.7, 127.9, 128.3, 128.7, 129.5, 129.5, 129.9, 131.1, 132.9, 133.3, 136.2, 140.2, 141.2, 144.3, 144.6, 167.7, 189.9; MS (m/z): 465 (M^++1).

Methyl (2E)-2-{[N-(2-formylphenyl)(4-methylbenzene)sulfo namido]methyl}-3-(2-methoxy phenyl)prop-2-enoate (3d):

Colourless solid; Yield: 97%; mp: 110-112 ºC; ^{1}H NMR ($CDCl_3$, 300 MHz): δ 2.41 (s, 3H), 3.69 (s, 3H), 3.70 (s, 3H), 4.45 (d, 1H, J = 13.5 Hz), 5.01 (d, 1H, J = 13.8 Hz), 6.38 - 7.87 (m, 13H), 9.85 (s, 1H); ^{13}C NMR ($CDCl_3$, 75 MHz): δ 21.6, 46.7, 52.2, 55.3, 110.7, 120.3, 123.1, 126.3, 127.5, 127.8, 128, 128.3, 129.5, 130, 130.9, 133.3 (m/z): 481 (M^++1).

Methyl (2E)-2-{[N-(2-formylphenyl)(4-methylbenzene)sulfo namido]methyl}-3-(4-methoxyphenyl)prop-2-enoat (3e):

Colourless solid; Yield : 97%; mp:110-112 ºC; 1H NMR (CDCl3, 300 MHz): δ 2.40 (s, 3H), 3.68 (s, 6H), 4.40 (d, 1H, J = 13.5Hz), 5.01 (d, 1H, J = 13.8Hz), 6.37 - 7.89 (m, 13H), 9.85 (s, 1H);13C NMR (CDCl3, 75 MHz): δ 21.6, 46.7, 52.2, 55.3, 110.7, 120.3, 123.1, 126.4, 127.4, 127.7, 128., 128.2, 129.5, 129.9, 130.9, 133.2, 133.3, 136.1, 140.9, 141.5, 144.1, 157.4, 167.4, 190;MS (m/z): 481 (M^++1).

Methyl (2E)-2-{[N-(2-formylphenyl)(4-methylbenzene)sulfo namido]methyl}-3-(2-chlorophenyl)prop-2-enoate (3f):

Colourless solid; Yield : 90%; mp: 142-144 ºC; ^{1}H NMR ($CDCl_3$, 300 MHz): δ 2.43 (s, 3H), 3.65 (s, 3H), 4.49 (d, 1H, J = 13.5 Hz), 5.01 (d, 1H, J = 13.8 Hz), 6.44-7.91 (m, 13H), 9.98 (s, 1H); ^{13}C NMR ($CDCl_3$, 75 MHz) : δ 21.6, 46.5, 52.4, 117.7, 123, 127.3, 128, 128.3, 128.5, 128.9, 129.6, 129.8, 130.9, 132.4, 133.5, 135.6, 136.1, 136.2, 141.3, 142.9, 144.5, 167.2, 189.8; MS(m/z): 485 (M^++1).

Methyl (2E)-2-{[N-(2-formylphenyl)(4-methylbenzene)sulfo namido]methyl}-3-(3-chlorophenyl)prop-2-enoate (3g):

Colourless solid; Yield: 90% ;mp: 142-144 ºC; ^{1}H NMR ($CDCl_3$, 300 MHz): δ 2.43 (s, 3H), 3.65 (s, 3H), 4.49 (d, 1H, J = 13.5 Hz), 5.00 (d, 1H, J = 13.5 Hz), 6.44-7.91 (m, 13H), 9.97 (s, 1H); ^{13}C NMR ($CDCl_3$, 75 MHz): δ 21.6, 46.4, 52.3, 126.9, 127.7, 128, 128.3, 128.5, 128.9, 129.6, 130.9, 132.4, 132.9, 133.50, 135.61, 136.07, 141.32, 142.87, 144.52, 167.22, 189.76; MS (m/z): 485 (M^++1).

Methyl (2E)-2-{[N-(2-formylphenyl)(4-methylbenzene)sulfo namido]methyl}-3-(4-chlorophenyl)prop-2-enoate (3h):

Colourless solid; Yield : 79%; mp:145-147ºC; ^{1}H NMR ($CDCl_3$, 300 MHz): δ 2.43 (s, 3H), 3.64 (s, 3H), 4.49 (d, 1H, *J* = 13.2 Hz), 5.00 (d, 1H, J = 12.9 Hz), 6.44-7.90 (m, 13H), 9.98 (s, 1H);^{13}C NMR ($CDCl_3$, 75 MHz): δ 21.6, 46.5, 52.3, 126.9, 127.7, 128, 128.3, 128.5, 128.9, 129.6, 130.9, 132.4, 132.9, 133.5, 135.6, 136.1, 141.3, 142.9, 144.5, 167.2, 189.8; MS (m/z): 485 (M^++1).

(E)-methyl3-(2,4-dichlorophenyl)-2-((N-(2-formylphenyl)-4-methylphenylsulfonamido)methyl)acrylate (3i):

Colourless solid; Yield : 80%, mp: 98-100ºC; ^{1}H NMR ($CDCl_3$, 300 MHz) : δ 2.48 (s, 3H), 3.72 (s, 3H), 4.34 (d, 1H, J = 13.5Hz), 4.89 (d, 1H, J = 13.8Hz), 6.36-7.95 (m, 12H), 10.02 (s, 1H); ^{13}C NMR ($CDCl_3$, 75 MHz) :δ 21.6, 46.8, 52.5, 117.7, 122.9, 127, 127.3, 128.1, 128.3, 128.6, 129.6, 129.8, 130.1, 131.1, 133.7, 134.9, 135.8, 136.1, 139.7, 141.4, 144.2, 189.7, 195; MS (m/z): 516 (M^++1).

(E)-methyl 2-((N-(2-formylphenyl)-4-methylphenylsulfo namido)methyl)-3-(4-isopropylphenyl)acrylate (3j):

Colourless solid; Yield: 88%; mp: 101-103 ºC; ^{1}H NMR ($CDCl_3$, 300 MHz,): δ 1.29 (s, 3H), 1.31 (s, 3H), 2.43 (s, 3H), 2.96 (sep, 1H, J = 6.9 Hz), 3.62 (s, 3H), 4.58 (d, 1H, J = 13.2 Hz), 5.06 (d, 1H, J = 13.5 Hz), 6.49 - 7.88 (m, 13H), 9.85 (s, 1H); ^{13C} NMR ($CDCl_3$, 75 MHz): δ 21.6, 23.8, 23.9, 34.1, 46.5, 52.2, 124.9, 126.9, 127.8, 127.9, 128.3, 128.4, 129.5, 130.1, 131.4, 132.9, 133.3, 136.2, 141, 144.3, 144.6, 151.1, 167.8, 189.8; MS (m/z) : 492 (M^++1).

Methyl (2E)-2-{[N-(2-formylphenyl)(4-methylbenzene)sulfo namido]methyl}-3-(4-fluorophenyl)prop-2-enoate (3k):

Colourless solid; Yield: 79%; mp:132-134ºC; ^{1}H NMR ($CDCl_3$, 300 MHz): δ 2.43 (s, 3H), 3.63 (s, 3H), 4.53 (d, 1H, J = 13.2 Hz), 5.03 (d, 1H, J = 13.5 Hz), 6.46-7.90 (m, 13H), 9.93 (s, 1H); ^{13}C NMR ($CDCl_3$, 75 MHz): δ 20.5, 45.2, 51.2, 114.7, 114.9, 124.8, 126.5, 126.9, 127.2, 127.3, 128.5, 128.9, 128.9, 130.7, 130.8, 131.8, 132.3, 135, 140.1, 142, 143.4, 160.5, 166.7, 188.6; MS (m/z): 469 (M^++1).

Methyl (2E)-2-{[N-(2-formylphenyl)(4-methylbenzene)sulfo namido]methyl}-3-(naphthalen-1-yl)prop-2-enoate) (3l):

Colourless solid; Yield: 97%; mp:139-141ºC; ^{1}H NMR ($CDCl_3$, 300 MHz): δ 2.36 (s, 3H), 3.85 (s, 3H), 4.43 (d, 1H, J = 13.5 Hz), 5.00 (d, 1H, J = 13.8 Hz), 6.03 - 8.22 (m, 15H), 10.08 (s, 1H);^{13}C NMR ($CDCl_3$, 75 MHz): δ 21.5, 46.9, 52.5, 124.6, 124.9, 126.4, 126.6, 126.7, 127.3, 127.9, 128, 128, 128.3, 129, 129.4, 131.3, 131.4, 133.2, 133.4, 135.8, 141.4, 142.9, 144, 166.9, 189.9; MS (m/z): 501 (M^++1).

Methyl (2E)-2-{[N-(2-formylphenyl)(4-methylbenzene)sulfo namido]methyl}-3-(3,4-dimethoxyphenyl)prop-2-enoate (3m):

Colourless solid; Yield:92%; mp:123-125ºC; ^{1}H NMR ($CDCl_3$, 300 MHz): δ 2.45 (s, 3H), 3.59 (s, 3H), 3.95 (s, 3H), 3.96(s, 3H), 4.67 (d, 1H, J = 13.2 Hz), 5.13 (d, 1H, J = 13.2 Hz), 6.51-7.89 (m, 12H), 9.89 (s, 1H);^{13}C NMR ($CDCl_3$, 75MHz): δ 21.6, 46.2, 52.2, 56.1, 56.3, 111.1, 112.9, 122.7, 124.6, 126.5, 127.91, 128.4, 128.4, 128.6, 129.6, 133.1, 133.3, 136.4, 140.76, 141.8, 144.4, 144.8, 150.9, 168.1, 189.8; MS (m/z) : 511 (M^++1).

Methyl (2E)-2-{[N-(2-formylphenyl)(4-methylbenzene)sulfo namido]methyl}-3-(4-methylphenyl)prop-2-enoate (3n):

Colourless solid; Yield:87%: mp:110-112 ºC; ^{1}H NMR ($CDCl_3$, 300 MHz) : δ 1.29 (t, 3H, J = 7.5 Hz), 2.46 (s, 3H), 2.71 (q, 2H, J = 7.5 Hz), 3.60 (s, 3H), 4.46 (d, 1H, J = 12.9 Hz), 4.97 (d, 1H, J = 12.9 Hz), 6.25-7.52 (m, 13H), 9.89 (s, 1H);^{13}C NMR ($CDCl_3$, 75 MHz) : δ 15.4, 21.6, 28.8, 47.2, 52.1, 125.5, 127.55, 127.8, 128.2, 128.5, 128.9, 129.5, 130, 130.8, 131.4, 133.6, 136.5, 142.7, 144.1, 144.2, 146.1, 168.1, 189.5; MS (m/z) 465 (M^++1).

Representative procedure for the synthesis of *Methyl 3-phenyl-5-tosyl-3,3a,4,5-tetrahydro isoxazolo[4,3-c]quinoline-3a-carboxylate* (5a):

To a solution of 2 mmol of *N*-allylated derivative (**3a**) in ethanol, $NH_2OH.HCl$ (6 mmol) was added and stirred well at room temperature for 1 h. After the completion of the reaction as evidenced by the tlc, ethanol was removed under reduced pressure and the crude thus obtained was further treated with 10 mL CCl_4 and NCS (5 mmol) and Et_3N (4 mmol) and the reaction mixture and stirred well at room temperature for 1 h. After completion of the reaction, reaction mixture was evaporated under reduced pressure and the resulting crude mass was diluted with water (15 mL) and extracted with ethyl acetate (3 × 15 mL). The combined organic layer was washed with brine (2 × 10 mL) and dried over anhydrous Na_2SO_4. The organic layer was evaporated and the crude mass was purified by column chromatography (silica gel 60-120 mesh 5% EtOAc in hexanes) to provide the desired pure product **5a (**0.36 g, 79% yield).

Methyl 3-phenyl-5-tosyl-3,3a,4,5-tetrahydroisoxazolo[4,3-c]quinoline-3a-carboxylate (5a):

Colourless solid; mp 163 – 165 ˚C; 1H NMR (300 MHz, CDCl3): δ 2.38 (s, 3H), 2.66 (d, 1H, J = 12.9 Hz), 3.80 (s, 3H), 4.74 (d, 1H, J = 12.9 Hz), 6.11 (s, 1H), 7.10 – 8.10 (m, 13H); 13C NMR (75 MHz, CDCl3): δ 21.5, 50.1, 53.6, 62.6, 88.2, 117.0, 119.8, 124.0,

125.4, 126.3, 126.7, 128.9, 129.0, 129.9, 131.1, 135.0, 136.6, 137.5, 144.2, 150.6, 170.6; IR (neat) : ν 1240, 1361, 1600 (medium), 1736 (strong) cm-1 ; HRMS (m/z) Calcd for $C_{25}H_{22}N_2O_5S$ [M + H]+ 463.1249, Found 463.1308.

Methyl 3-o-tolyl-5-tosyl-3,3a,4,5-tetrahydroisoxazolo[4,3-c]quinoline-3a- carboxylate (5b):

Colourless solid; Yield: 72%; mp 168 – 170ºC ; ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.35 (s, 3H), 2.50(s, 3H), 2.77 (d, 1H, J = 12.9 Hz), 3.86 (s, 3H), 4.75 (d, 1H, J = 12.9 Hz) 6.30 (s, 1H), 7.11 – 8.10 (m, 12H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 18.4, 20.6, 23.7, 48.6, 52.7, 61.7, 115.7, 116.0, 118.5, 119.3, 123.0, 124.6, 125.6, 127.5, 128.0, 128.9, 130.0, 130.1, 133.2, 135.7, 136.5, 143.2, 149.4, 169.8; IR (neat): ν 1252, 1458, 1598 (medium), 1735 (strong) cm^{-1} ; HRMS (m/z) Calcd for $C_{26}H_{24}N_2O_5S$ $[M + H]^+$ 477.1342, Found 477.1474.

Methyl 3-p-tolyl-5-tosyl-3,3a,4,5-tetrahydroisoxazolo[4,3-c] quinoline-3a-carboxylate (5c):

Colourless solid; Yield: 76%; mp 170-172 ºC; ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.26 (s, 3H), 2.31(s, 3H), 2.63 (d, 1H, J = 12.9 Hz), 3.70 (s, 3H), 4.66 (d, 1H, J = 12.9.1 Hz), 5.99 (s, 1H), 7.01 – 8.01 (m, 12H);^{13}C NMR (75 MHz $CDCl_3$): δ 21.1, 21.5, 50.1, 53.6, 62.5, 88.2, 117.0, 119.8, 124.0, 125.3, 126.8, 126.8, 129.7,129.9, 131.1, 132.0, 136.6, 137.6, 138.8, 144.2, 150.6, 170.7; IR (neat): ν 1244, 1464, 1636 (medium), 1740 (strong) cm^{-1} ; HRMS (m/z) Calcd for $C_{26}H_{24}N_2O_5S$ $[M + H]^+$ 477.1362, Found 477.1478.

Methyl 3-(2-methoxyphenyl)-5-tosyl-3,3a,4,5-tetrahydro isoxazolo[4,3-c]quinoline-3a-carboxylate (5d): Colourless solid; Yield: 80%; mp 132-134 ºC; ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.39 (s, 3H), 2.81 (d, 1H, J = 12.9 Hz), 3.80 (s, 6H), 5.10 (d, 1H, J = 12.9 Hz), 6.51 (s, 1H), 7.09 – 8.05 (m, 12H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 21.5, 48.8, 53.6, 63.0, 85.8, 116.6, 120.0, 124.0, 126.3, 126.8, 127.5, 128.0, 129.9, 130.0, 130.1, 131.3, 131.4, 131.5, 132.9, 136.9, 137.5, 144.2, 150.9, 169.6; IR (neat):ν 1224, 1461, 1622 (medium), 1736 (strong) cm^{-1} ; HRMS (m/z) Calcd for $C_{26}H_{24}N_2O_6S$ $[M + H]^+$ 493.1433, Found; 493.1533.

Methyl 3-(4-methoxyphenyl)-5-tosyl-3,3a,4,5-tetrahydro isoxazolo[4,3-c]quinoline-3a-carboxylate (5e): Colourless solid; Yield: 84%; mp 140-142 ºC; ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.39 (s, 3H), 2.72 (d, 1H, J = 12.6 Hz), 3.78 (s, 3H), 3.80 (s, 3H), 4.72 (d, 1H, J = 12.9 Hz), 6.06 (s, 1H), 6.88 – 8.09 (m, 12H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 21.5, 50.1, 53.6, 55.3, 62.5, 88.1, 114.4, 117.1, 119.8, 124.0, 126.3, 126.7, 126.8, 127.1, 129.9, 131.2, 136.6, 137.6, 144.2, 150.6, 160.0, 170.7; IR (neat):ν 1287, 1513, 1613 (medium), 1740 (strong) cm^{-1} ; HRMS (m/z) Calcd for $C_{26}H_{24}N_2O_6S$ $[M + H]^+$ 493.1344, Found 493.1433.

Methyl 3-(2-chlorophenyl)-5-tosyl-3,3a,4,5-tetrahydro isoxazolo[4,3-c]quinoline-3a-carboxylate (5f): Colourless solid; Yield: 78%; mp 155-157 ºC; ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.39 (s, 3H), 2.81 (d, 1H, J = 12.9 Hz), 3.80 (s, 3H), 5.10 (d, 1H, J = 12.9 Hz), 6.51 (s, 1H), 7.09 – 8.08 (m, 12H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 21.5, 48.6, 53.6, 62.9, 85.8, 116.6, 120.0, 124.4, 126.8, 127.5, 128.0, 129.4, 129.9, 130.0, 130.1, 131.3, 131.4, 132.9.136.9, 137.5, 144.2, 150.7, 169.6; IR (neat): ν 1241, 1461, 1601 (medium), 1736 (strong) cm^{-1} ; HRMS (m/z) Calcd for $C_{25}H_{21}ClN_2O_5S$ $[M + H]^+$ 497.0816, Found 497.0932.

Methyl 3-(3-chlorophenyl)-5-tosyl-3,3a,4,5-tetrahydro isoxazolo[4,3-c]quinoline-3a-carboxylate (5g): Colourless solid; Yield: 82%; mp 160-162 ºC; ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.39 (s, 3H), 2.67 (d, 1H, J = 12.9 Hz), 3.79 (s, 3H), 4.72 (d, 1H. J = 12.9 Hz), 6.09 (s, 1H), 7.10 – 8.08 (m, 12H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 21.5, 50.1, 53.7, 62.6, 87.4, 116.8, 120.0, 124.2, 126.3, 126.7, 126.9, 126.9, 129.2, 129.3, 130.0, 131.3, 133.6, 134.9, 136.6, 137.5, 144.4, 150.7, 170.4; IR (neat):ν 1246, 1479, 1636 (medium), 1732 (strong) cm^{-1} ; HRMS (m/z) Calcd for $C_{25}H_{21}ClN_2OS$ $[M + H]^+$ 497.0812, Found 497.0930.

Methyl 3-(4-chlorophenyl)-5-tosyl-3,3a,4,5-tetrahydro isoxazolo[4,3-c]quinoline-3a-carboxylate (5h): Colourless solid; Yield: 85%; mp 159-161 ºC; ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.40 (s, 3H), 2.66 (d, 1H, J = 12.6 Hz), 3.80 (s, 3H), 4.72 (d, 1H, J = 12.9 Hz), 6.09 (s, 1H), 7.11 – 8.08 (m, 12H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 21.5, 50.1, 53.7, 62.6, 87.4, 116.8, 120.0, 124.2, 126.3, 126.7, 126.9, 129.3, 130.0, 131.3, 133.6, 134.9, 136.6, 137.6, 144.3, 150.7, 170.7; IR (neat): ν 1243, 1490, 1616 (medium), 1740 (strong) cm^{-1} ; HRMS (m/z) Calcd for $C_{25}H_{21}ClN_2O_5S$ $[M + H]^+$ 497.0924, Found 497.0932.

Methyl 3-(2,4-dichlorophenyl)-5-tosyl-3,3a,4,5-tetrahydro isoxazolo[4,3-c]quinoline-3a-carboxylate (5i): Colourless solid; Yield: 79%; mp 157-159 ºC; ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.40 (s, 3H), 2.81 (d, 1H, J = 12.9 Hz), 3.80 (s, 3H), 5.06 (d, 1H, J = 12.6 Hz), 6.46 (s, 1H), 7.10 – 8.07 (m, 11H); ^{13}C NMR (75 MHz, $CDCl_3$) : δ 21.6, 48.8, 53.7, 63.0, 85.4, 116.5, 120.1, 124.1, 126.3, 126.8, 127.9, 129.1, 129.8, 130.0, 131.5, 131.6, 132.1, 135.4, 137.0, 137.5, 144.3, 151.1, 169.5; IR (neat): ν 1244, 1463, 1636 (medium), 1737 (strong) cm^{-1} ; HRMS (m/z) Calcd for $C_{25}H_{20}Cl_2N_2O_5S$ $[M + H]^+$ 531.0436, Found 531.0549.

Methyl 3-(4-isopropylphenyl)-5-tosyl-3,3a,4,5-tetrahydro isoxazolo[4,3-c]quinoline-3a-carboxylate (5j): Colourless solid; Yield: 86%; mp 152-154 ºC; ^{1}H NMR (300 MHz, $CDCl_3$): δ 1.16 (d, 6H, J = 6.9 Hz), 2.31 (s, 3H), 2.83 (sep, 1H, J = 6.9 Hz), 2.61 (d, 1H, J

= 12.9 Hz), 3.71 (s, 3H), 4.68 (d, 1H, J = 12.9 Hz), 5.99 (s, 1H), 7.02 – 8.02 (m, 12H).^{13}C NMR (75 MHz $CDCl_3$): δ 21.5, 23.8, 23.9, 33.8, 50.1, 53.6, 62.5, 88.3, 117.0, 119.7, 124.0, 125.4, 126.3, 126.8, 127.0, 129.9, 131.1, 132.3, 136.6, 137.4, 144.2, 149.7, 150.63, 170.7; IR (neat): ν 1260, 1461, 1606 (medium), 1742 (strong) cm^{-1} ; HRMS (m/z) Calcd for $C_{28}H_{28}N_2O_5S$ $[M + H]^+$ 505.1674, Found 505.1795.

Methyl 3-(4-fluorophenyl)-5-tosyl-3,3a,4,5-tetrahydro isoxazolo[4,3-c]quinoline-3a-carboxylate (5k): Colourless solid; Yield: 81%; mp 139-141 ºC; ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.39 (s, 3H), 2.66 (d, 1H, J = 12.6 Hz), 3.79 (s, 3H), 4.72 (d, 1H, J = 12.9 Hz), 6.09 (s, 1H), 7.05 – 8.08 (m, 12H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 21.5, 50.1, 53.7, 62.6, 87.5, 115.9, 116.2, 116.8, 119.9, 124.1, 126.3, 126.7, 127.3, 127.4, 130.0, 130.9, 131.2, 136.6, 137.5, 144.4, 150.7, 170.5; IR (neat): ν 1240, 1508, 1603 (medium), 1746 (strong) cm^{-1} ; HRMS (m/z) Calcd for $C_{25}H_{21}FN_2O_5S$ $[M + H]^+$ 481.1124, Found 481.1235.

Methyl 3-(naphthalen-2-yl)-5-tosyl-3,3a,4,5-tetrahydro isoxazolo[4,3-c]quinoline-3a-carboxylate (5l): Colourless solid; Yield: 84%; mp 155-157 ºC; ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.34 (s, 3H), 2.62 (d, 1H, J = 12.9 Hz), 3.87 (s, 3H), 4.69 (d, 1H, J = 12.9 Hz), 6.96 (s, 1H), 7.11 – 7.93 (m, 15H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 21.4, 50.2, 53.8, 63.3, 86.2, 117.4, 120.2, 122.5, 124.0, 124.2, 125.5, 126.2, 126.0, 126.5, 127.4, 129.0, 129.2, 129.7, 129.8, 130.2, 131.0, 133.6, 136.9, 137.6, 144.1, 150.6, 171.1; IR (neat): ν 1240, 1486, 1600 (medium), 1738 (strong) cm^{-1} ; HRMS (m/z) Calcd for $C_{29}H_{24}N_2O_5S$ $[M + H]^+$ 513.1370, Found 513.1488.

Methyl 3-(3,4-dimethoxyphenyl)-5-tosyl-3,3a,4,5-tetrahydro isoxazolo[4,3-c]quinoline-3a-carboxylate (5m): Colourless solid; Yield: 79%; mp 156-158 ºC; ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.39 (s, 3H), 2.73 (d, 1H, J = 12.9 Hz), 3.79 (s, 3H), 3.87 (d, 6H, J = 4.8 Hz), 4. 73 (d, 1H, J = 12.9 Hz), 6.06 (s, 1H), 6.75 – 8.08 (m, 11H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 20.5, 28.6, 49.1, 52.6, 54.9, 55.1, 61.5, 87.1, 107.3, 110.5, 116.0, 116.8, 118.9, 123.0, 125.2, 127.7, 126.5, 129.0, 130.1, 135.6, 136.6, 143.3, 148.4, 149.7, 169.7; IR (neat):ν 1237, 1512, 1623 (medium), 1737 (strong) cm^{-1} ; HRMS (m/z) Calcd for $C_{27}H_{26}N_2O_7S$ $[M + H]^+$ 523.1422, Found 523.1534.

Methyl 3-(4-ethylphenyl)-5-tosyl-3,3a,4,5-tetrahydro isoxazolo[4,3-c]quinoline-3a-carboxylate (5n): Colourless solid; Yield: 74%; mp 163-165 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 1.24 (t, 3H, J = 7.5 Hz), 2.38 (s, 3H), 2.67 (q, 3H, J = 7.5 Hz), 3.78 (s, 3H), 4.75 (d, 1H, J = 12.9 Hz), 6.07 (s, 1H), 7.11 – 8.09 (m, 12H); ^{13}CNMR (75 MHz, $CDCl_3$): δ 15.4, 21.5, 28.5, 50.1, 53.6, 62.5, 88.3, 117.0,

119.8, 122.4, 124.0, 125.4, 126.3, 126.8, 128.5, 129.9, 131.1, 132.2, 136.6, 137.5, 144.2, 145.1, 170.7; IR (KBr): ν 1245, 1486, 1606 (medium), 1737 (strong) cm^{-1} ; HRMS (m/z) Calcd for $C_{27}H_{26}N_2O_5S$ $[M + H]^+$491.1523, Found 491.1639.

Typical experimental procedure for the synthesis of (Z)-N-(2-cyano-3-phenylallyl)-N-(2-formylphenyl)-4-methylbenzenesulfonamide (7a): A solution of N-Ts aminobenzaldehyde (**1**) (1 mmol, 0.28g) and potassium carbonate (2 mmol, 0.29 g) in acetonitrile solvent was stirred for 15 min at room temperature. To this solution, (E)-2-(bromomethyl)-3-arylacrylonitrile (**6a**) (1.2 mmol, 0.27 g) was added drop wise till the addition is complete. After the completion of the reaction as indicated by TLC, the reaction mixture was concentrated and extracted with ethylacetate (2x15 mL). The organic layer thus obtained was washed with water (2x10 mL), followed by brine solution (2x 10 mL) and dried over anhydrous sodium sulphate. Then the crude sample was purified by a pad of silica gel (100-200 mesh) column chromatography using ethylacetate and Hexane (1:9) to afford the pure product (**7a**) as a colourless solid (0.38 g, 92% yield).

(Z)-N-(2-cyano-3-phenylallyl)-N-(2-formylphenyl)-4-methylbenzenesulfonamide (7a):

Colorless solid; Yield:92%; mp:126-128°C; 1H NMR (300 MHz, CDCl3): δ 2.44 (s, 3H), 4.27 (d, 1H, J = 14.4Hz), 4.82 (d, 1H, J = 13.8Hz), 6.85–8.03 (m, 14H), 10.46 (s, 1H); 13C NMR (CDCl3, 75 MHz): δ 21.7, 55.8, 105.5, 117.5, 128.1, 128.3, 128.9, 129, 129.3, 129.4, 129.9, 131.2, 132.4, 134, 134.3, 135.9, 140.3, 144.8, 147.9, 189,6; MS (m/z):417 (M^++1).

(2Z)-2-{[N-(2-Formylphenyl)(4-methylbenzene)sulfonamido]methyl}-3-(2-chlorophenyl) prop-2-enenitrile (7b):

Colorless solid; Yield :92%; mp: 134-136°C; ^{1}H NMR (300 MHz, $CDCl_3$) : δ 2.46 (s, 3H), 4.30 (d, 1H, J = 13.1 Hz), 4.87 (d, 1H, J = 13.8 Hz), 6.86–8.03 (m, 13H), 10.46 (s, 1H); ^{13}C NMR ($CDCl_3$, 75 MHz) : δ 21.7, 55.3, 109.1, 116.6, 127.3, 128.1, 129.2, 129.3, 129.5, 129.8, 129.9, 130.8, 131.9, 133.9, 134.2, 134.3, 135.9, 140.1, 144.5, 144.8, 189.5; MS (m/z): 452 (M^++1).

(2Z)-2-{[N-(2-Formylphenyl)(4-methylbenzene)sulfonamido]methyl}-3-(4-chlorophenyl) prop-2-enenitrile (7c):

Colorless solid; Yield: 92%; mp: 131-133°C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.45 (s, 3H), 4.30 (d, 1H, J = 13.1 Hz), 4.87 (d, 1H, J = 13.8 Hz), 6.86–8.03 (m, 13H), 10.42 (s, 1H); ^{13}C NMR ($CDCl_3$, 75 MHz): δ 21.7, 55.8, 106.3, 117.2, 128, 128.4, 129.3, 129.3, 129.5, 129.9, 130.3, 130.8, 133.9, 134.4, 135.8, 137.2, 140.3, 144.9, 146.3, 189.5; MS (m/z) :452 (M^++1).

(2Z)-3-(2H-1,3-Benzodioxol-5-yl)-2-{[N-(2-formylphenyl)(4-methylbenzene)sulfonamido] methyl}prop-2-enenitrile (7d):

Colorless solid; Yield :92%; mp:136-138°C; ^{1}HNMR (300 MHz, $CDCl_3$) : δ 2.45 (s, 3H), 4.24 (d, 1H, J = 13.5 Hz), 4.77 (d, 1H, J = 13.5 Hz), 5.99 (s, 2H), 6.75-8.00 (m, 12H), 10.40 (s, 1H);^{13}C NMR ($CDCl_3$, 75 MHz): δ 21.7, 55.9, 101.8, 102.5, 107.8, 108.6, 117.8, 125.9, 126.6, 127.3, 128, 128.4, 129.3, 129.4, 129.8, 134.2, 135.9, 140.3, 144.7, 147.5, 148.3, 150.3, 189.6; MS (m/z) : 462 (M^++1).

(Z)-N-(2-cyano-3-(2,4-dichlorophenyl)allyl)-N-(2-formylphenyl)-4-methylbenzenesulfonamide (7e):

Colorless solid; Yield:92%; mp:126-132°C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.46 (s, 3H), 4.30 (d, 1H, J = 14.4Hz), 4.80 (d, 1H, J = 14.7Hz), 6.87–8.01 (m, 12H), 10.42 (s, 1H);^{13}C NMR ($CDCl_3$, 75 MHz): δ 21.7, 55.8, 106.2, 117.2, 125.6, 127.4, 128, 128.4, 129.1, 129.3, 129.4, 129.5, 129.7, 129. 9, 130.3, 130.8, 130.9, 134.4, 135.8, 137.2, 140.3. 144.9, 146.3, 189.6; MS (m/z): 483 (M^++1).

((Z)-N-(2-cyano-3-(4-isopropylphenyl)allyl)-N-(2-formylphenyl)-4-methylbenzenesulfonamide(7f):

Colorless solid; Yield: 88%; mp:132-136 ºC ^{1}H NMR ($CDCl_3$, 300 MHz,): δ 1.29 (s, 6H), 2.46 (s, 3H), 2.42 (sep, J = 6.3 Hz, 1H), 4.27 (d, 1H, J = 14.1Hz), 4.84 (d, 1H, J = 13.8Hz), 6.86 - 8.01 (m, 13H), 10.45 (s, 1H).^{13}C NMR ($CDCl_3$, 75 MHz): δ 21.7, 23.7, 23.8, 34.1, 55.8, 103.9, 117.7, 127.1, 128.1, 128.3, 129.3, 129.3, 129.6, 129.8, 129.9, 129.9, 134.1, 134.3, 135.9, 140.3, 144.7, 147.9, 152.7, 189.6; MS (m/z); 457 (M^++1).

(2Z)-2-{[N-(2-Formylphenyl)(4-methylbenzene)sulfonamido]methyl}-3-(2-methylphenyl) prop-2-enenitrile (7g):

Colorless solid; Yield: 92%; mp:121-123°C; ^{1}H NMR (300 MHz, $CDCl_3$) : δ 2.06 (s, 3H), 2.46 (s, 3H), 4.30 (s, 1H), 4.88 (d, 1H, J = 11.7 Hz), 6.87–8.03 (m, 13H), 10.49 (s, 1H); ^{13}C NMR ($CDCl_3$, 75 MHz) : δ 19.5, 21.7, 55.4, 107.7, 117.1, 126.4, 127.8, 128.1, 129.2, 129.3, 129.9, 130.5, 130.7, 131.8, 133.8, 134.3, 136, 137.1, 140.2, 144.9, 147.3, 189.6; MS (m/z); 432 (M^++1).

(2Z)-2-{[N-(2-formylphenyl)(4-methylbenzene)sulfonamido]methyl}-3-(3-chlorophenyl) prop-2-enenitrile (7h):

Colorless solid; Yield: 92%; mp: 124-228°C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.45 (s, 3H), 4.29 (d, 1H, J = 14.1Hz), 4.81 (d, 1H, J = 14.1Hz), 6.87–8.01 (m, 13H), 10.43 (s, 1H); ^{13}C NMR (CDCl3, 75 MHz): δ 21.7, 55.8, 105.5, 117.5, 127.3, 128.1, 128.4, 128.9, 129, 129.3, 129.5, 129.9, 131.2, 132.3, 134.1, 134.3, 135.8, 140.3, 144.8, 147.9, 189.6; MS (m/z); 452 (M^++1).

(2Z)-2-{[N-(2-Formylphenyl)(4-methylbenzene)sulfonamido]methyl}-3-(3,4-dimethoxyphenyl)prop-2-enenitrile (7i):

Colorless; solid; Yield: 92%; mp: 139-141°C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.45 (s, 3H), 3.86 (s, 3H), 3.88 (s, 3H), 4.23 (d, 1H, J = 14.4 Hz), 4.83 (d, 1H, J = 13.1 Hz), 6.80–8.01 (m, 12H), 10.47 (s, 1H); ^{13}C NMR ($CDCl_3$, 75 MHz) : δ 21.6, 55.9, 55.9, 55.9, 60.9, 101.9, 110.5, 110.8, 118.2, 124.4, 125.3, 128, 128.2, 129.2, 129.8, 129.9, 134.1, 134.3, 135.9, 140.4, 144.7, 147.8, 149, 151.7, 189.7; MS (m/z): 478 (M^++1).

Representative procedure for the synthesis of 3-Phenyl-5-tosyl-3,3a,4,5-tetrahydroisoxazolo[4,3-c]quinoline-3a-carbonitrile (9a):

To a solution of 2 mmol of N-allylated derivative (**7a**) in ethanol, $NH_2OH.HCl$ (6 mmol) was added and stirred well at room temperature for 1 h. After the completion of the reaction as evidenced by the tlc, ethanol was removed under reduced pressure and the crude thus obtained was further treated with 10 mL CCl_4 and NCS (5 mmol) and Et_3N (4 mmol) and the reaction mixture and stirred well at room temperature for 1 h. After completion of the reaction, reaction mixture was evaporated under reduced pressure and the resulting crude mass was diluted with water (15 mL) and extracted with ethyl acetate (3 × 15 mL). The combined organic layer was washed with brine (2 × 10 mL) and dried over anhydrous Na_2SO_4. The organic layer was evaporated and the crude mass was purified by column chromatography (silica gel 60-120 mesh 5% EtOAc in hexanes) to provide the desired pure product **9a (**0.29 g, 67% yield).

3-Phenyl-5-tosyl-3,3a,4,5-tetrahydroisoxazolo[4,3-c]quinoline-3a-carbonitrile(9a):

Colourless solid; Yield: 67%; mp 136 - 138 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.38, (s, 3H), 3.90 (d, 1H, J = 12.6 Hz), 5.30 (d, 1H, J = 12.9 Hz), 5.49 (s, 1H), 7.12 – 7.95 (m, 13H); ^{13}CNMR (75 MHz, $CDCl_3$): δ 21.6, 51.0, 54.2, 89.4, 113.8, 114.0, 119.7, 124.5, 126.7, 126.8, 128.8, 129.1, 130.2, 131.5, 132.7, 135.5, 136.7, 145.5, 151.6; IR (KBr): ν1262, 1444, 1603, 2837 (medium) cm^{-1} ; HRMS (m/z) Calcd for $C_{24}H_{19}N_3O_3S$ $[M + H]^+$ 430.1168, Found 430.1203.

3-(2-Chlorophenyl)-5-tosyl-3,3a,4,5-tetrahydroisoxazolo[4,3-c]quinoline-3a-carbonitrile (9b):

Colourless solid; Yield: 64%; mp 160-162 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.32 (s, 3H), 2.76 (d, 1H, J = 13.2 Hz), 5.10 (d, 1H, J = 12.9 Hz), 6.49 (s, 1H), 7.02 – 7.93 (m, 12H); ^{13}CNMR (75 MHz, $CDCl_3$): δ 21.6, 43.7, 48.5, 50.9, 86.3, 113.7, 116.6, 119.4, 124.2, 127.1, 127.8, 128.1, 129.9, 130.9, 131.1, 131.4, 131.1, 132.4, 135.7, 136.5, 145.0, 148.0; IR (KBr): ν 1261, 1523, 1633, 2057 (medium) cm^{-1}; HRMS (m/z) Calcd for $C_{24}H_{18}ClN_3O_3S$ $[M + H]^+$ 464.0767, Found 464.0842.

3-(4-Chlorophenyl)-5-tosyl-3,3a,4,5-tetrahydroisoxazolo[4,3-c]quinoline-3a-carbonitrile (9c):

Colourless solid; Yield: 66%; mp 158-160°C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.31 (s, 3H), 3.81 (d, 1H, J = 12.9 Hz), 5.21 (d, 1H, J = 12.6 Hz), 5.40 (s, 1H), 7.05 – 7.98 (m, 12H); ^{13}CNMR (75 MHz, $CDCl_3$): δ 20.5, 28.6, 49.9, 53.2, 87.6, 112.6, 112.9, 118.7, 123.6, 125.8, 127.0, 127.2, 128.4, 128.9, 131.8, 134.5, 135.3, 135.7, 144.2, 150.6; IR (KBr): ν 1284, 1491, 1636, 2925 (medium) cm^{-1} ; HRMS (m/z) Calcd for $C_{24}H_{18}ClN_3O_3S$ $[M + H]^+$ 464.0756, Found 464.0833.

3-(Benzo[d][1,3]dioxol-5-yl)-5-tosyl-3,3a,4,5-tetrahydroisoxazolo[4,3-c]quinoline-3a-carbonitrile (9d): Colourless solid; Yield: 61%; mp 175-177 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.39 (s, 3H), 3.84 (d, 1H, J = 12.9 Hz), 5.27 (d, 1H, J = 12.9 Hz), 5.40 (s, 1H), 6.05 (s, 2H), 6.90 – 7.96 (m, 11H); ^{13}CNMR (75 MHz, $CDCl_3$): δ 21.6, 51.0, 54.0, 57.2, 89.3, 101.6, 107.2, 108.7, 113.8, 119.7, 121.0, 124.5, 124.8, 126.7, 128.1, 129.9, 132.7, 135.5, 136.7, 145.1, 148.3, 149.2, 151.6; IR (KBr): ν 1024, 1362, 1605, 2830 (medium)cm^{-1} ; HRMS (m/z) Calcd for $C_{25}H_{19}N_3O_5S$ $[M + H]^+$ 474.1045, Found 474.1125.

3-(2,4-dichlorophenyl)-5-tosyl-3,3a,4,5-tetrahydroisoxazolo[4,3-c]quinoline-3a-carbonitrile (9e): Colourless solid; Yield: 63%; mp 152-154 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.38 (d, 3H), 3.87 (d, 1H, J = 12.9 Hz), 5.28 (d, 1H, J = 12.9 Hz), 5.46 (s, 1H), 7.11 – 7.96 (m, 11H); ^{13}CNMR (75 MHz, $CDCl_3$): δ 15.3, 21.6, 28.7, 51.0, 54.1, 89.5, 113.9, 114.2, 119.7, 124.5, 126.7, 126.9, 128.0, 128.5, 128.6, 129.9, 132.6, 135.6, 136.7, 145.1, 146.5, 151.6; IR (KBr): ν 1286, 1462, 1604, 2963 (medium) cm^{-1} ; HRMS (m/z) Calcd for $C_{24}H_{17}Cl_2N_3O_3S$ $[M + H]^+$ 498.0346, Found 498.0460.

3-(4-Isopropylphenyl)-5-tosyl-3,3a,4,5-tetrahydroisoxazolo[4,3-c]quinoline-3a-carbonitrile (9f): Colourless solid; Yield: 66%; mp 183-185 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 1.30 (d, 6H, J = 15.0 Hz), 2.38 (s, 3H), 2.83 (sep, 1H, J = 6.6 Hz), 3.87 (d, 1H, J =

11.7 Hz), 5.26 (d, 1H, J = 9.9 Hz), 5.40 (s, 1H), 7.13 – 7.96 (m, 12H); ^{13}CNMR (75 MHz, $CDCl_3$): δ 21.6, 23.8, 23.9, 34.0, 51.0, 54.0, 89.5, 113.9, 114.2, 119.7, 124.5, 126.7, 127.0, 128.5, 129.9, 132.6, 135.6, 136.7, 145.1, 151.6; IR (KBr): ν 1269, 1463, 1637, 2398 (medium) cm^{-1} ; HRMS (m/z) Calcd for $C_{27}H_{25}N_3O_3S$ $[M + H]^+$ 472.1578, Found 472.1694.

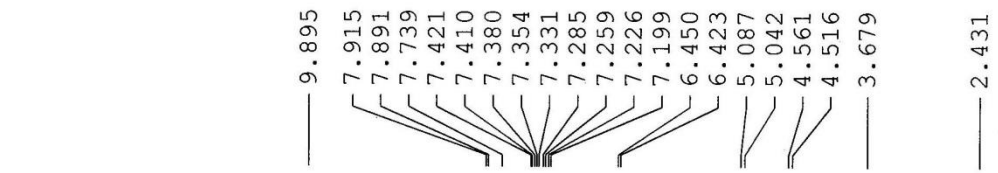
3-o-Tolyl-5-tosyl-3,3a,4,5-tetrahydroisoxazolo[4,3-c]quinoline-3a-carbonitrile (9g):

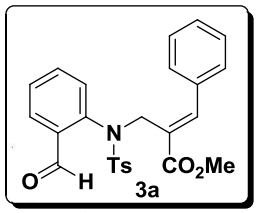
Colourless solid; Yield: 65%; mp 190-192 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.30 (s, 3H), 2.31 (s, 3H), 3.85 (d, 1H, J = 12.6 Hz), 5.28 (d, 1H, J = 12.9 Hz), 5.75 (s, 1H), 7.03 – 7.8 (m, 12H); ^{13}CMR (75 MHz, $CDCl_3$): δ 14.1, 19.7, 21.6, 29.7, 51.1, 54.3, 86.5, 113.8, 119.6, 124.5, 126.7, 127.5, 128.1, 129.7, 130.9, 132.6, 135.4, 135.5, 136.5, 145.1, 151.1; IR (KBr): ν 1287, 1489, 1633, 2852 (medium) cm^{-1} ; HRMS (m/z) Calcd for $C_{25}H_{21}N_3O_3S$ $[M + H]^+$ 444.1254, Found 444.1379.

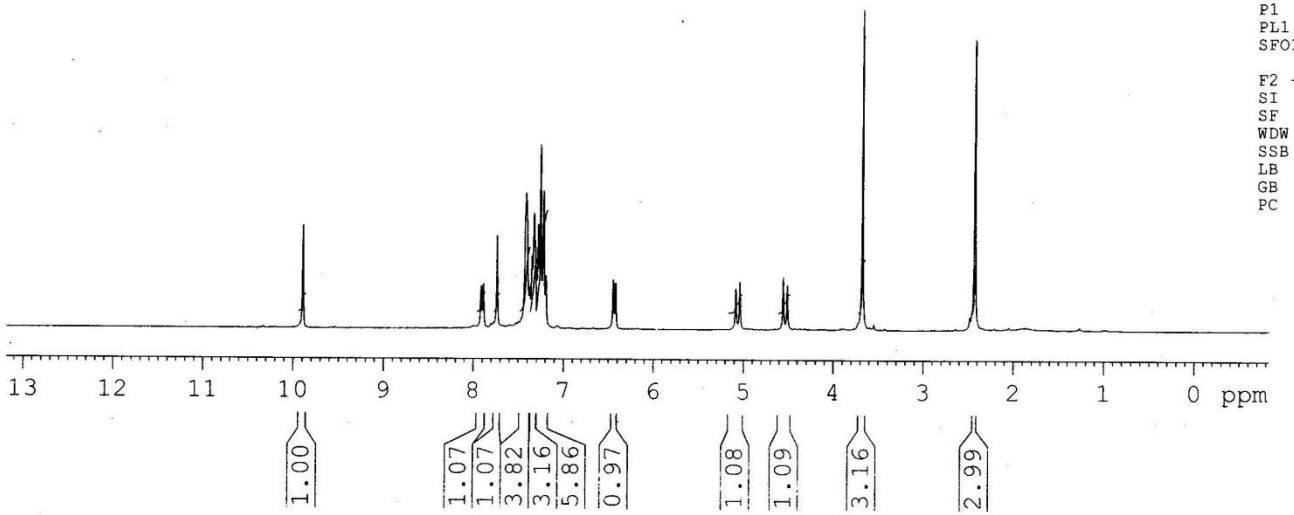
3-(3-Chlorophenyl)-5-tosyl-3,3a,4,5-tetrahydroisoxazolo[4,3-c]quinoline-3a-carbonitrile (9h):

Colourless solid; Yield: 67%; mp 155-157 °C; 1H NMR (300 MHz, CDCl3): δ 2.30 (s, 3H), 3.83 (d, 1H, J = 5.1 Hz), 5.23 (d, 1H, J = 5.1 Hz), 5.43 (s, 1H), 7.02 – 7.86 (m, 12H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 21.6, 28.6, 50.0, 53.2, 88.3, 112.8, 118.7, 123.5, 125.8, 127.0, 128.1, 128.8, 128.9, 129.2, 130.6, 130.5, 131.7, 134.5, 135.7, 144.1, 150.6; IR (KBr): ν 1260, 1521, 1635, 2923 (medium) cm^{-1} ; HRMS (m/z) Calcd for $C_{24}H_{18}ClN_3O_3S$ $[M + H]^+$ 464.0746, Found 464.0829.

3-(3,4-Dimethoxyphenyl)-5-tosyl-3,3a,4,5-tetrahydroisoxazolo[4,3-c]quinoline-3a-carbonitrile (9i): Colourless solid; Yield: 62%; mp 180-182 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.33 (s, 3H), 3.94 (d, 1H, J = 21.6 Hz), 3.95 (s, 6H), 5.54 (d, 1H, J = 13.2 Hz), 5.95 (s, 1H), 7.10 – 7.97 (m, 11H); ^{13}CNMR (75 MHz, $CDCl_3$): δ 21.5, 51.4, 54.5, 56.3, 88.2, 111.5, 112.9, 113.7, 114.1, 115.4, 119.8, 122.9, 124.5, 126.6, 128.0, 129.9, 132.7, 135.8, 136.8, 145.0, 148.9, 150.8, 151.6; IR (KBr): ν 1268, 1461, 1637, 2925 (medium) cm^{-1} ; HRMS (m/z) Calcd for $C_{26}H_{23}N_3O_5S$ $[M + H]^+$ 490.1324, Found 490.1431.







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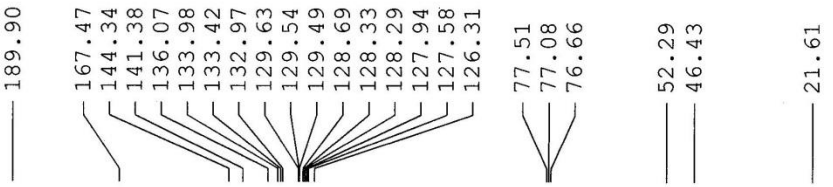
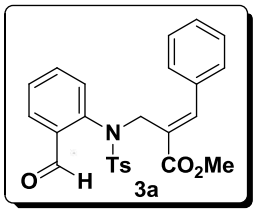
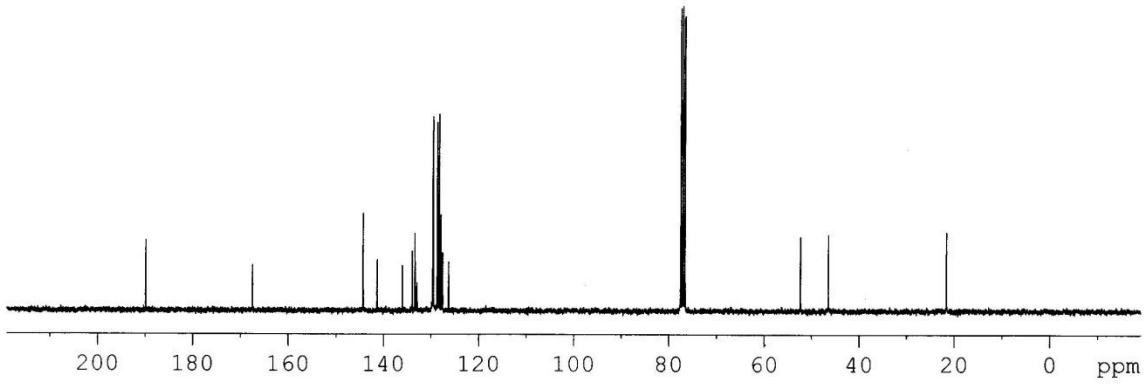
AQ 5.3084660 sec
RG 64
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 13.15 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

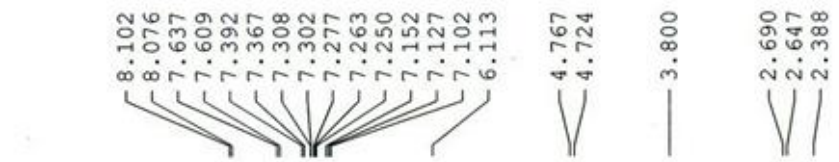


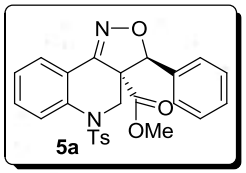




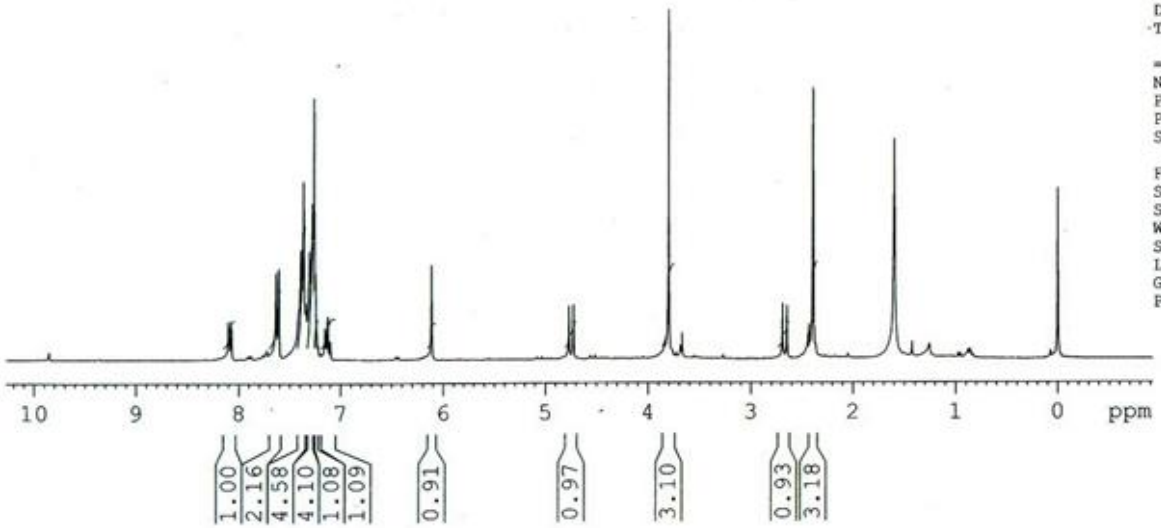
BRUKER

```
Current Data Parameters
NAME      DK-V-N-Ts-H-EST
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_            20110910
Time                16.24
INSTRUM             spect
PROBHD   5 mm DUL 13C-1
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   230
DS                     4
SWH          17985.611 Hz
FIDRES         0.274439 Hz
AQ             1.8219508 sec
RG                5792.6
DW                27.800 usec
DE                 6.00 usec
TE                300.0 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                 9.30 usec
PL1                0.00 dB
SFO1         75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             80.00 usec
PL2                0.00 dB
PL12              15.68 dB
PL13              16.00 dB
SFO2        300.1312005 MHz

F2 - Processing parameters
SI                 32768
SF          75.4677490 MHz
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                 1.40
```



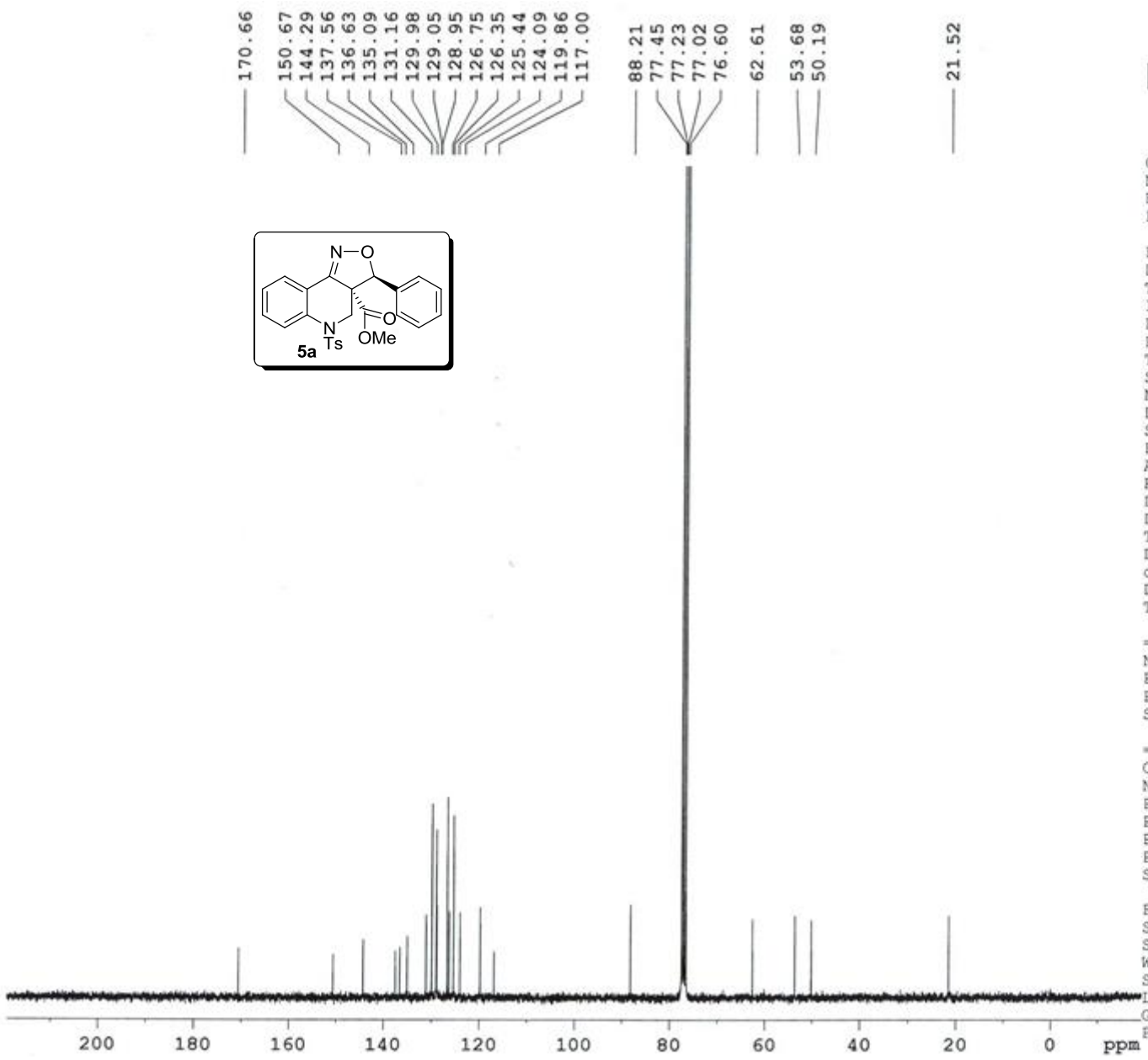


5a



BRUKER

```
Current Data Parameters
NAME                  VV-27F
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20120825
Time                  11.14
INSTRUM               spect
PROBHD   5 mm DUL 13C-1
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                        8
DS                        2
SWH               6172.839 Hz
FIDRES            0.094190 Hz
AQ                5.3084660 sec
RG                    322.5
DW                 81.000 usec
DE                  6.00 usec
TE                  300.0 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                 13.15 usec
PL1                 0.00 dB
SFO1          300.1318534 MHz

F2 - Processing parameters
SI                    32768
SF            300.1300055 MHz
WDW                      EM
SSB                       0
LB                 0.30 Hz
GB                        0
PC                     1.00
```



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Current Data Parameters
NAME vv-27
EXPNO 2
PROCNO 1

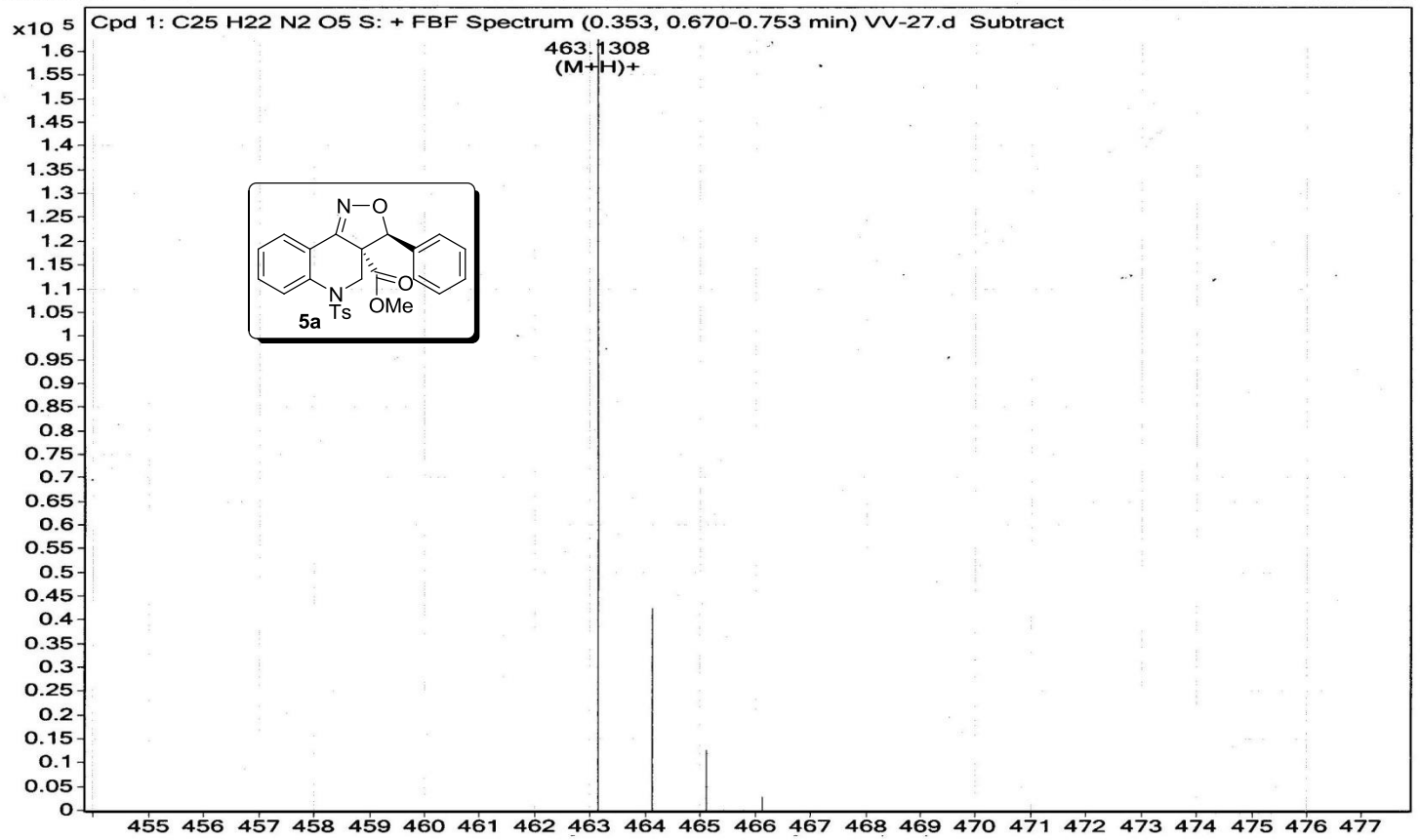
F2 - Acquisition Parameters
Date_ 20130730
Time 20.39
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 825
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 574.7
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

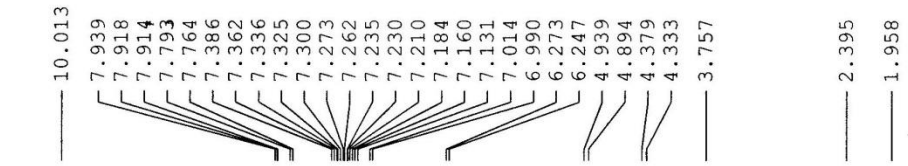
======== CHANNEL f1 ========
NUC1 13C
P1 9.30 usec
PL1 0.00 dB
SFO1 75.4752953 MHz

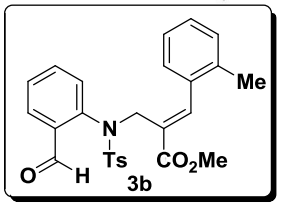
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.68 dB
PL13 16.00 dB
SFO2 300.1312005 MHz

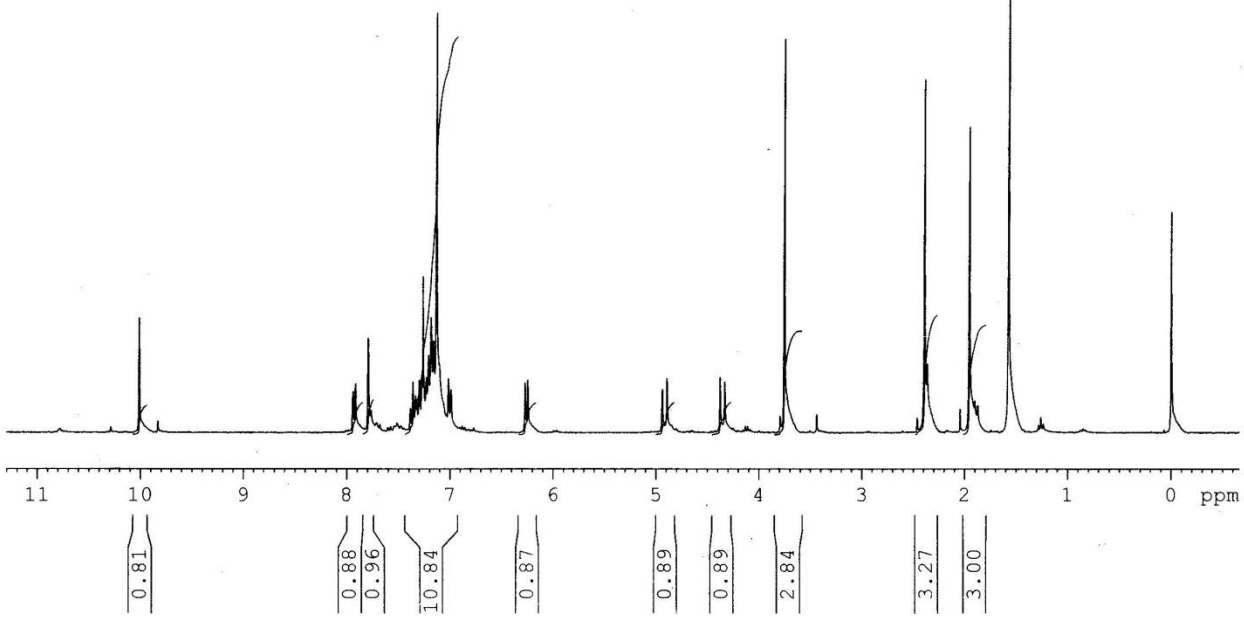
F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Sample Name	VV-27	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	VV-27.d	**ACQ Method**	Pondicherry Universi	**Comment**	MM-MB-462.1249	**Acquired Time**	18-11-2014 15:05:37







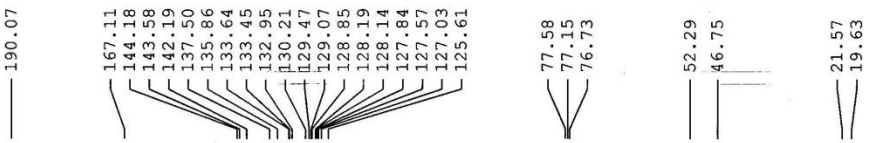


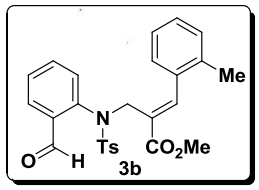
Current Data Parameters
NAME DK-V-77
EXPNO 1
PROCNO 1

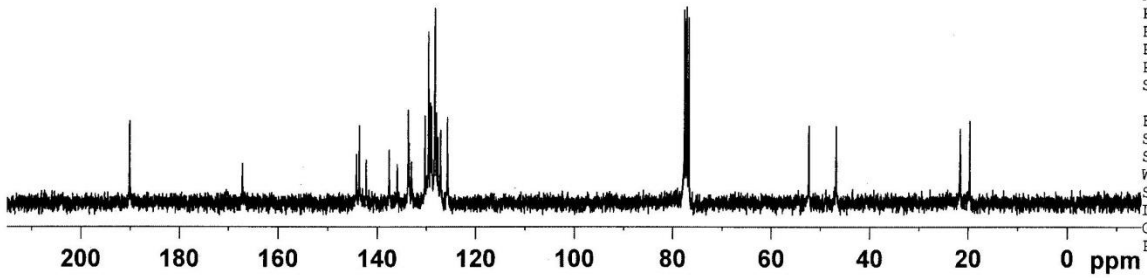
F2 - Acquisition Parameters
Date_ 20100701
Time 18.02
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 456.1
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 13.15 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300060 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00







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```
Current Data Parameters
NAME      DK-V-2-Me-Est-CHO
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_             20100914
Time                 13.50
INSTRUM              spect
PROBHD   5 mm DUL 13C-1
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                    111
DS                      4
SWH             17985.611 Hz
FIDRES              0.274439 Hz
AQ                1.8219508 sec
RG                    512
DW                  27.800 usec
DE                   6.00 usec
TE                  300.0 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   13C
P1                    7.40 usec
PL1                  -2.00 dB
SFO1           75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                   1H
PCPD2                80.00 usec
PL2                   0.00 dB
PL12                 15.68 dB
PL13                 16.00 dB
SFO2          300.1312005 MHz

F2 - Processing parameters
SI                    32768
SF             75.4677490 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```

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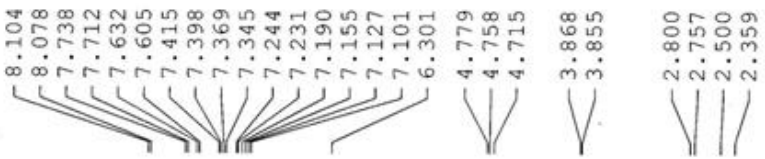
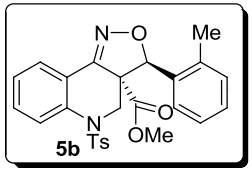
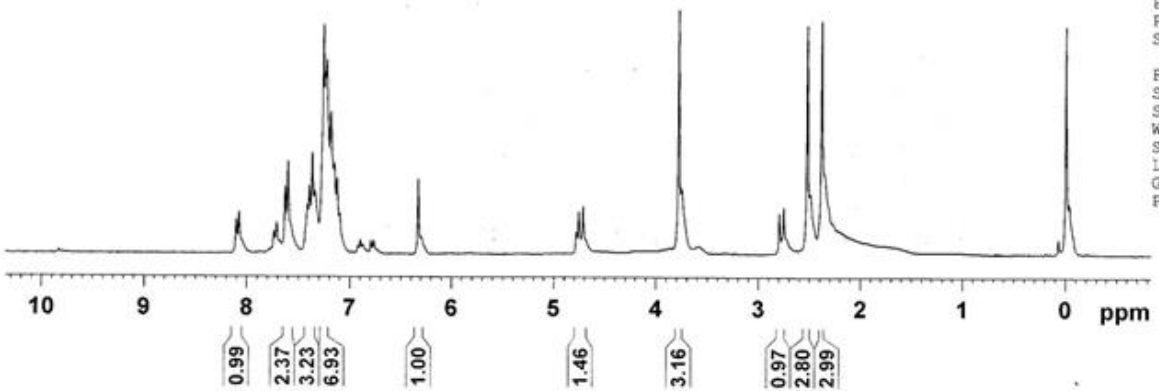






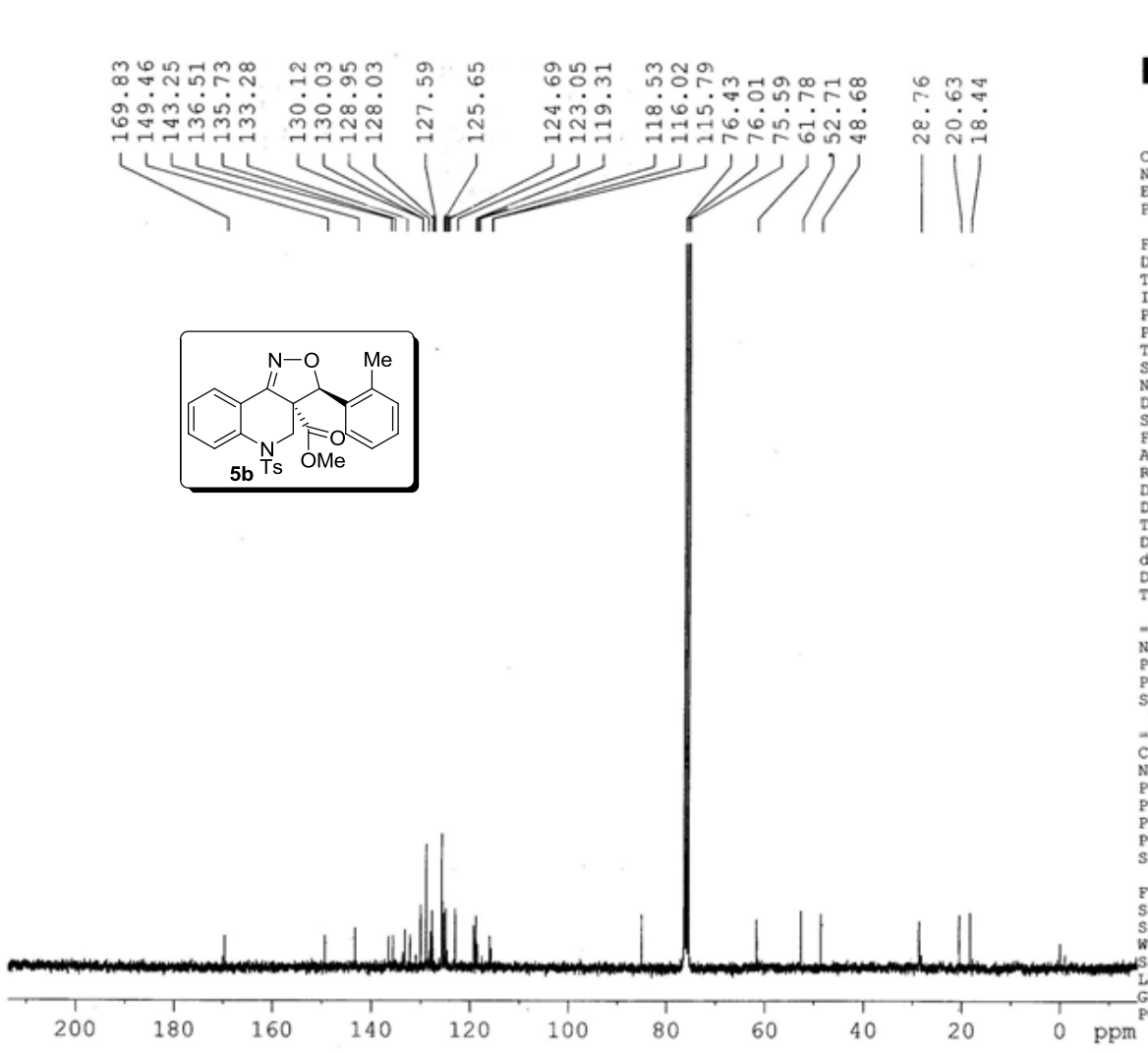
BRUKER

```
Current Data Parameters
NAME                  VV-55F
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20150422
Time                  12.21
INSTRUM               spect
PROBHD   5 mm DUL 13C-1
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                6172.839 Hz
FIDRES            0.094190 Hz
AQ                5.3084660 sec
RG                    203.2
DW                   81.000 usec
DE                    6.00 usec
TE                   300.0 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                    13.15 usec
PL1                    0.00 dB
SFO1          300.1318534 MHz

F2 - Processing parameters
SI                    32768
SF            300.1300082 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```



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Current Data Parameters

NAME	VV-55-F
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20130307
Time	17.56
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	17985.611 Hz
FIDRES	0.274439 Hz
AQ	1.8219508 sec
RG	574.7
DW	27.800 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1

======== CHANNEL f1 ========

NUC1	13C
P1	9.30 usec
PL1	0.00 dB
SFO1	75.4752953 MHz

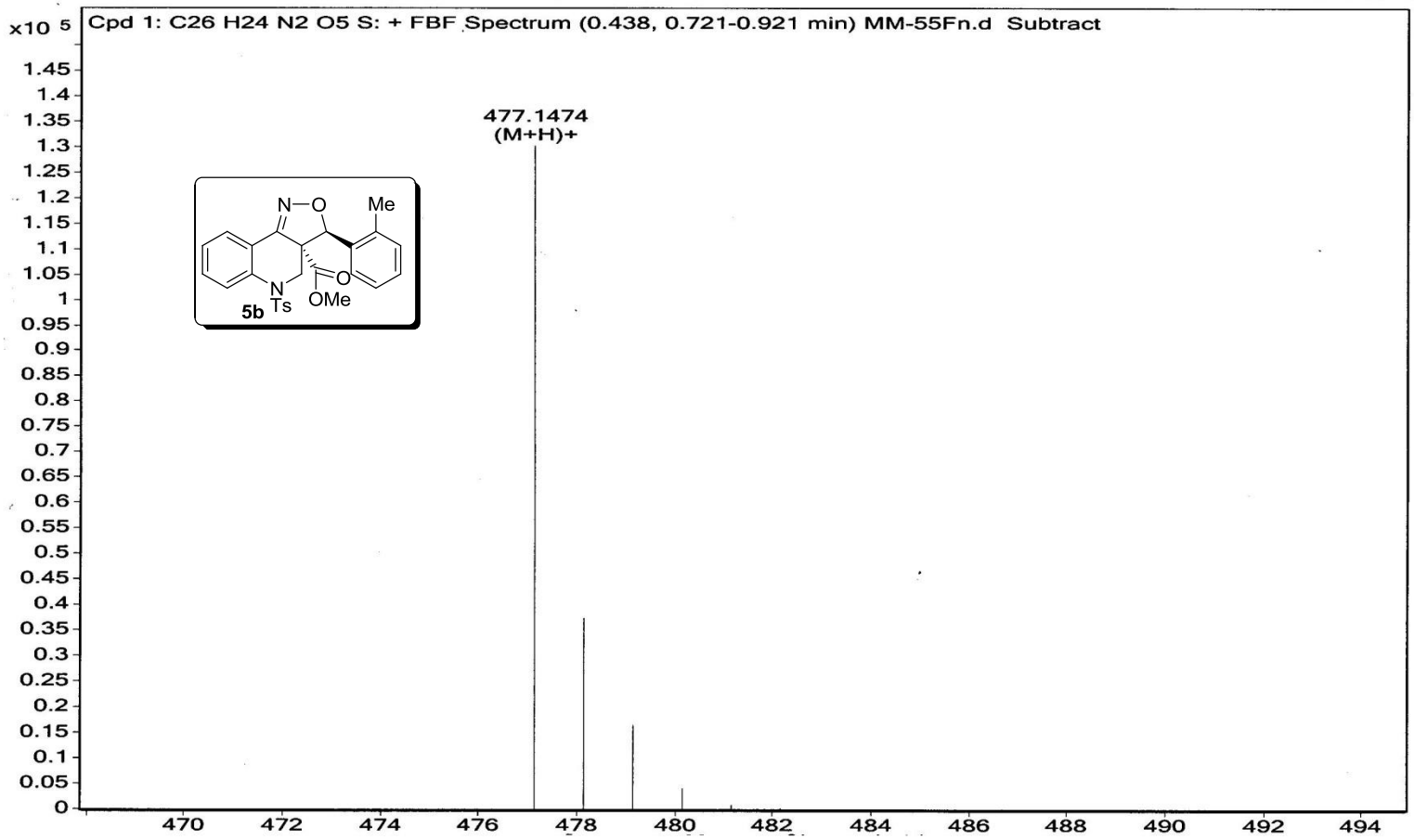
======== CHANNEL f2 ========

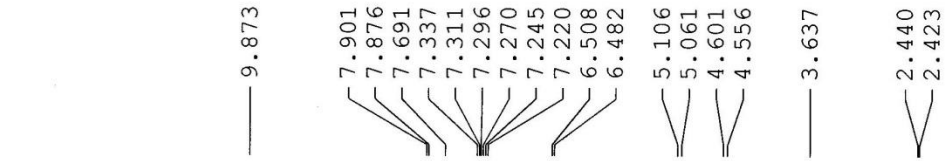
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.00 dB
PL12	15.68 dB
PL13	16.00 dB
SFO2	300.1312005 MHz

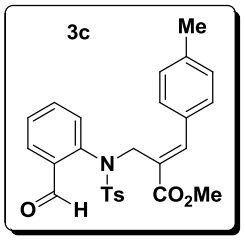
F2 - Processing parameters

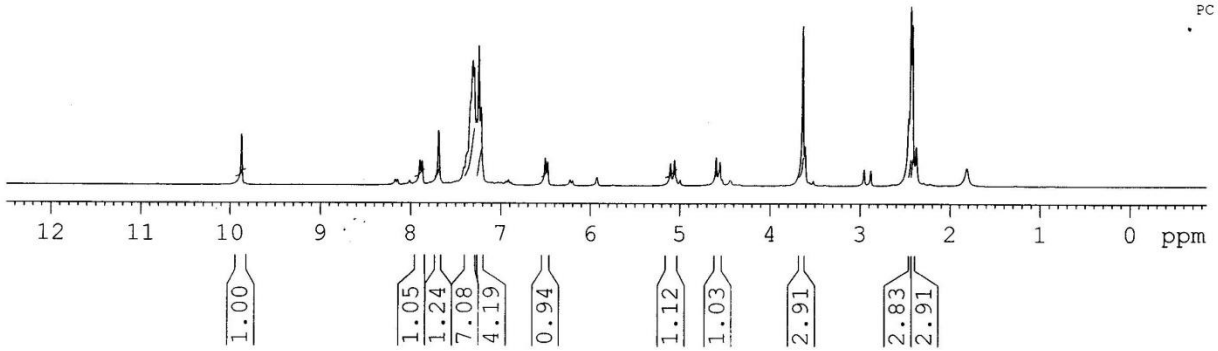
SI	32768
SF	75.4678253 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

Sample Name	MM-55F	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	MM-55Fn.d	**ACQ Method**	Pondicherry Universi	**Comment**	MSK-MB-476.1406	**Acquired Time**	05-06-2015 12:58:29







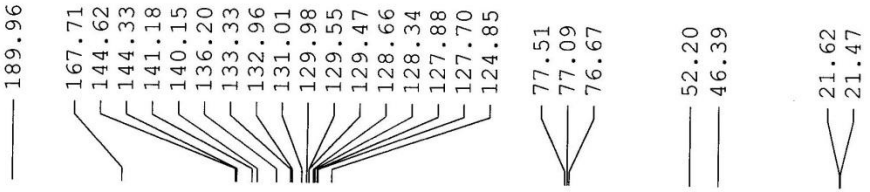


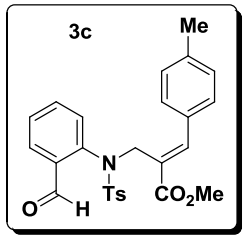
Current Data Parameters
NAME DK-V-4-OMe EST Ts-CHO
EXPNO 1
PROCNO 1

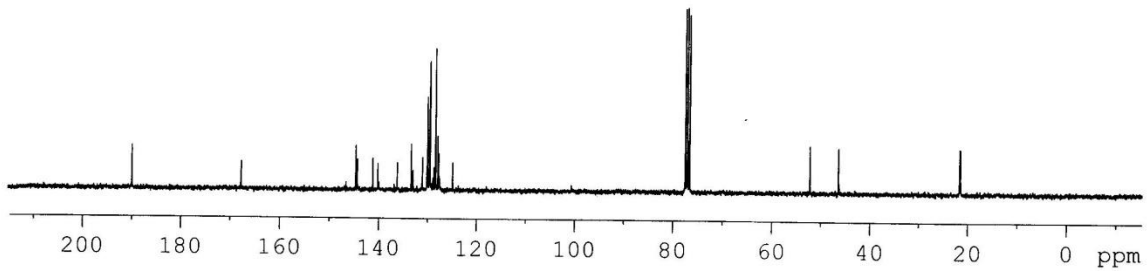
F2 - Acquisition Parameters
Date_ 20111009
Time 17.42
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 40.3
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 13.15 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

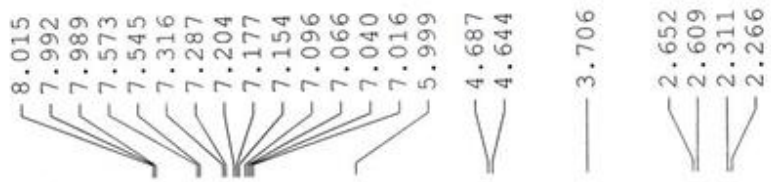
F2 - Processing parameters
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

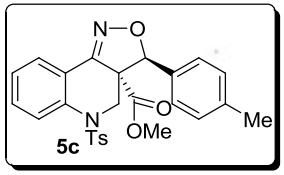


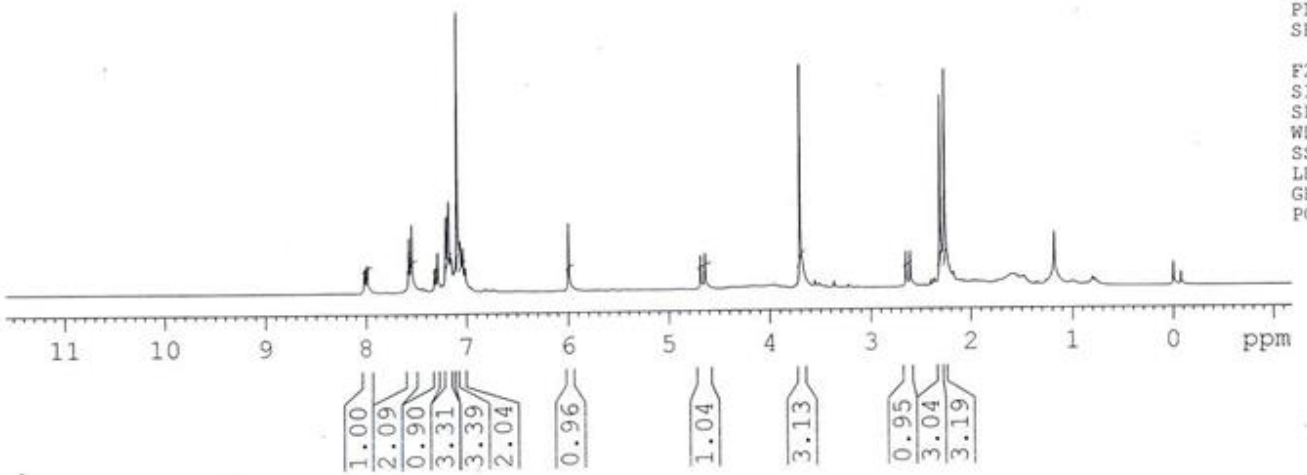





```
Current Data Parameters
NAME      DK-V-4-OMe EST Ts-CHO
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20111009
Time               17.50
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  200
DS                    4
SWH           17985.611 Hz
FIDRES         0.274439 Hz
AQ             1.8219508 sec
RG                1290.2
DW                27.800 usec
DE                 6.00 usec
TE                300.0 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                  9.30 usec
PL1                 0.00 dB
SFO1         75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              80.00 usec
PL2                 0.00 dB
PL12               15.68 dB
PL13               16.00 dB
SFO2        300.1312005 MHz

F2 - Processing parameters
SI                32768
SF         75.4677490 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```





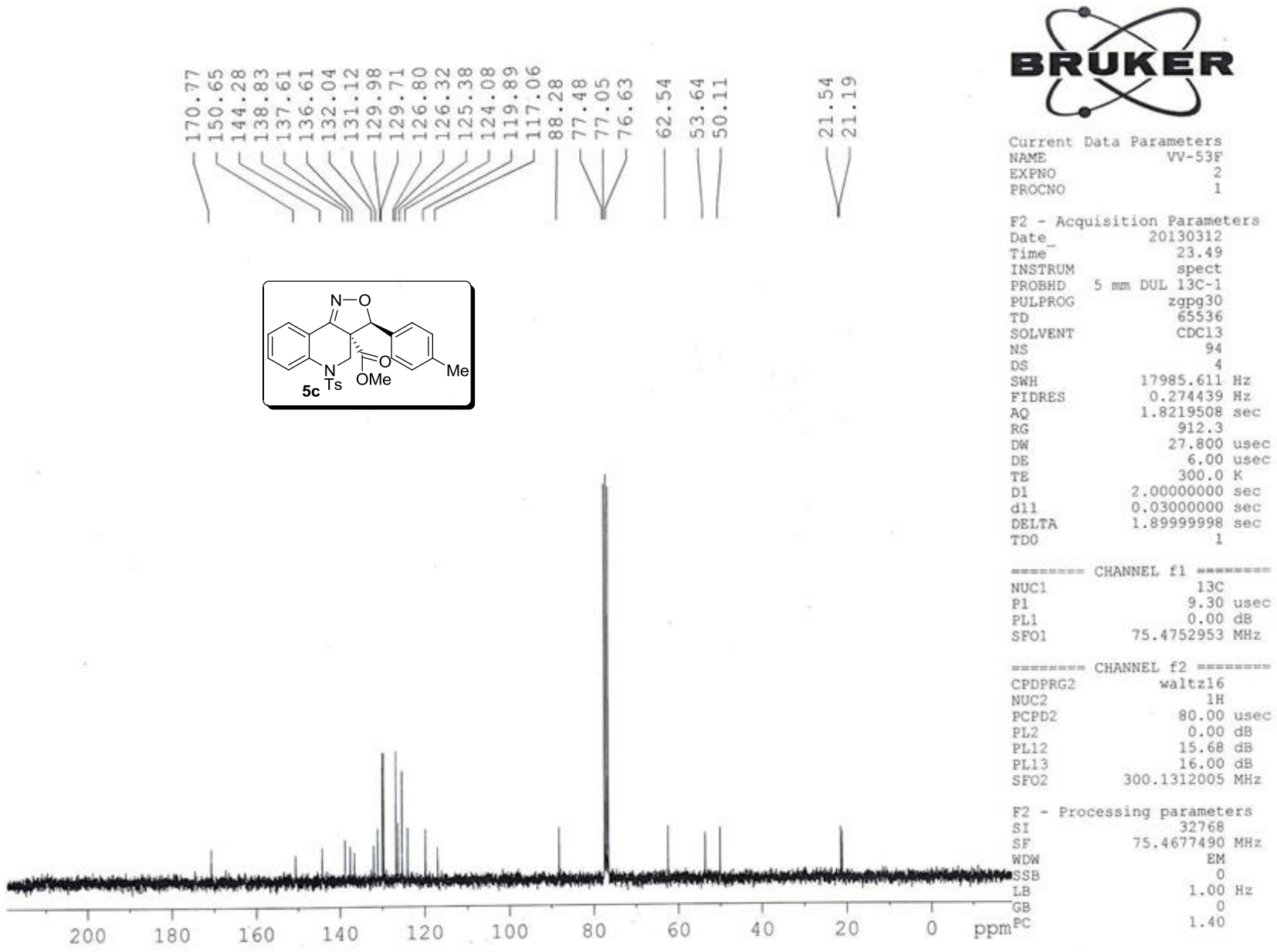


Current Data Parameters
NAME VV-53F
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130312
Time 23.44
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 8
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 90.5
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 13.15 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300297 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



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Current Data Parameters
NAME VV-53F
EXPNO 2
PROCNO 1

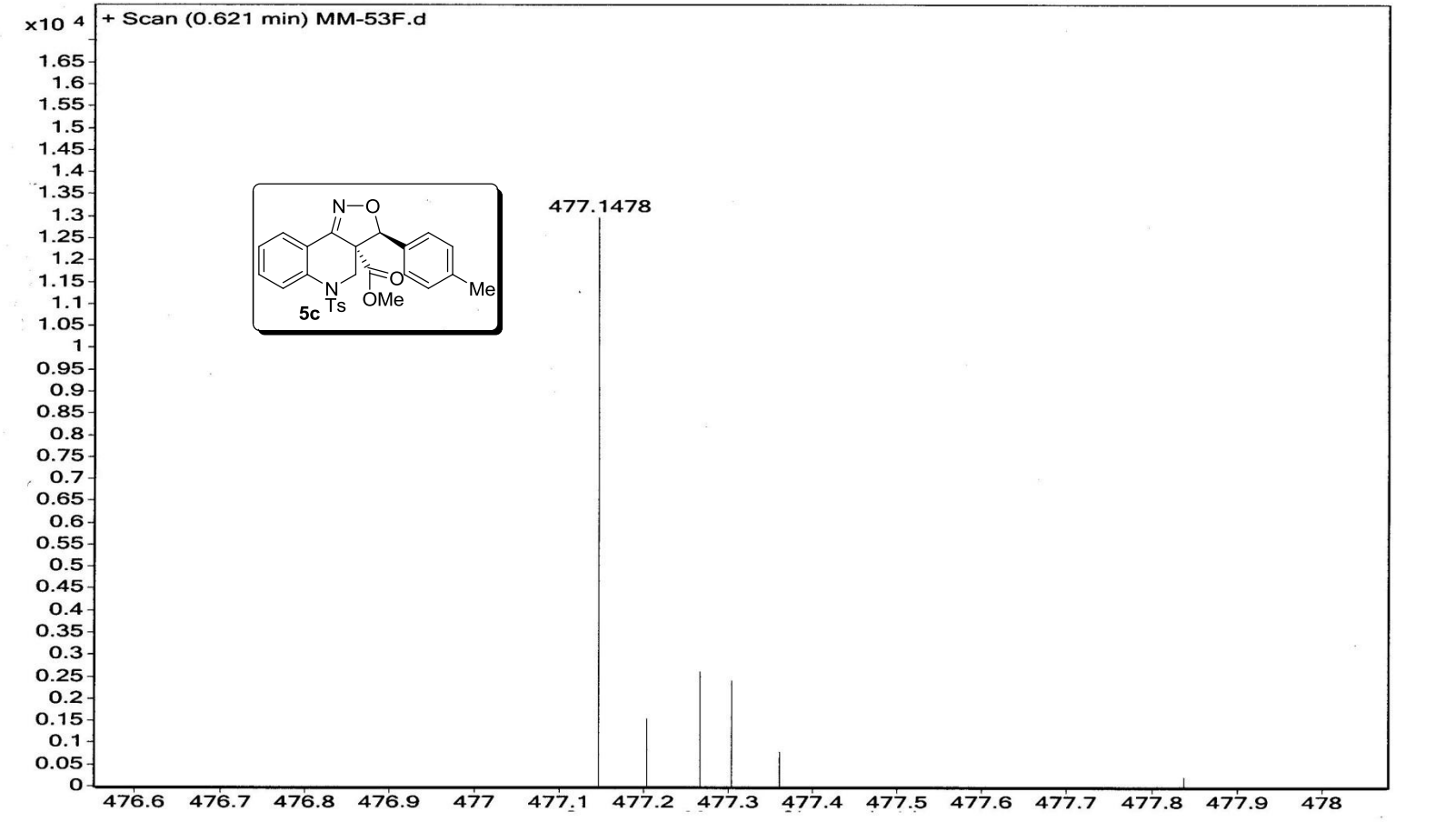
F2 - Acquisition Parameters
Date_ 20130312
Time 23.49
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 94
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 912.3
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

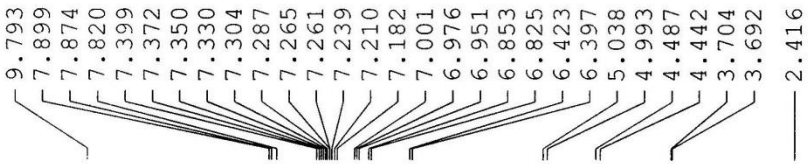
======== CHANNEL f1 ========
NUC1 13C
P1 9.30 usec
PL1 0.00 dB
SFO1 75.4752953 MHz

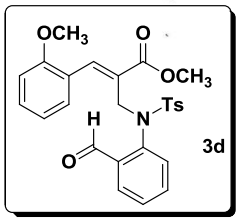
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.68 dB
PL13 16.00 dB
SFO2 300.1312005 MHz

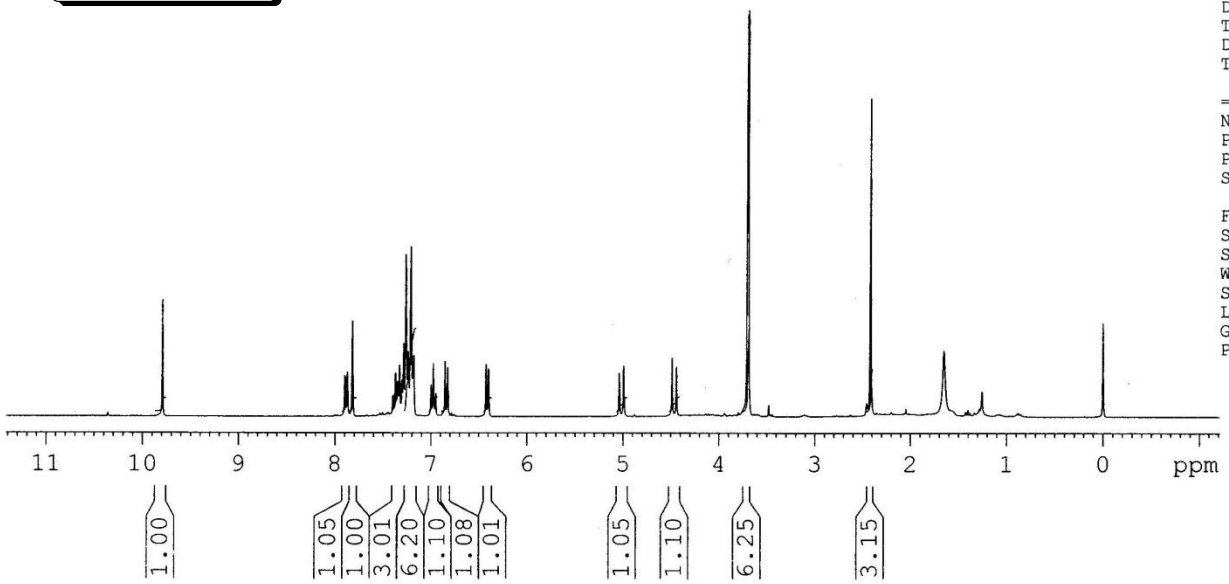
F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Sample Name	MM-53F	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	MM-53F.d	**ACQ Method**	Pondicherry Universi	**Comment**	MSK-MB-476.1406	**Acquired Time**	05-06-2015 13:32:25







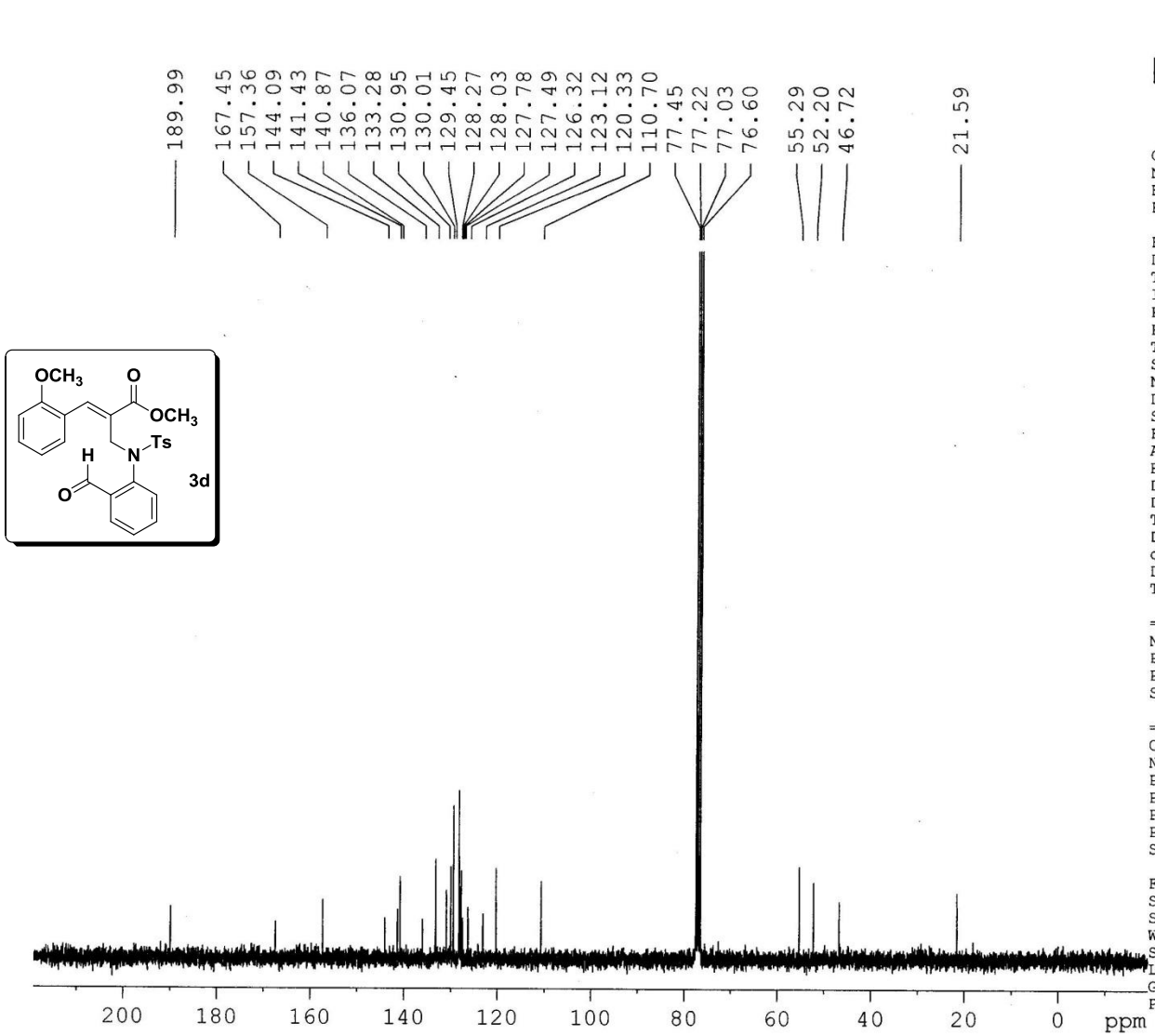


Current Data Parameters
NAME VV-57
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121201
Time 19.10
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 181
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 13.15 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300050 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



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Current Data Parameters

NAME	VV-57
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date_	20121201
Time	19.13
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	214
DS	4
SWH	17985.611 Hz
FIDRES	0.274439 Hz
AQ	1.8219508 sec
RG	574.7
DW	27.800 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1

======== CHANNEL f1 ========

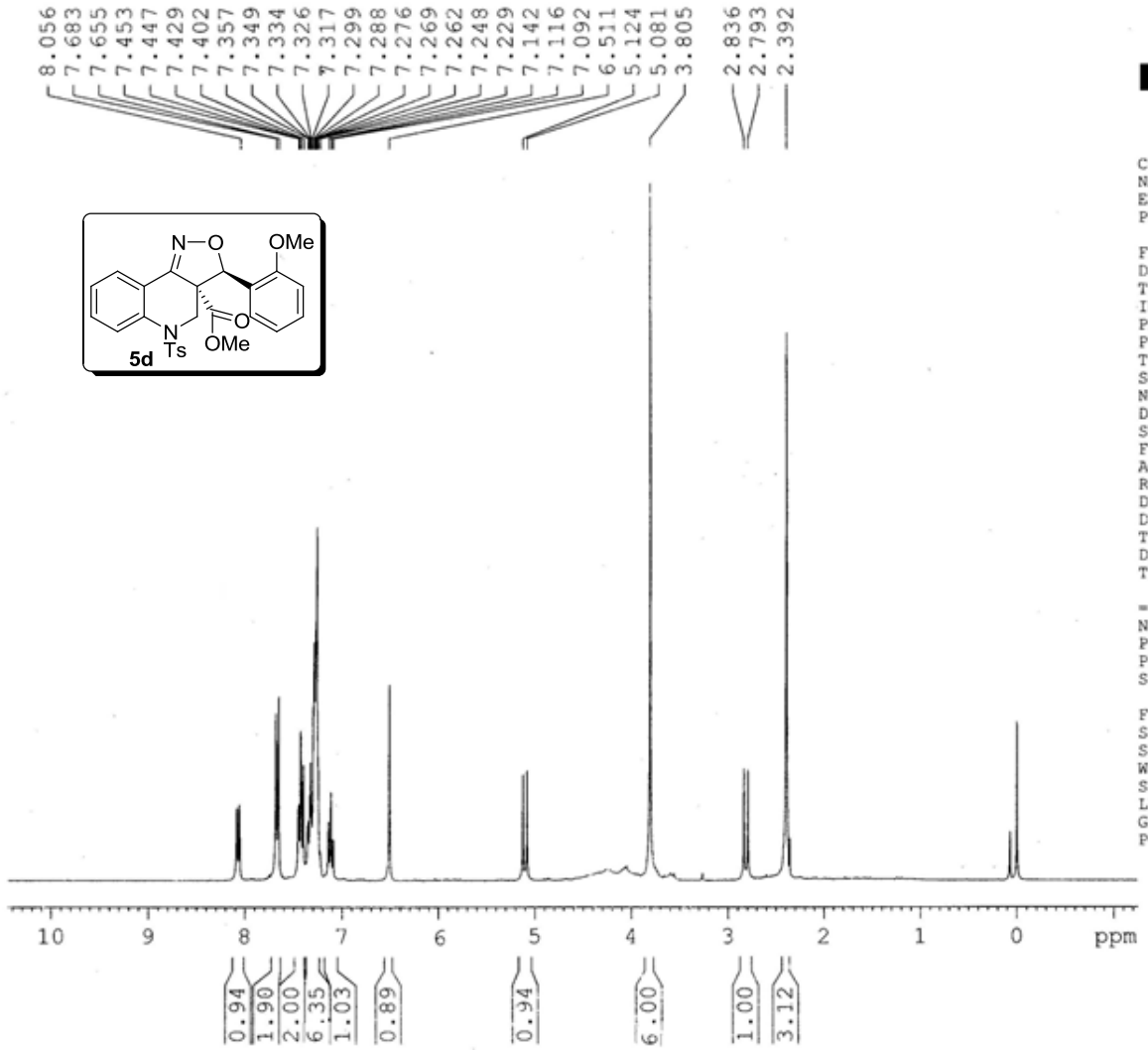
NUC1	13C
P1	9.30 usec
PL1	0.00 dB
SFO1	75.4752953 MHz

======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.00 dB
PL12	15.68 dB
PL13	16.00 dB
SFO2	300.1312005 MHz

F2 - Processing parameters

SI	32768
SF	75.4677490 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



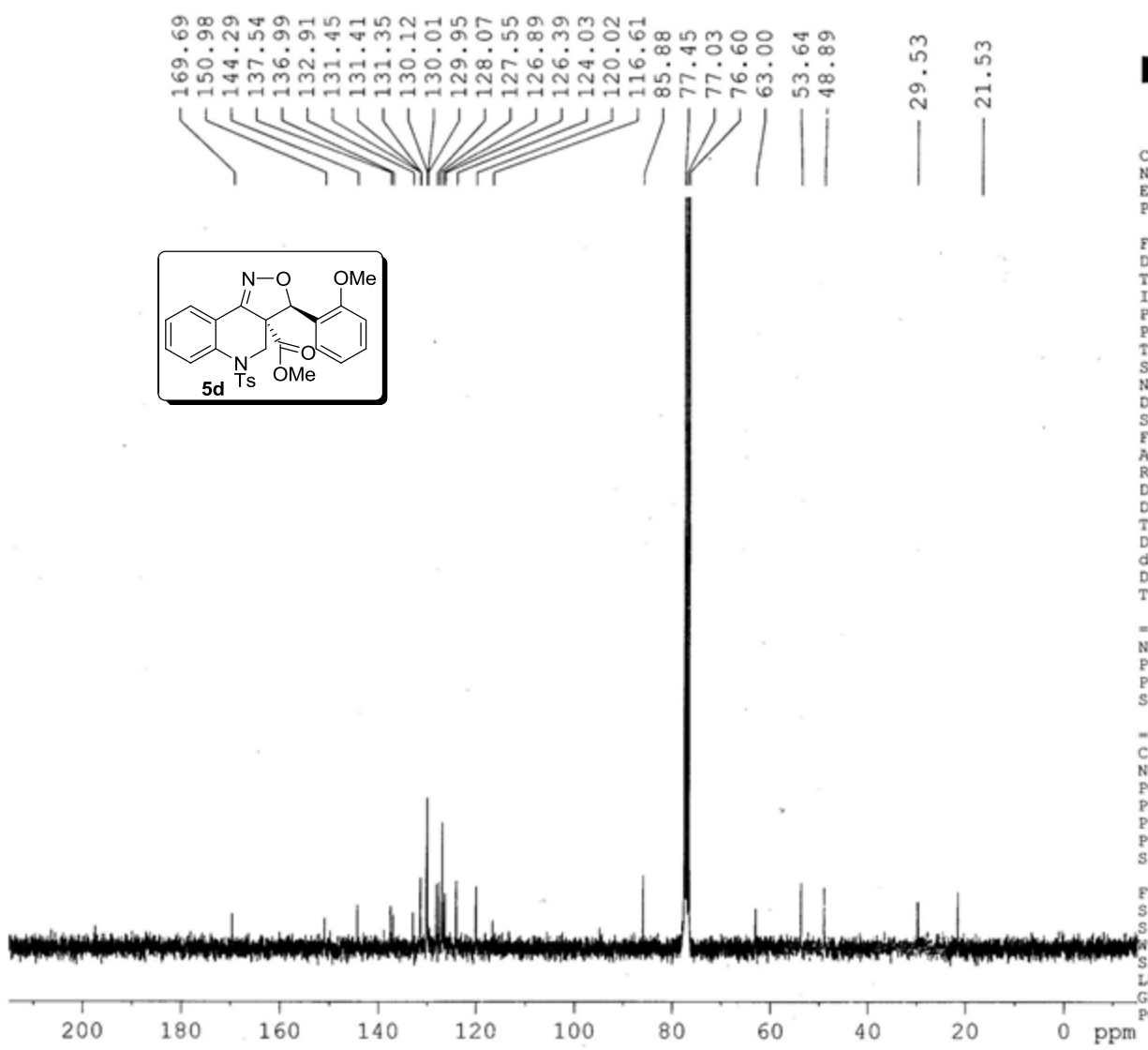
BRUKER

Current Data Parameters
NAME VV-57F
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130205
Time 22.01
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 13
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 161.3
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 13.15 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

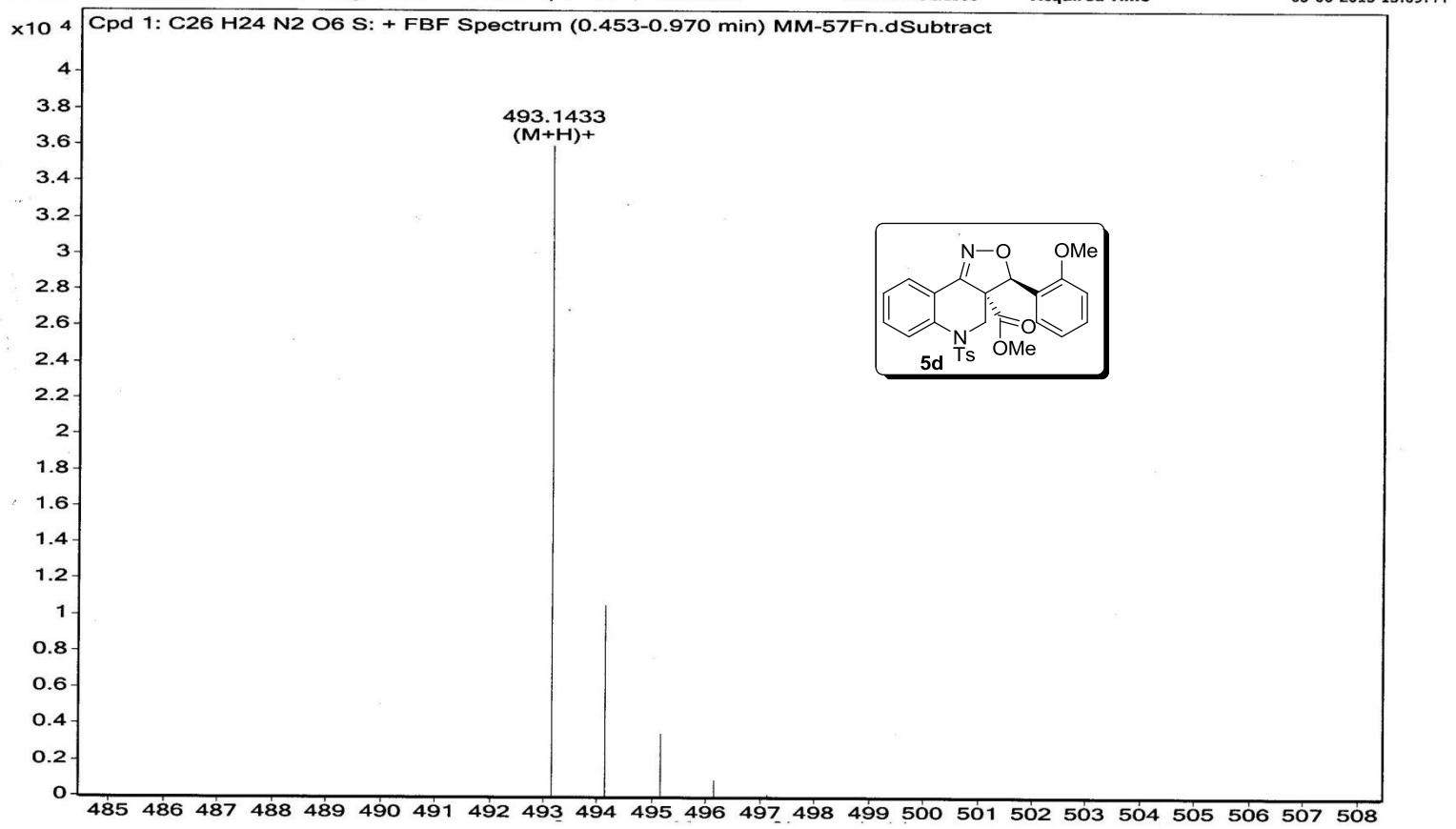
F2 - Processing parameters
SI 32768
SF 300.1300060 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

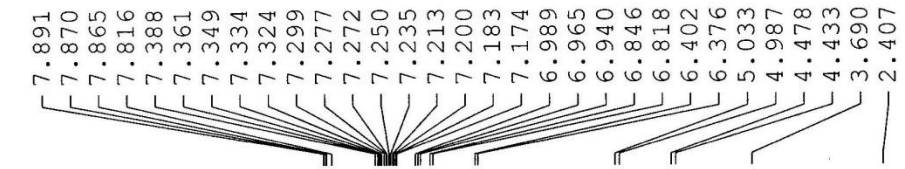


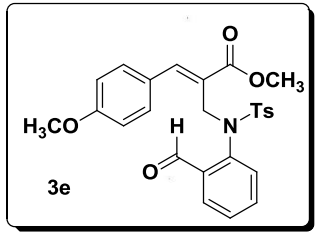
BRUKER

```
Current Data Parameters
NAME                  V.V.57F
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_                20130206
Time                    19.26
INSTRUM                 spect
PROBHD    5 mm DUL 13C-1
PULPROG                zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                        902
DS                          4
SWH                17985.611 Hz
FIDRES             0.274439 Hz
AQ                 1.8219508 sec
RG                    1290.2
DW                    27.800 usec
DE                     6.00 usec
TE                    300.0 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                      13C
P1                       9.30 usec
PL1                      0.00 dB
SFO1              75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                   80.00 usec
PL2                      0.00 dB
PL12                    15.68 dB
PL13                    16.00 dB
SFO2             300.1312005 MHz

F2 - Processing parameters
SI                        32768
SF                75.4677490 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40
```

Sample Name	MM-57F	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	MM-57Fn.d	**ACQ Method**	Pondicherry Universi	**Comment**	MSK-MB-492.1355	**Acquired Time**	05-06-2015 13:09:44







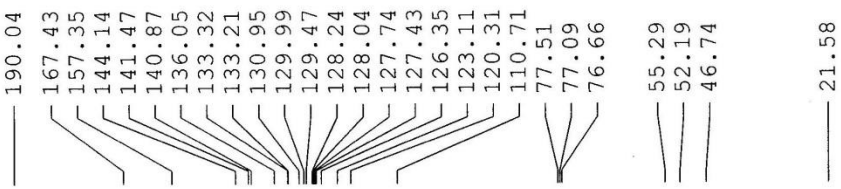
BRUKER

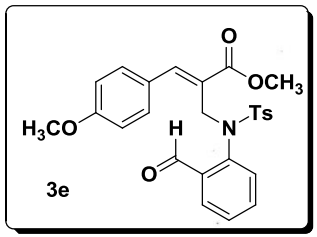
Current Data Parameters
NAME DK-V-4-OME-TS-CHO
EXPNO 1
PROCNO 1

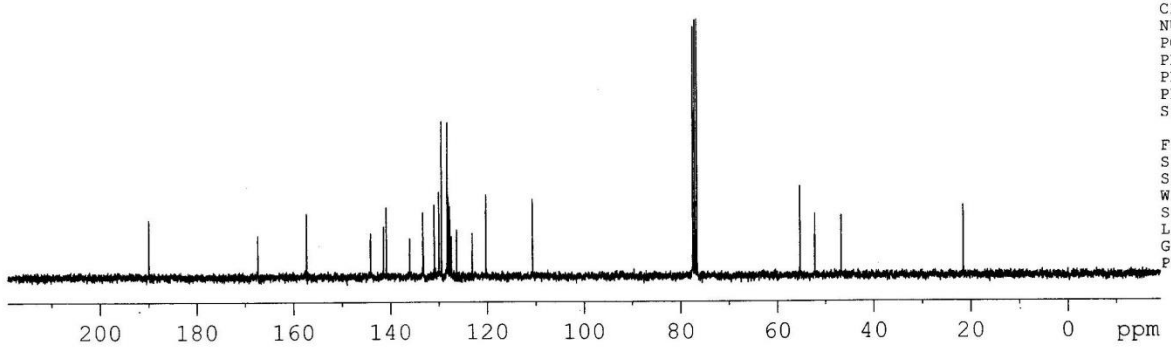
F2 - Acquisition Parameters
Date_ 20130305
Time 22.29
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 64
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 13.15 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300036 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00







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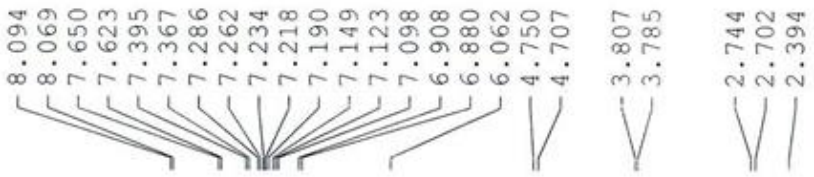
Current Data Parameters
NAME DK-V-4-OME-TS-CHO
EXPNO 2
PROCNO 1

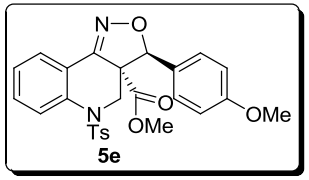
F2 - Acquisition Parameters
Date_ 20130305
Time 22.36
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 96
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 574.7
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.30 usec
PL1 0.00 dB
SFO1 75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.68 dB
PL13 16.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





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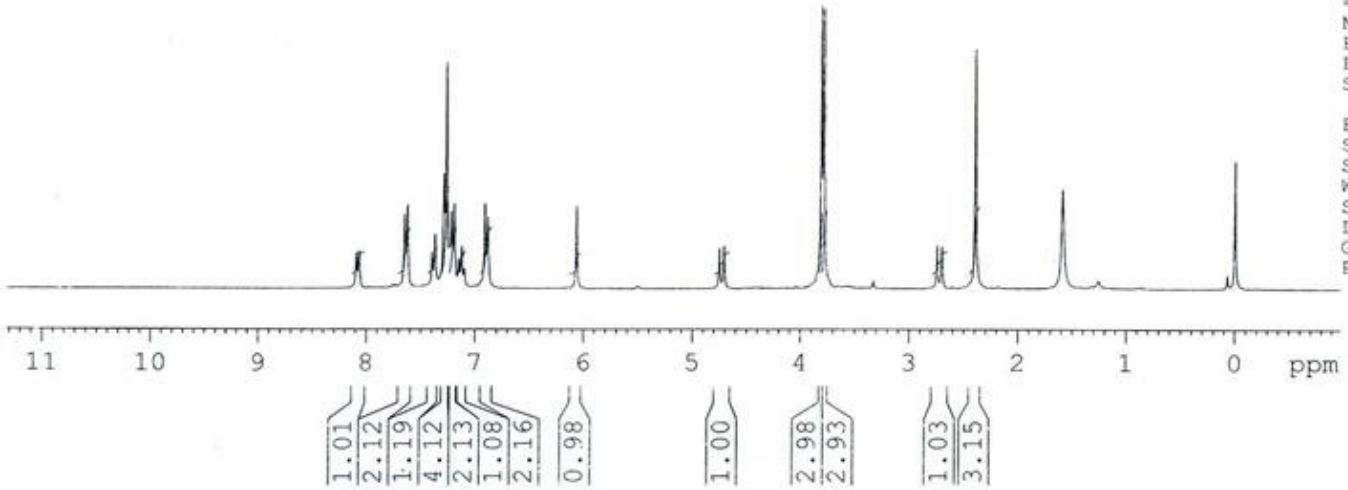


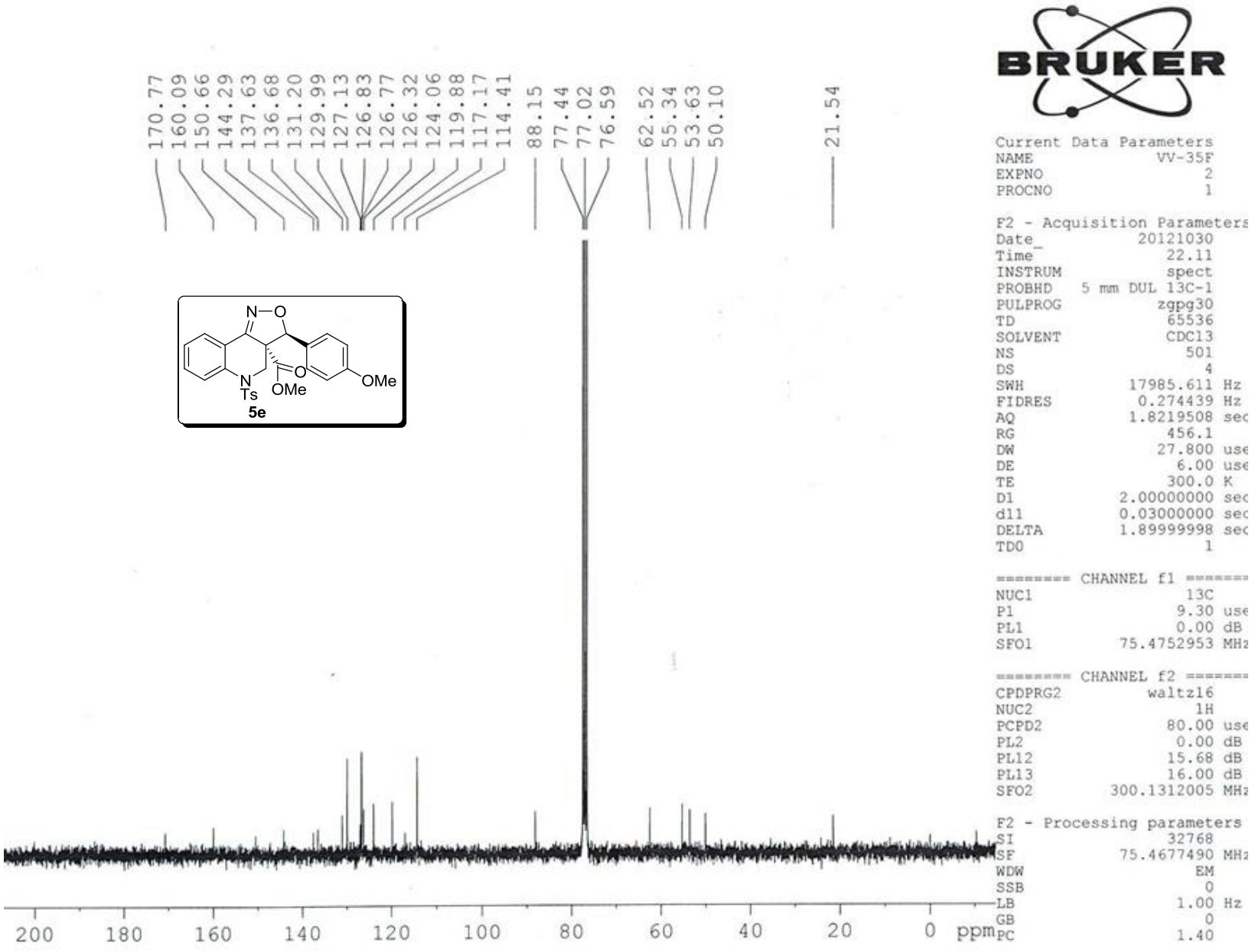
BRUKER

```
Current Data Parameters
NAME                  VV-35F
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20121030
Time                  21.38
INSTRUM               spect
PROBHD   5 mm DUL 13C-1
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                        16
DS                         2
SWH                6172.839 Hz
FIDRES             0.094190 Hz
AQ                 5.3084660 sec
RG                     406.4
DW                    81.000 usec
DE                     6.00 usec
TE                    300.0 K
D1                 1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     13.15 usec
PL1                     0.00 dB
SFO1          300.1318534 MHz

F2 - Processing parameters
SI                        32768
SF            300.1300063 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00
```



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Current Data Parameters
NAME VV-35F
EXPNO 2
PROCNO 1

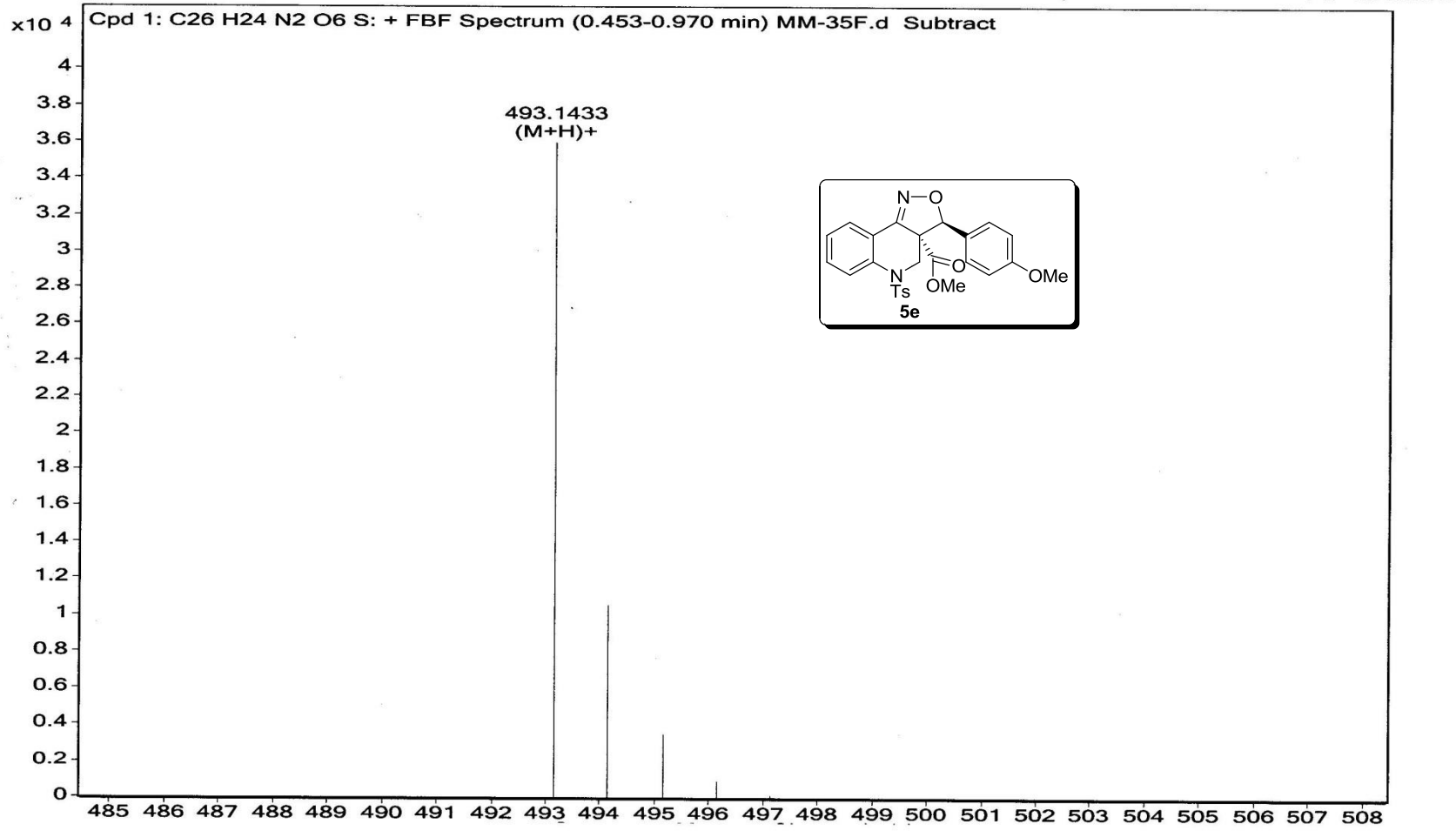
F2 - Acquisition Parameters
Date_ 20121030
Time 22.11
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 501
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 456.1
DW 27.800 use
DE 6.00 use
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

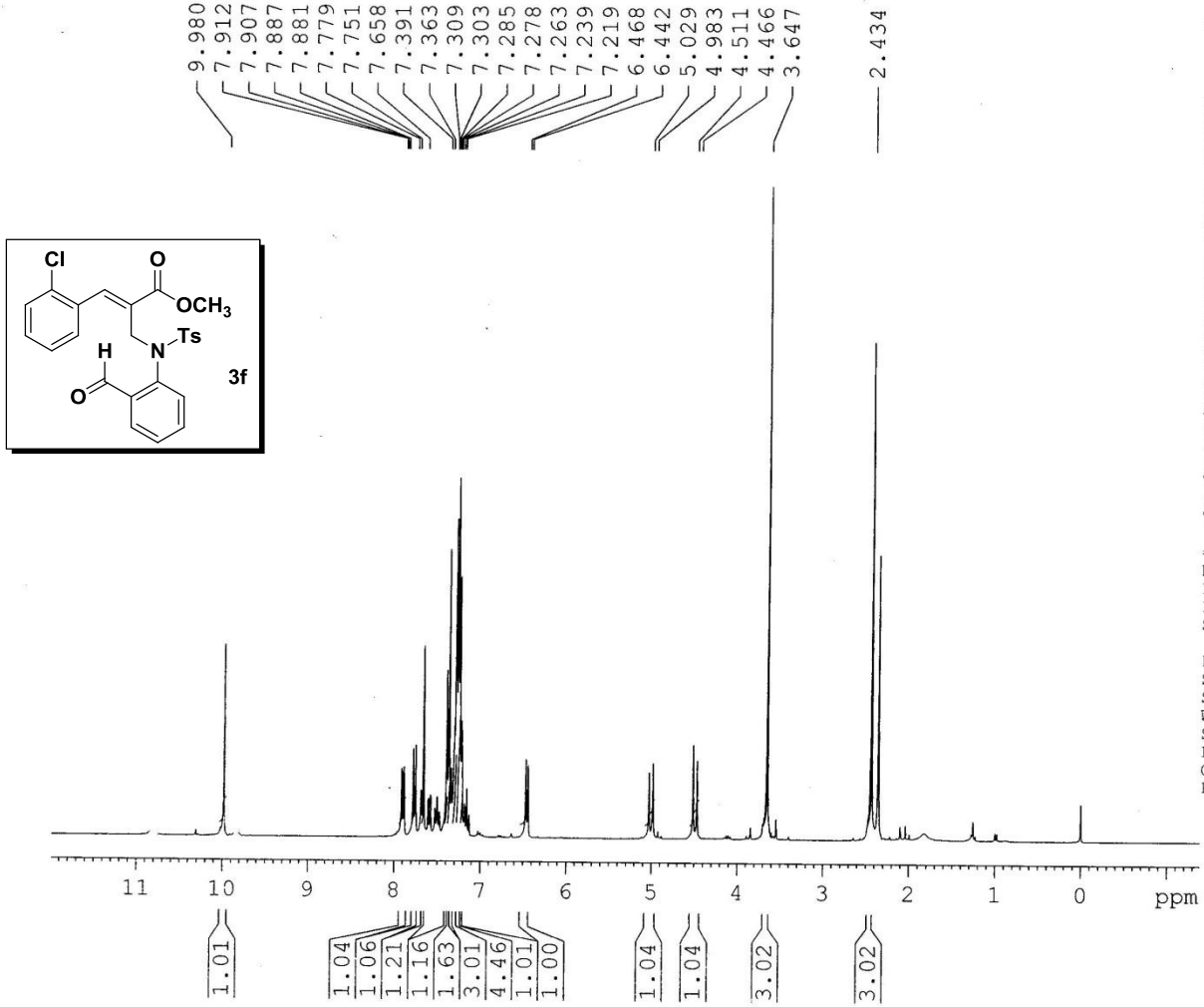
======== CHANNEL f1 ========
NUC1 13C
P1 9.30 use
PL1 0.00 dB
SFO1 75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 use
PL2 0.00 dB
PL12 15.68 dB
PL13 16.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Sample Name	MM-35F	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	MM-35F.d	**ACQ Method**	Pondicherry Universi	**Comment**	MSK-MB-492.1355	**Acquired Time**	05-06-2015 13:09:44





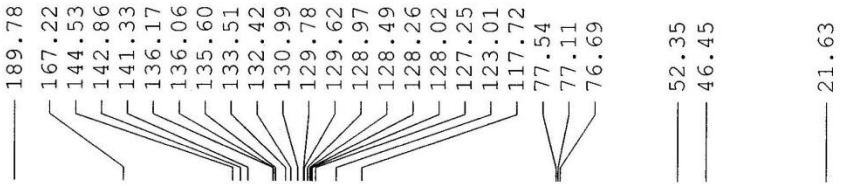
BRUKER

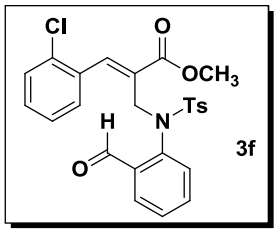
Current Data Parameters
NAME DK-V-2-Cl-EST-CHO
EXPNO 2
PROCNO 1

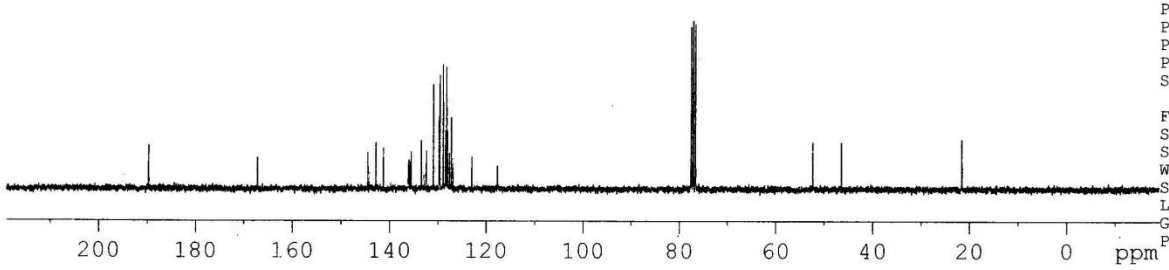
F2 - Acquisition Parameters
Date_ 20130303
Time 23.29
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 45.3
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 13.15 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300011 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00







BRUKER

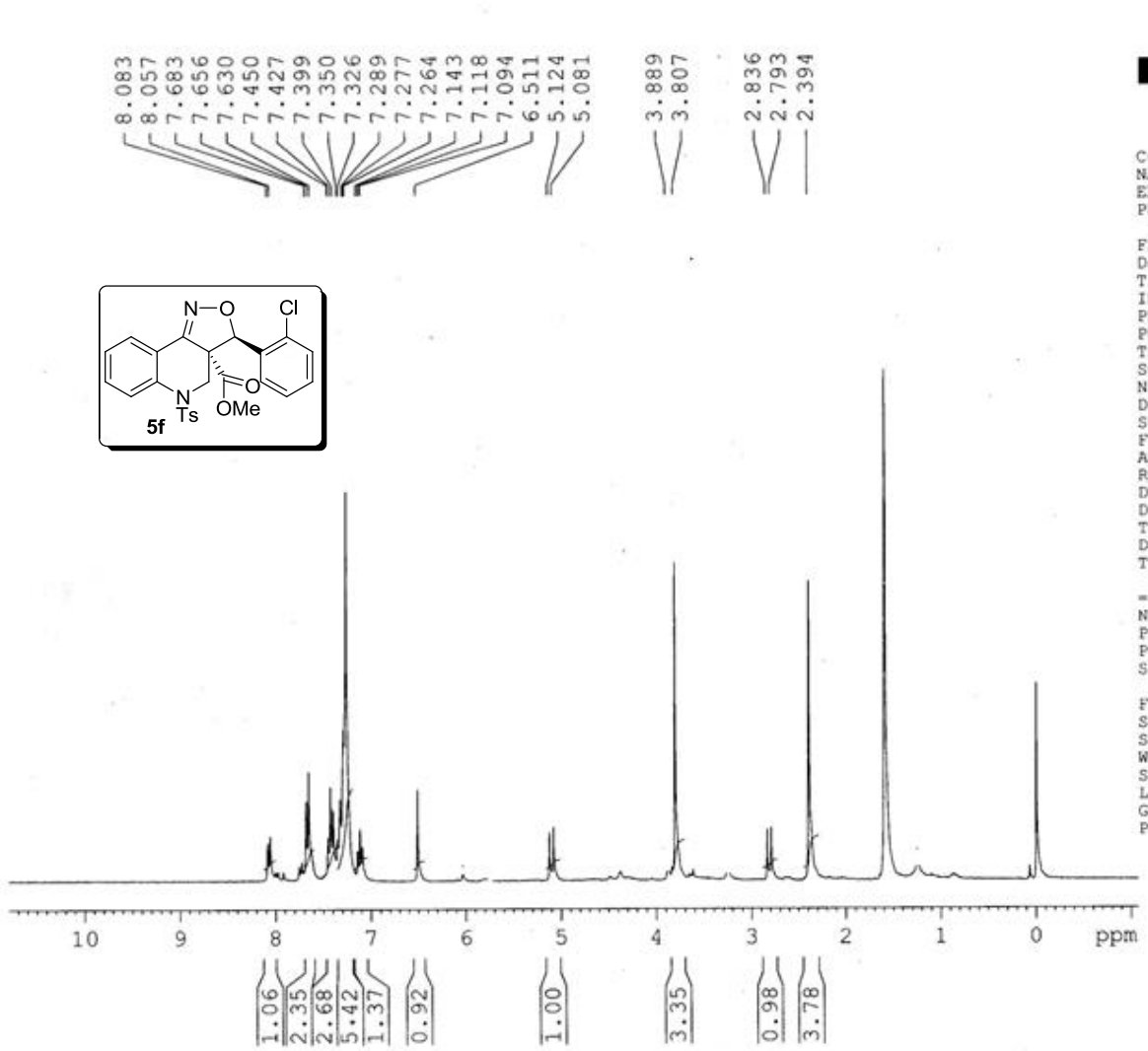
Current Data Parameters
NAME DK-V-2-Cl-EST-CHO
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130303
Time 23.33
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 58
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 912.3
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.30 usec
PL1 0.00 dB
SFO1 75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.68 dB
PL13 16.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



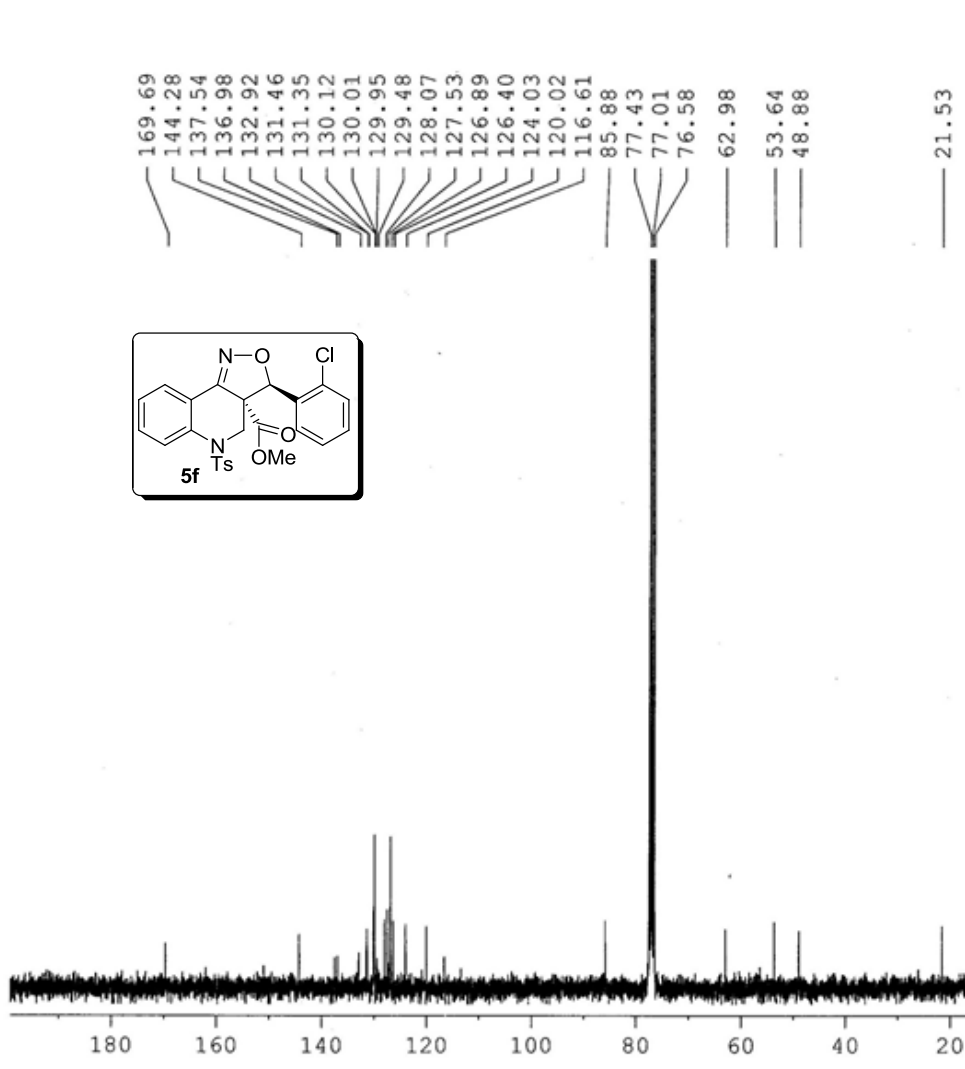
BRUKER

Current Data Parameters
NAME VV-33F
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120904
Time 13.18
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 456.1
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 13.15 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

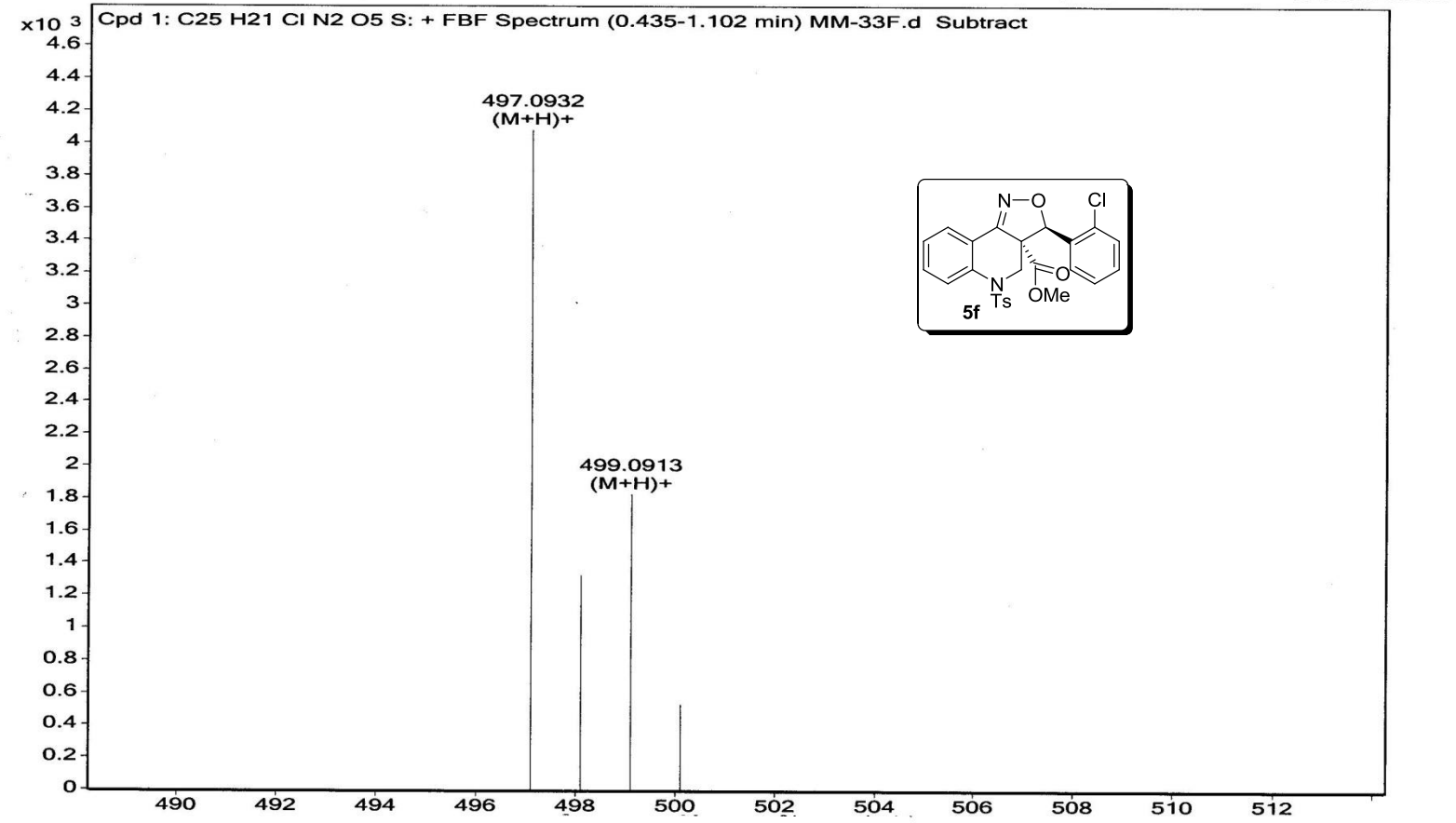
F2 - Processing parameters
SI 32768
SF 300.1300063 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

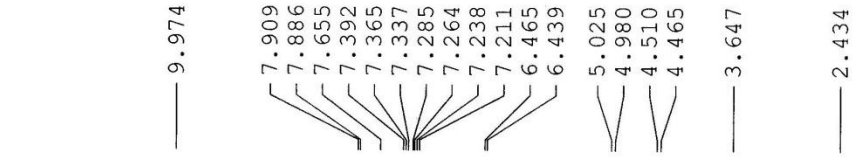


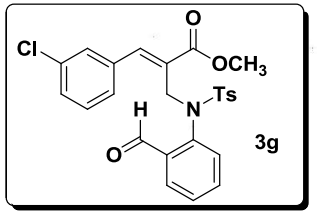
BRUKER

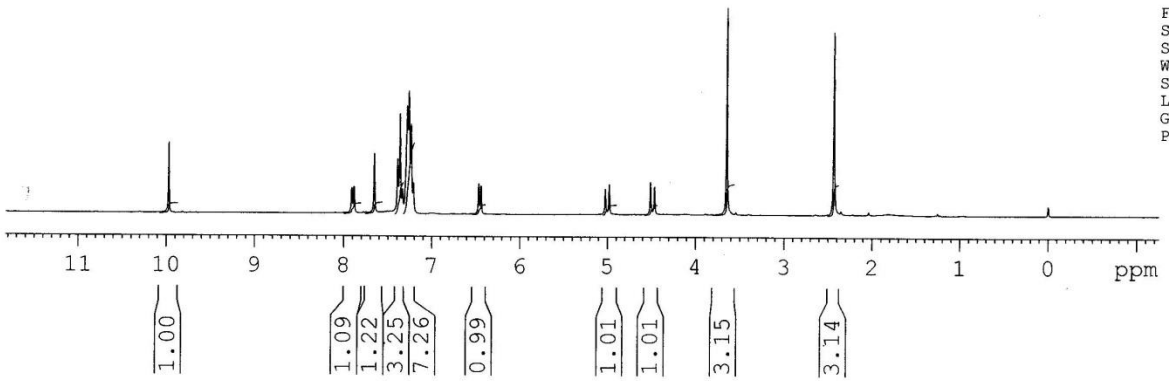
```
Current Data Parameters
NAME                  VV-33F
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20121204
Time                  22.08
INSTRUM               spect
PROBHD    5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT              CDC13
NS                    1024
DS                       4
SWH              17985.611 Hz
FIDRES            0.274439 Hz
AQ                1.8219508 sec
RG                     512
DW                  27.800 usec
DE                   6.00 usec
TE                  300.0 K
D1               2.00000000 sec
d11              0.03000000 sec
DELTA            1.89999998 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                     13C
P1                    9.30 usec
PL1                   0.00 dB
SFO1            75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                     1H
PCPD2                80.00 usec
PL2                   0.00 dB
PL12                 15.68 dB
PL13                 16.00 dB
SFO2           300.1312005 MHz

F2 - Processing parameters
SI                       32768
SF              75.4677490 MHz
WDW                         EM
SSB                          0
LB                    1.00 Hz
GB                           0
PC                    1.40
```

Sample Name	MM-33F	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	MM-33F.d	**ACQ Method**	Pondicherry Universi	**Comment**	MSK-MB-496.0859	**Acquired Time**	05-06-2015 13:06:04







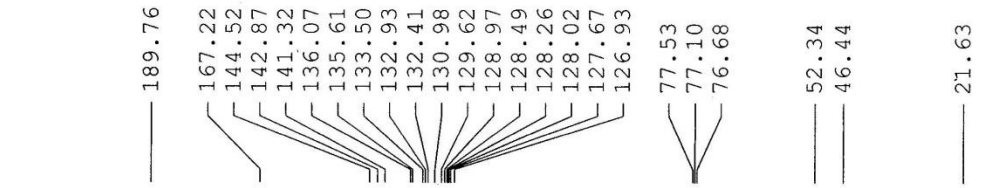


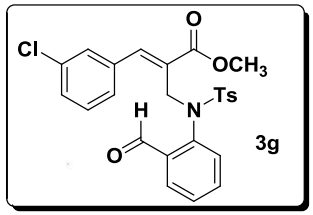
Current Data Parameters
NAME DK-V-3-Cl-EST-TS-CHO
EXPNO 1
PROCNO 1

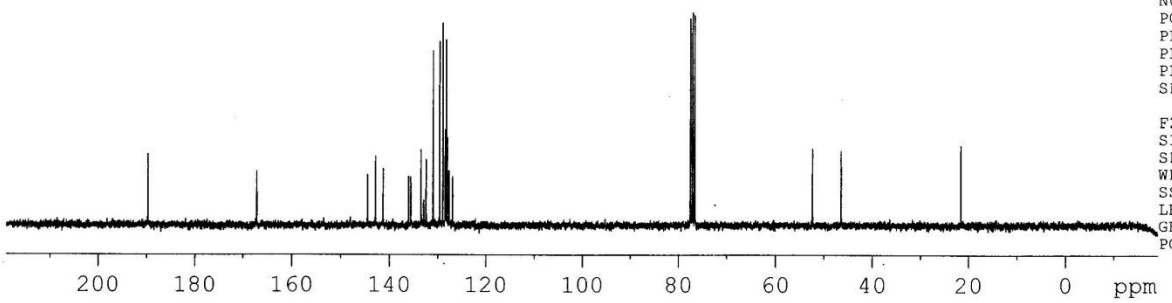
F2 - Acquisition Parameters
Date_ 20130305
Time 22.46
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 57
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 13.15 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300016 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

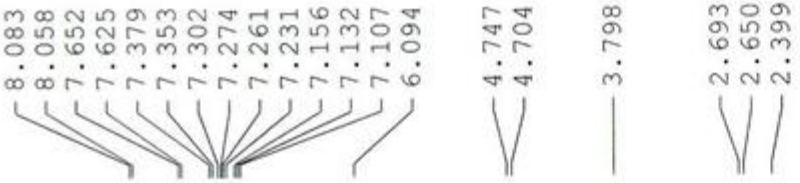


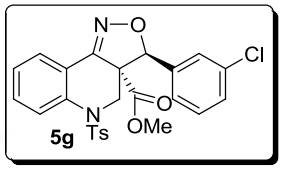


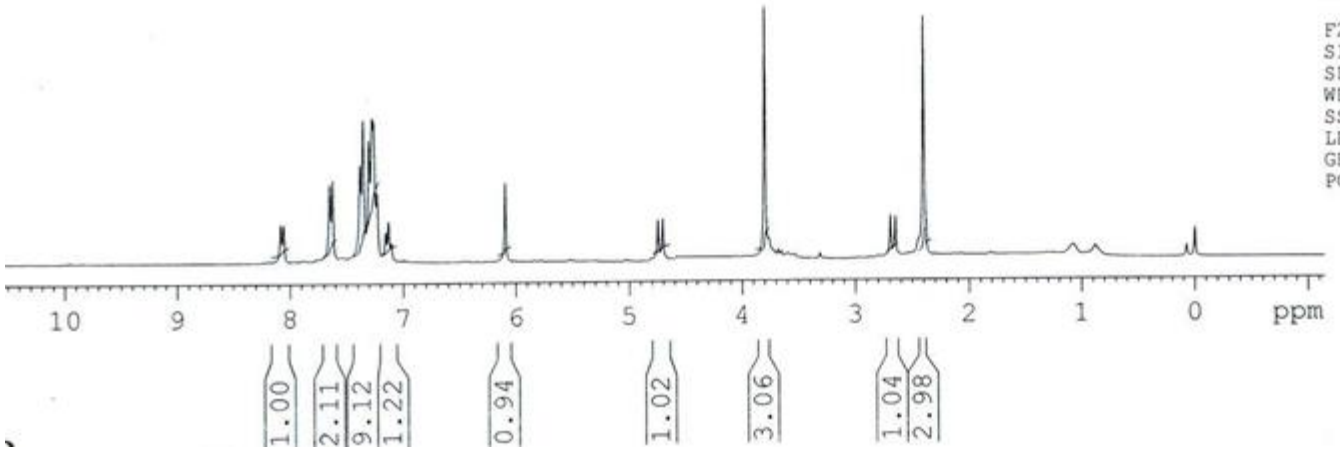


BRUKER

```
Current Data Parameters
NAME      DK-V-3-Cl-EST-TS-CHO
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_              20130305
Time                  22.52
INSTRUM                spect
PROBHD   5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                      93
DS                       4
SWH              17985.611 Hz
FIDRES            0.274439 Hz
AQ                1.8219508 sec
RG                    724.1
DW                  27.800 usec
DE                   6.00 usec
TE                  300.0 K
D1               2.00000000 sec
d11              0.03000000 sec
DELTA            1.89999998 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                    9.30 usec
PL1                   0.00 dB
SFO1           75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                   1H
PCPD2                80.00 usec
PL2                   0.00 dB
PL12                 15.68 dB
PL13                 16.00 dB
SFO2          300.1312005 MHz

F2 - Processing parameters
SI                    32768
SF             75.4677490 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```







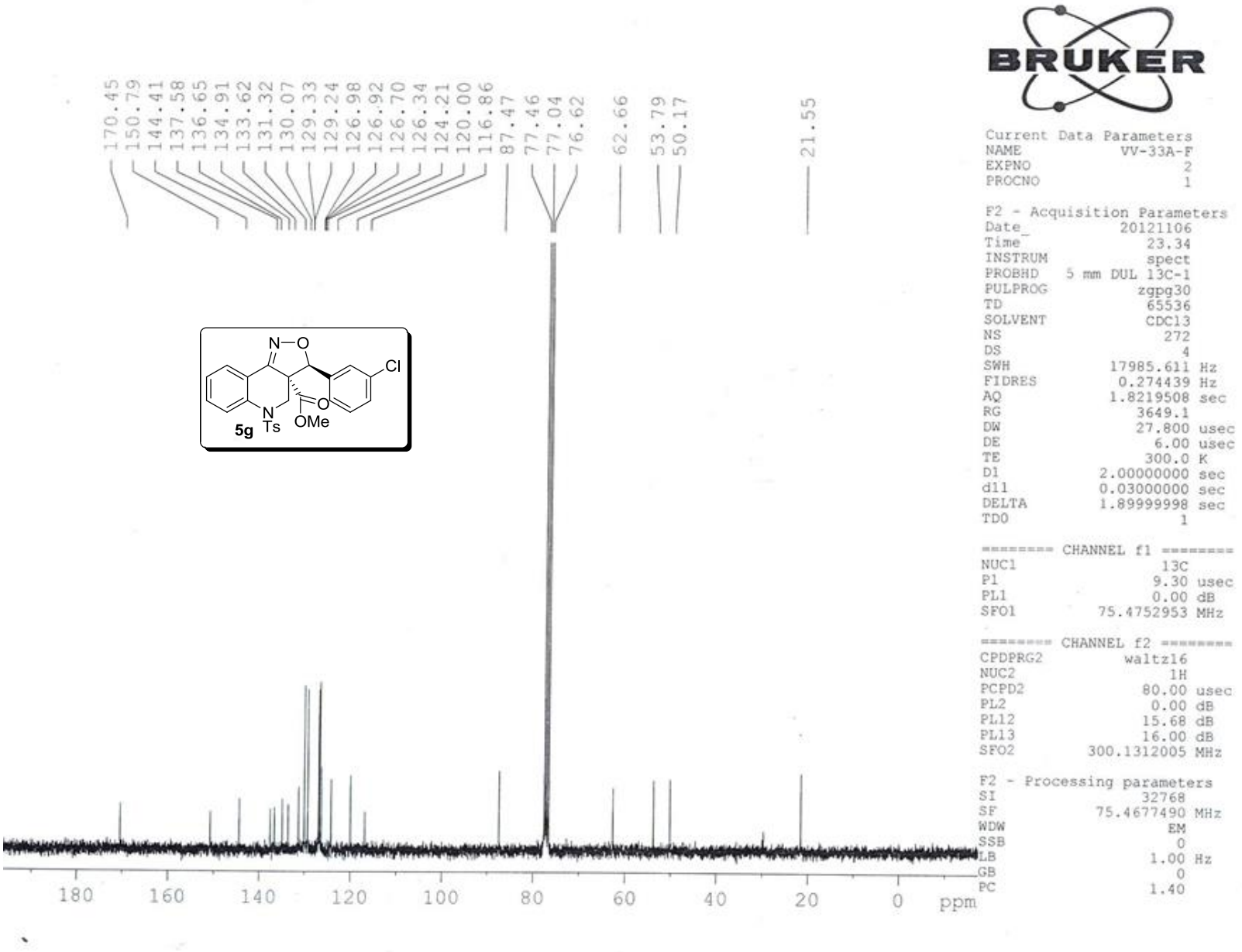
BRUKER

Current Data Parameters
NAME VV-33A-F
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121106
Time 23.27
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 7
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 101.6
DW 81.000 use
DE 6.00 use
TE 300.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 13.15 use
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300056 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



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Current Data Parameters
NAME VV-33A-F
EXPNO 2
PROCNO 1

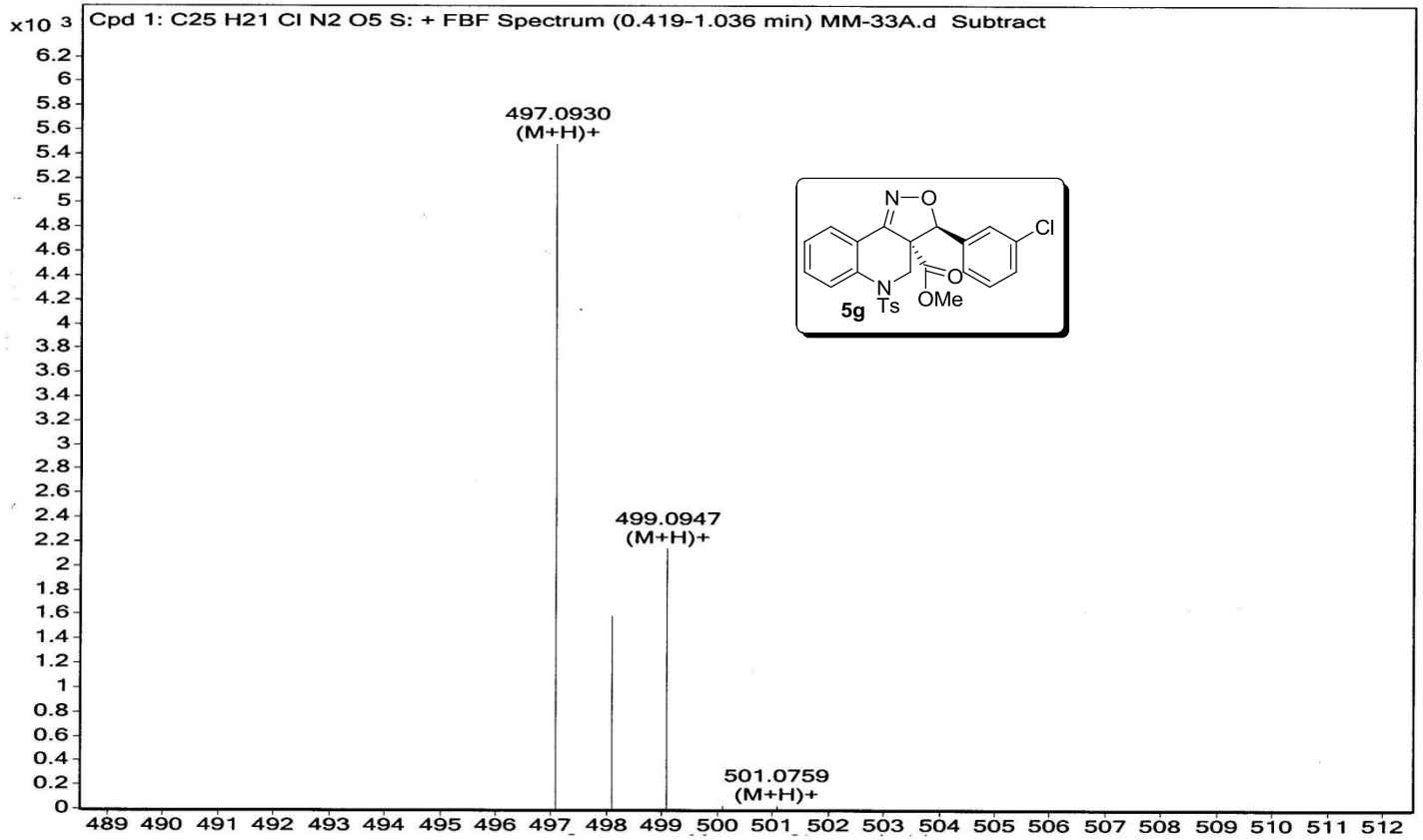
F2 - Acquisition Parameters
Date_ 20121106
Time 23.34
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 272
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 3649.1
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

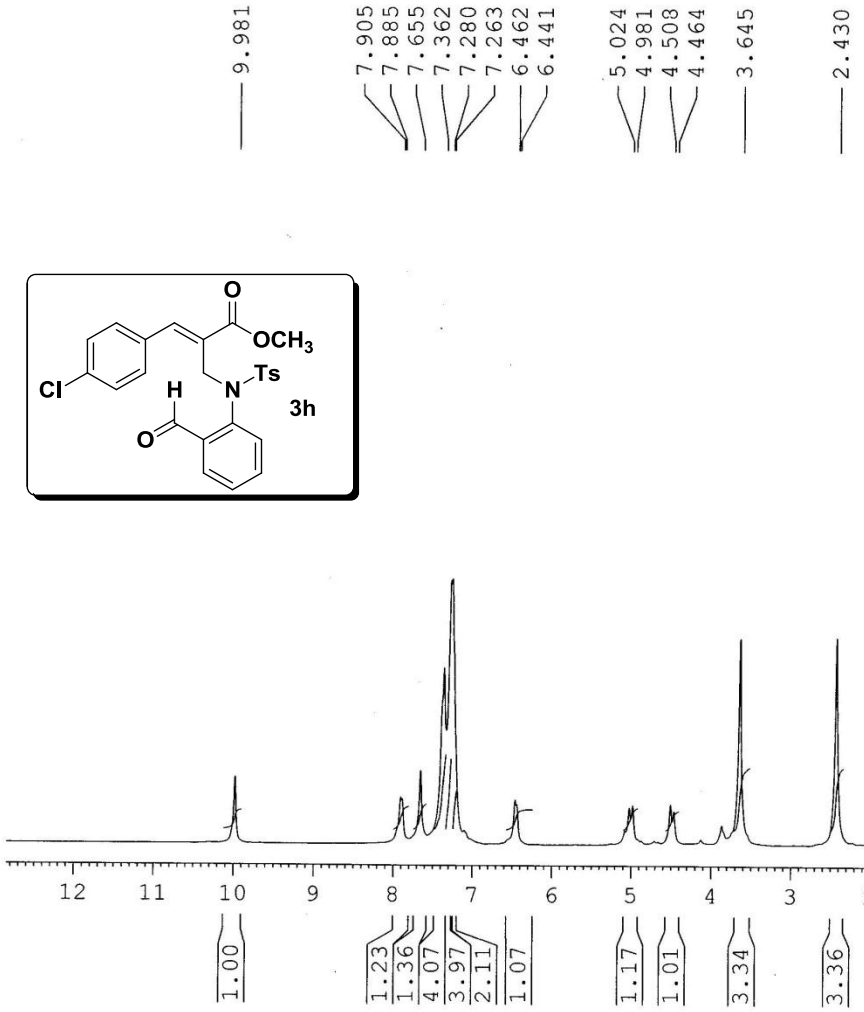
======== CHANNEL f1 ========
NUC1 13C
P1 9.30 usec
PL1 0.00 dB
SFO1 75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.68 dB
PL13 16.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Sample Name	MM-33A	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	MM-33A.d	**ACQ Method**	Pondicherry Universi	**Comment**	MSK-MB-496.0859	**Acquired Time**	05-06-2015 13:02:28





BRUKER

Current Data Parameters
NAME DK-V-4-Cl-EST-CHO
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

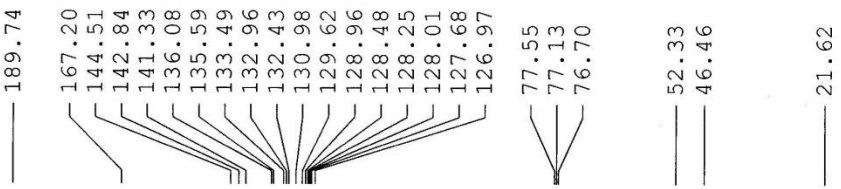
Date_	20130305
Time	19.52
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	6172.839 Hz
FIDRES	0.094190 Hz
AQ	5.3084660 sec
RG	40.3
DW	81.000 usec
DE	6.00 usec
TE	300.0 K
D1	1.00000000 sec
TD0	1

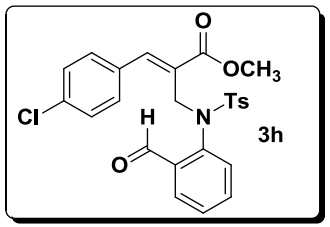
======== CHANNEL f1 ========

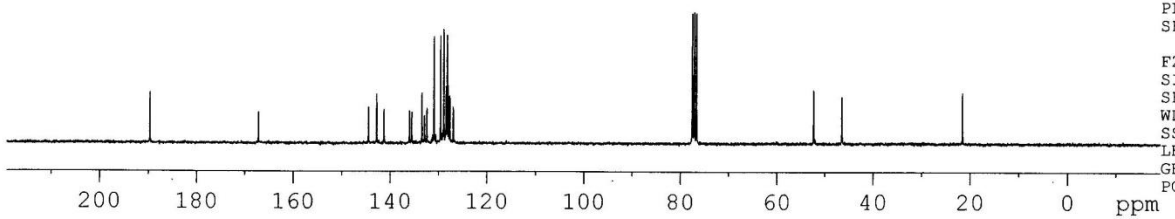
NUC1	1H
P1	13.15 usec
PL1	0.00 dB
SFO1	300.1318534 MHz

F2 - Processing parameters

SI	32768
SF	300.1300015 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00







BRUKER

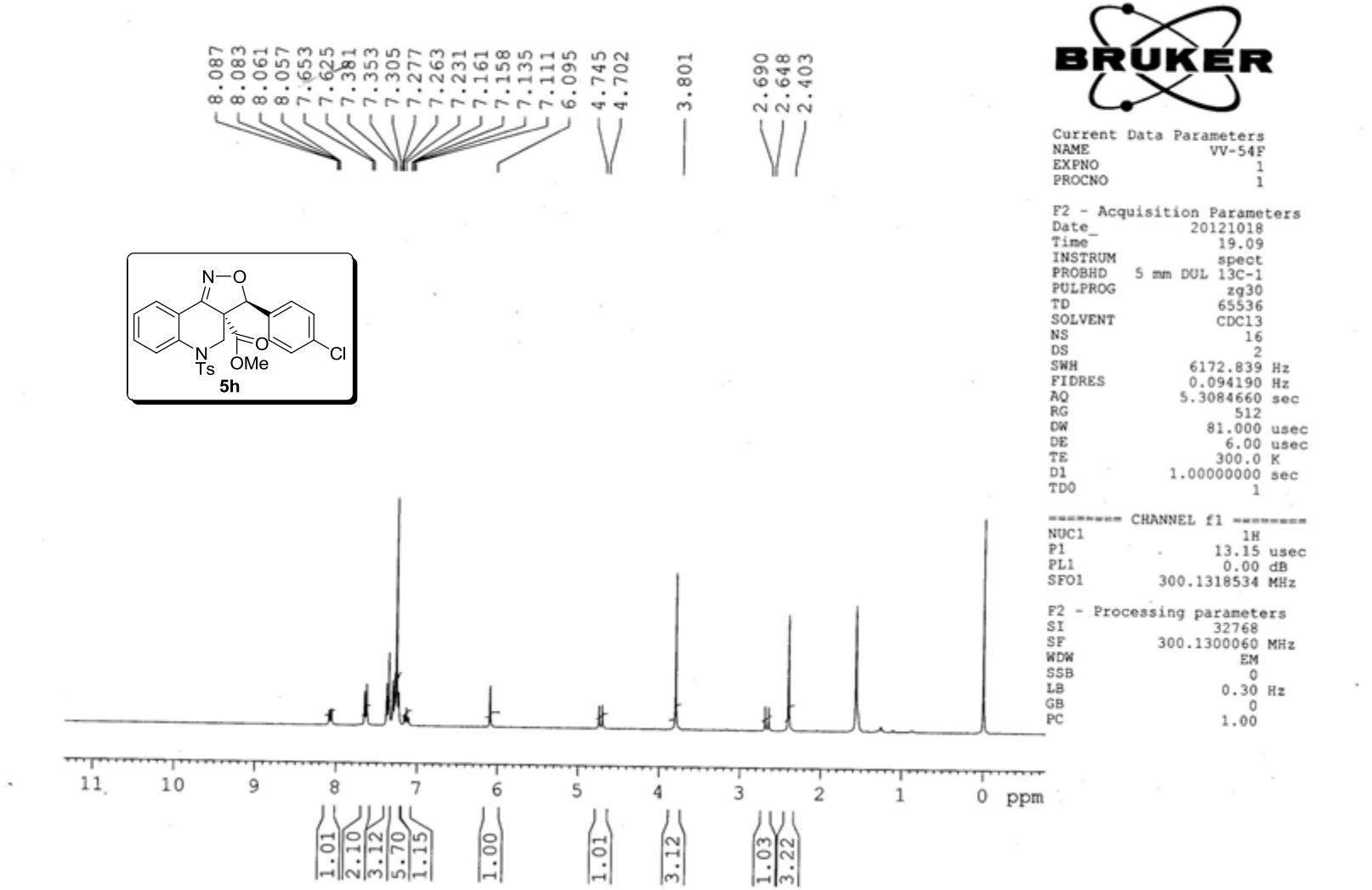
```
Current Data Parameters
NAME      DK-V-4-Cl-EST-CHO
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_             20130305
Time                 20.23
INSTRUM              spect
PROBHD   5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT                CDC13
NS                     460
DS                       4
SWH              17985.611 Hz
FIDRES               0.274439 Hz
AQ                1.8219508 sec
RG                   1625.5
DW                  27.800 usec
DE                   6.00 usec
TE                  300.0 K
D1               2.00000000 sec
d11              0.03000000 sec
DELTA            1.89999998 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    13C
P1                    9.30 usec
PL1                   0.00 dB
SFO1           75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                   0.00 dB
PL12                 15.68 dB
PL13                 16.00 dB
SFO2          300.1312005 MHz

F2 - Processing parameters
SI                   32768
SF             75.4677490 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```



BRUKER

Current Data Parameters
NAME VV-54F
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121018
Time 19.09
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 512
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 13.15 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300060 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

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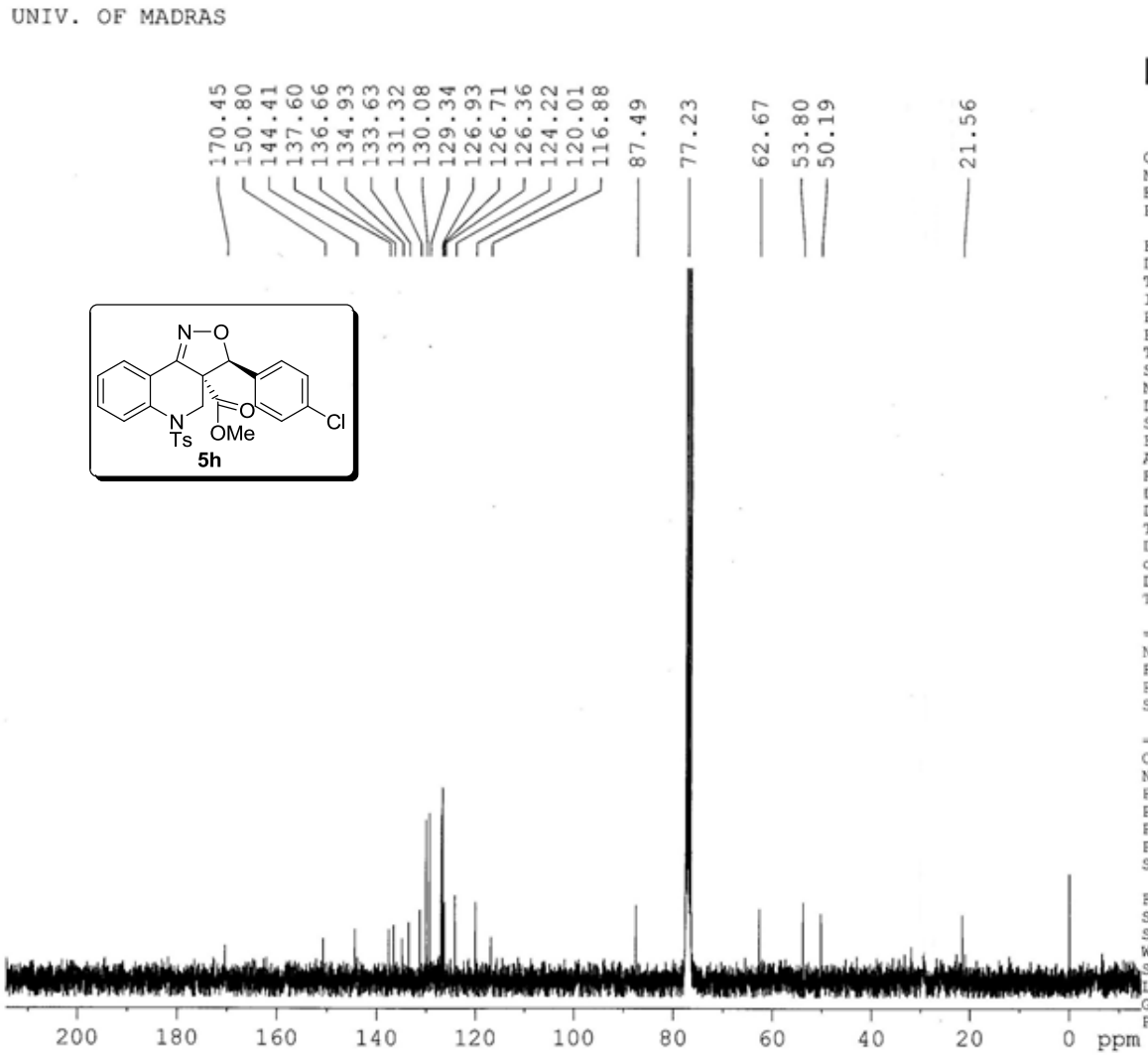
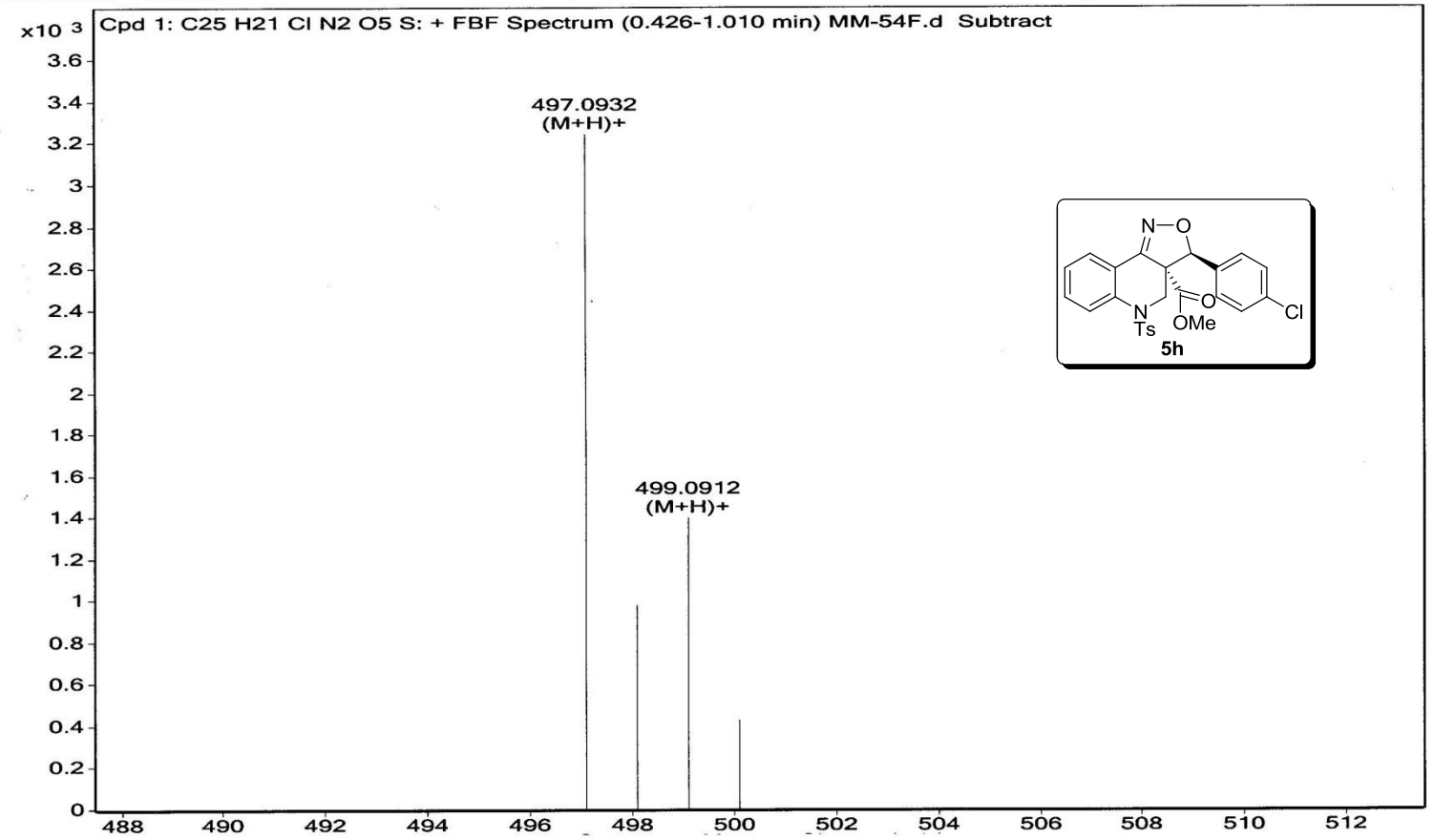
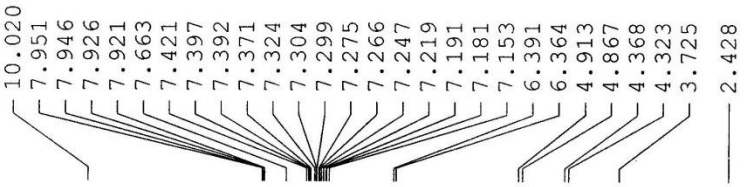


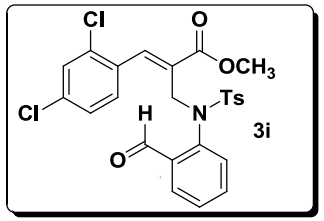
BRUKER

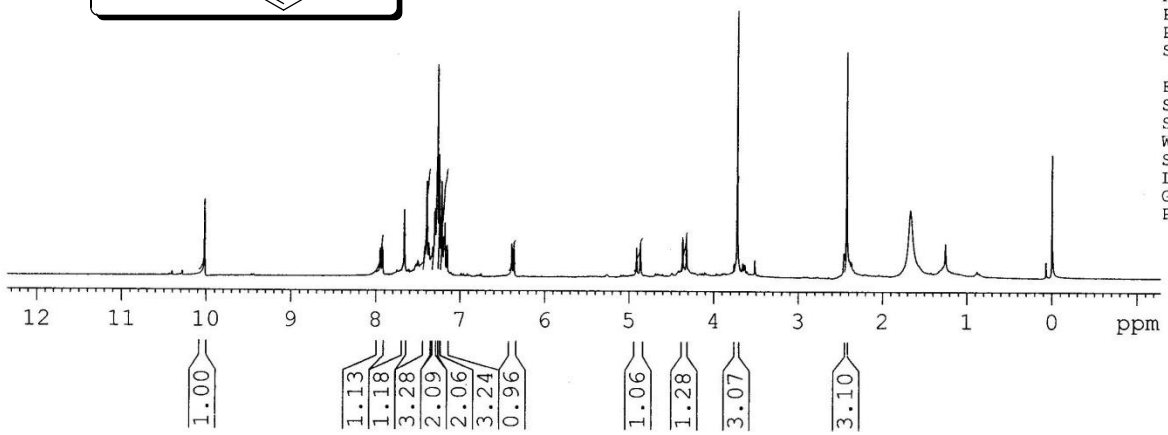
```
Current Data Parameters
NAME                  VV-54F
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20150422
Time                  12.32
INSTRUM               spect
PROBHD   5 mm DUL 13C-1
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     2310
DS                        4
SWH               17985.611 Hz
FIDRES            0.274439 Hz
AQ                1.8219508 sec
RG                     3251
DW                   27.800 usec
DE                    6.00 usec
TE                   300.0 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                    13C
P1                     9.30 usec
PL1                    0.00 dB
SFO1           75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                    0.00 dB
PL12                  15.68 dB
PL13                  16.00 dB
SFO2          300.1312005 MHz

F2 - Processing parameters
SI                     32768
SF             75.4677482 MHz
WDW                       EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.40
```

Sample Name	MM-54F	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	MM-54F.d	**ACQ Method**	Pondicherry Universi	**Comment**	MSK-MB-496.0859	**Acquired Time**	05-06-2015 14:49:27



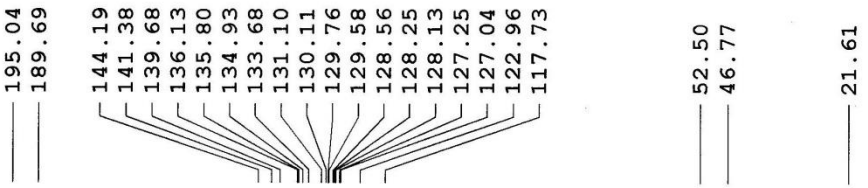


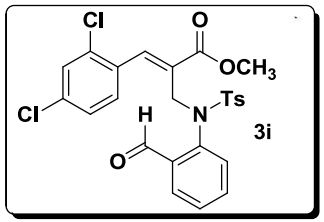


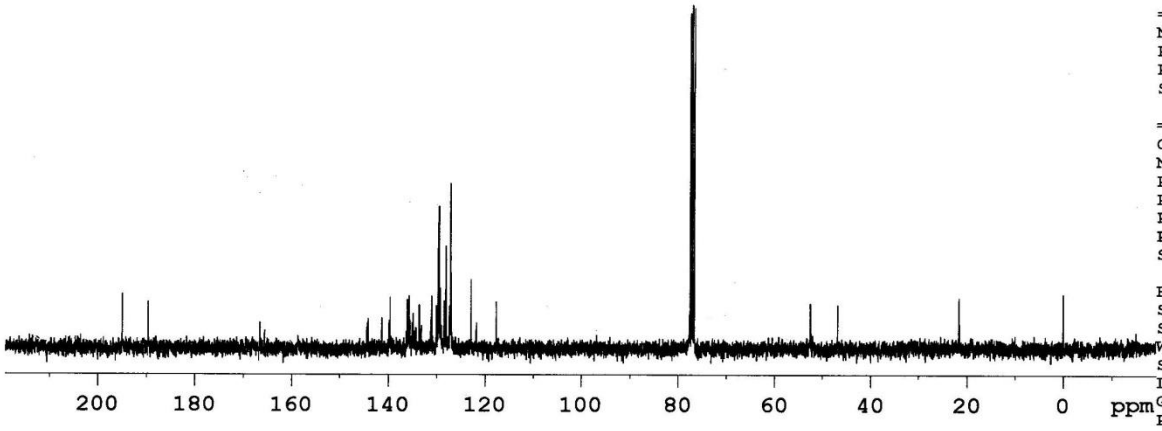


BRUKER

```
Current Data Parameters
NAME                  VV-52
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20121204
Time                  23.13
INSTRUM               spect
PROBHD    5 mm DUL 13C-1
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                6172.839 Hz
FIDRES             0.094190 Hz
AQ                 5.3084660 sec
RG                     287.4
DW                    81.000 usec
DE                     6.00 usec
TE                     300.0 K
D1                 1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                    13.15 usec
PL1                    0.00 dB
SFO1          300.1318534 MHz

F2 - Processing parameters
SI                    32768
SF            300.1300049 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```







BRUKER

Current Data Parameters

NAME	VV-237
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20150622
Time	20.26
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	78
DS	4
SWH	17985.611 Hz
FIDRES	0.274439 Hz
AQ	1.8219508 sec
RG	20642.5
DW	27.800 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1

======== CHANNEL f1 ========

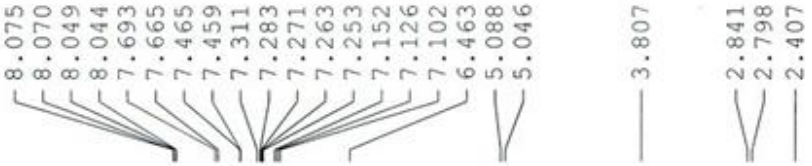
NUC1	13C
P1	10.38 usec
PL1	0.00 dB
SFO1	75.4752953 MHz

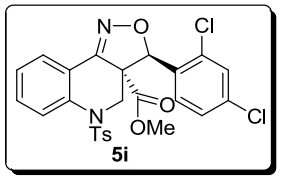
======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.00 dB
PL12	15.21 dB
PL13	16.00 dB
SFO2	300.1312005 MHz

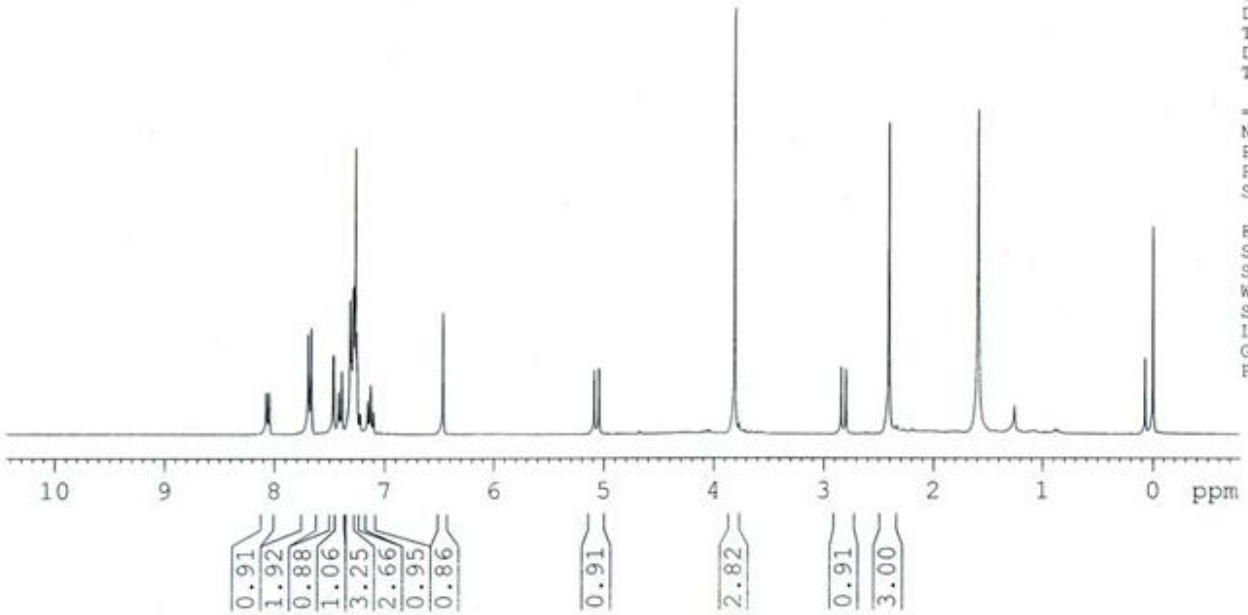
F2 - Processing parameters

SI	32768
SF	75.4677496 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



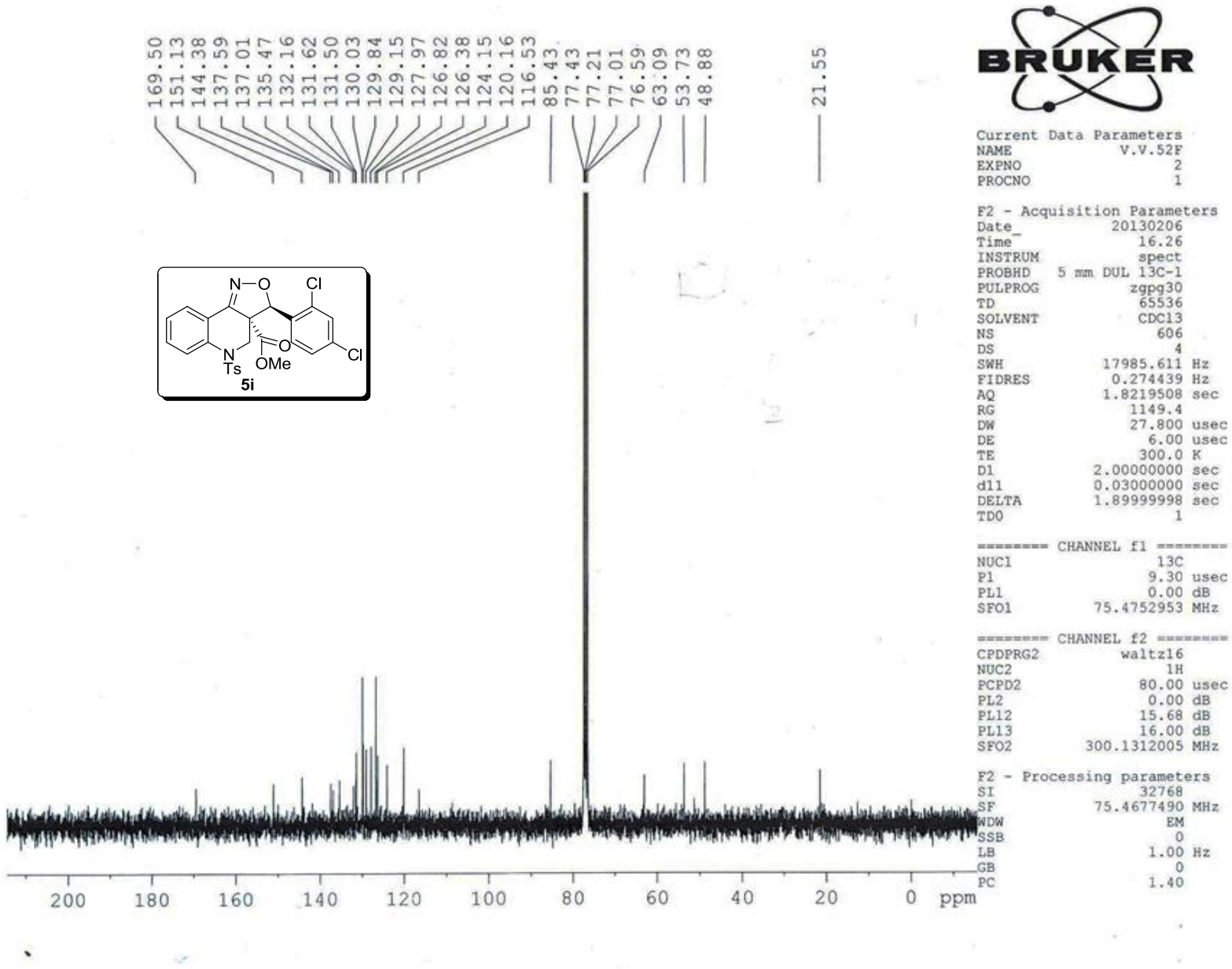


5i



BRUKER

```
Current Data Parameters
NAME                  V.V.52F
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20130206
Time                  16.21
INSTRUM               spect
PROBHD    5 mm DUL 13C-1
PULPROG               zg30
TD                    65536
SOLVENT               CDCl3
NS                       11
DS                        2
SWH                6172.839 Hz
FIDRES            0.094190 Hz
AQ                5.3084660 sec
RG                    322.5
DW                   81.000 usec
DE                    6.00 usec
TE                   300.0 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     1H
P1                   13.15 usec
PL1                   0.00 dB
SFO1          300.1318534 MHz

F2 - Processing parameters
SI                    32768
SF            300.1300058 MHz
WDW                      EM
SSB                       0
LB                    0.30 Hz
GB                        0
PC                    1.00
```



BRUKER

Current Data Parameters
NAME V.V.52F
EXPNO 2
PROCNO 1

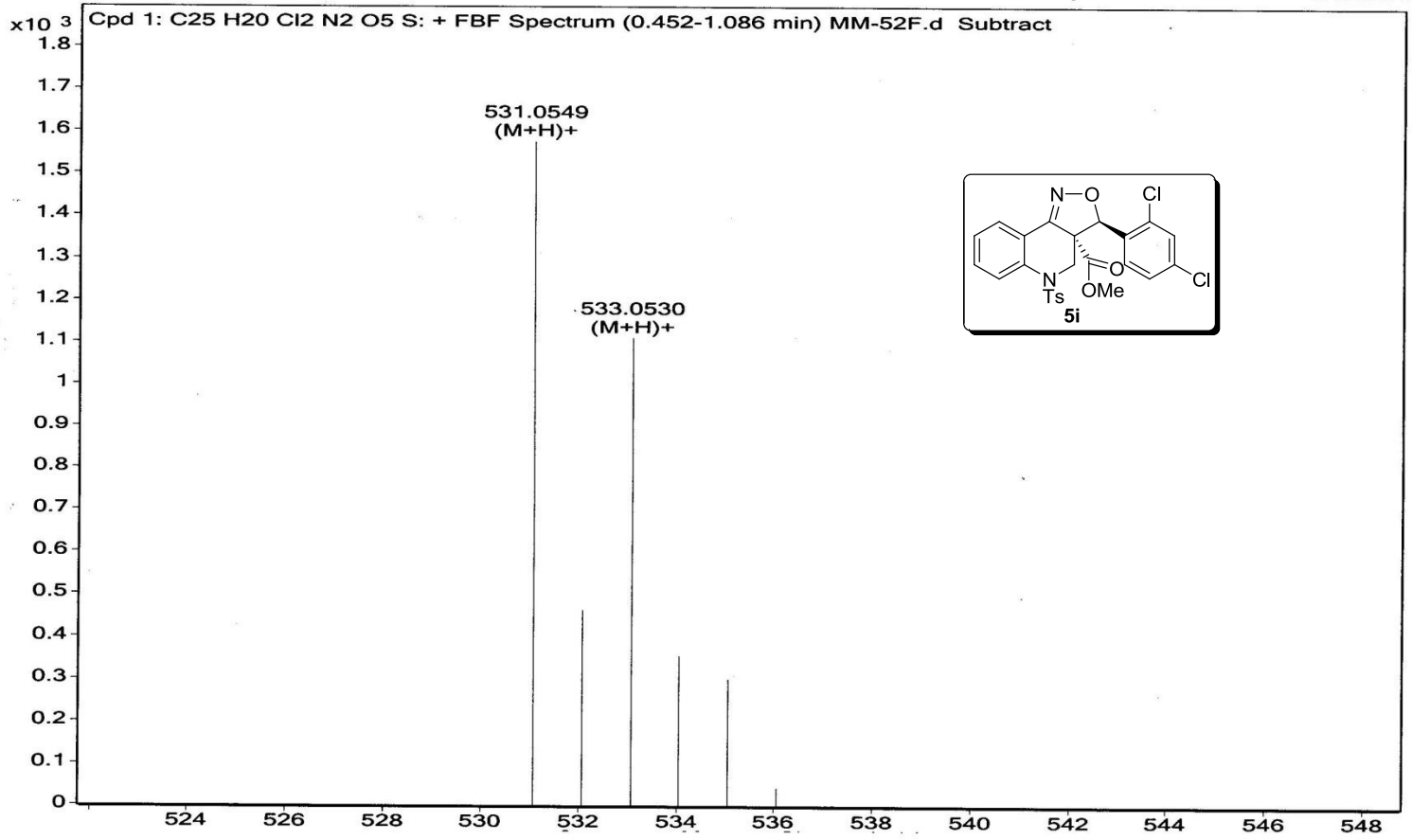
F2 - Acquisition Parameters
Date_ 20130206
Time 16.26
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 606
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 1149.4
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

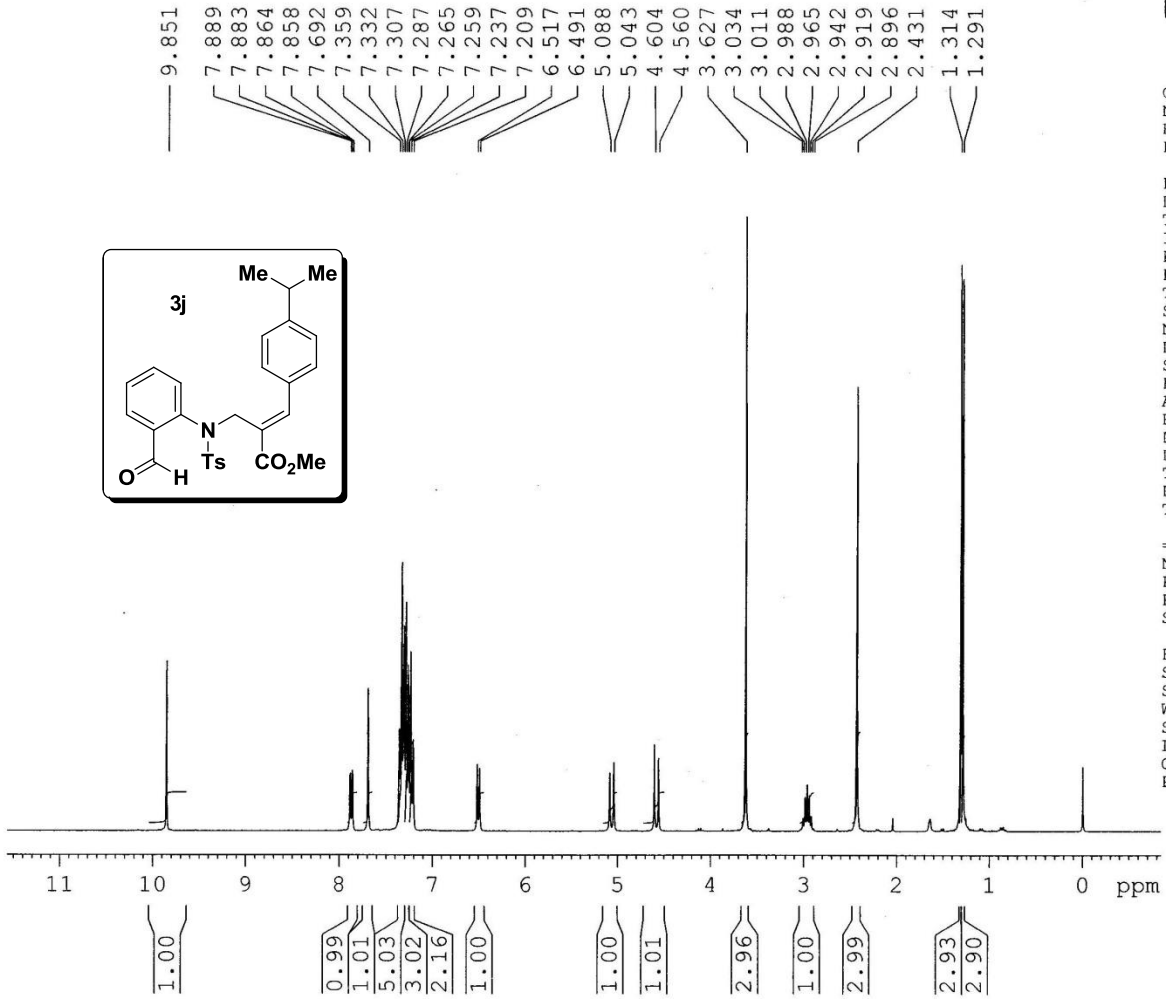
======== CHANNEL f1 ========
NUC1 13C
P1 9.30 usec
PL1 0.00 dB
SFO1 75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.68 dB
PL13 16.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

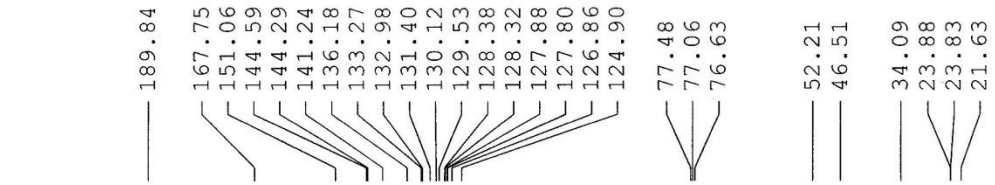
Sample Name	MM-52F	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	MM-52F.d	**ACQ Method**	Pondicherry Universi	**Comment**	MSK-MB-530.0470	**Acquired Time**	05-06-2015 13:27:49

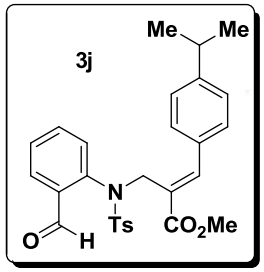


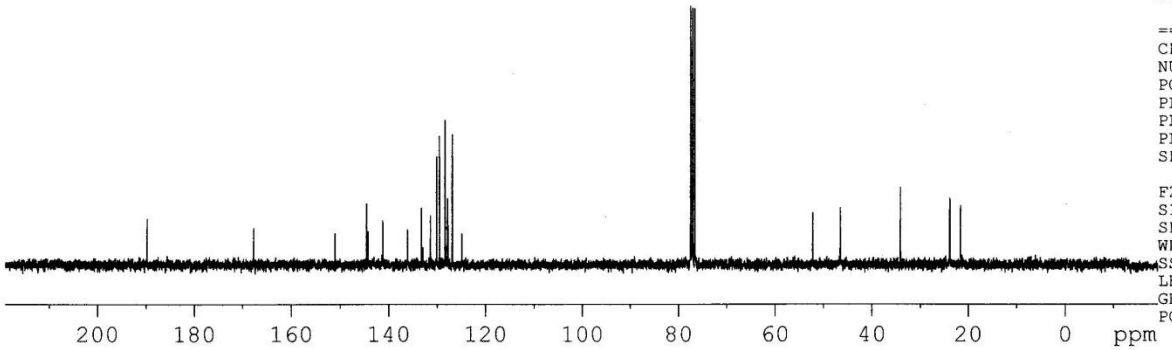


BRUKER

```
Current Data Parameters
NAME      DK-V-PIP-EST-TS-CHO
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20121211
Time                  19.57
INSTRUM               spect
PROBHD    5 mm DUL 13C-1
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      12
DS                       2
SWH                6172.839 Hz
FIDRES             0.094190 Hz
AQ                 5.3084660 sec
RG                      80.6
DW                    81.000 usec
DE                     6.00 usec
TE                    300.0 K
D1                 1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                      13.15 usec
PL1                      0.00 dB
SFO1            300.1318534 MHz

F2 - Processing parameters
SI                      32768
SF              300.1300051 MHz
WDW                        EM
SSB                         0
LB                       0.30 Hz
GB                          0
PC                       1.00
```

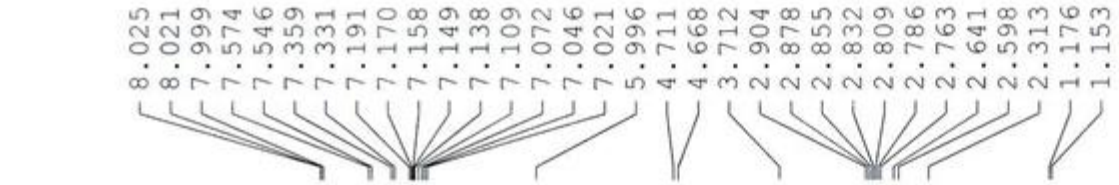


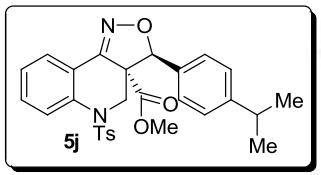


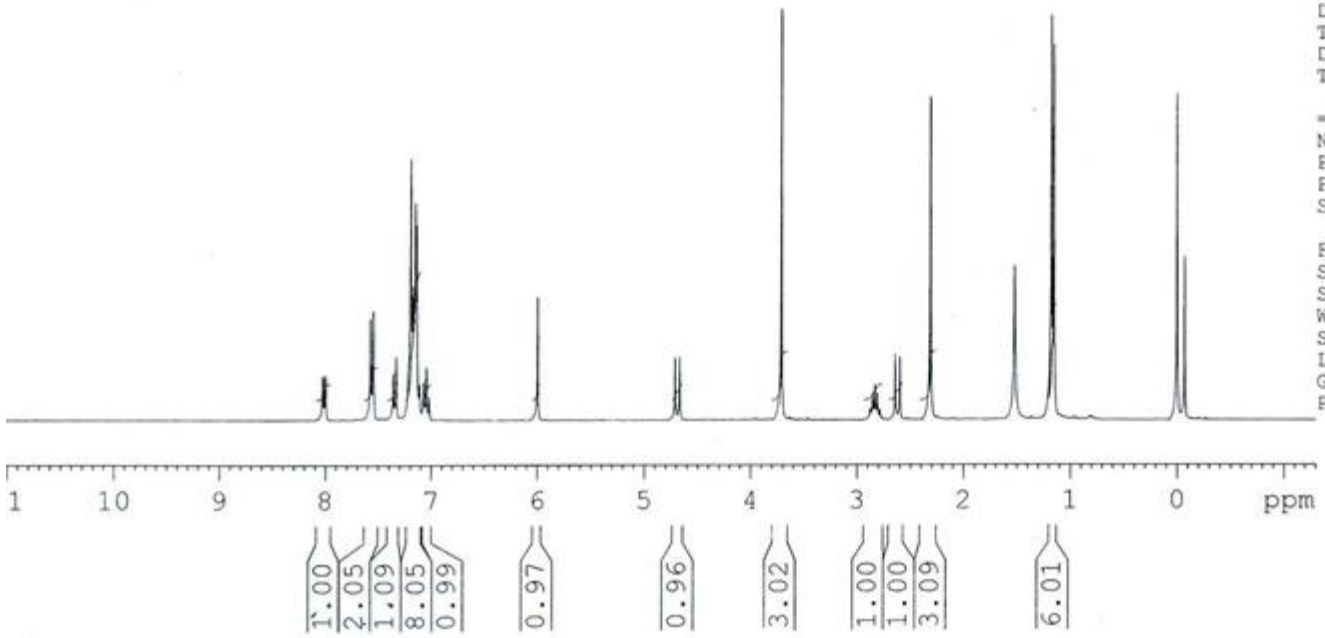


BRUKER

```
Current Data Parameters
NAME      DK-V-PIP-EST-TS-CHO
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_              20121211
Time                  20.02
INSTRUM               spect
PROBHD   5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT              CDC13
NS                      65
DS                       4
SWH               17985.611 Hz
FIDRES             0.274439 Hz
AQ                1.8219508 sec
RG                      512
DW                   27.800 usec
DE                    6.00 usec
TE                   300.0 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   13C
P1                    9.30 usec
PL1                   0.00 dB
SFO1           75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                   1H
PCPD2                80.00 usec
PL2                   0.00 dB
PL12                 15.68 dB
PL13                 16.00 dB
SFO2          300.1312005 MHz

F2 - Processing parameters
SI                    32768
SF             75.4677490 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```

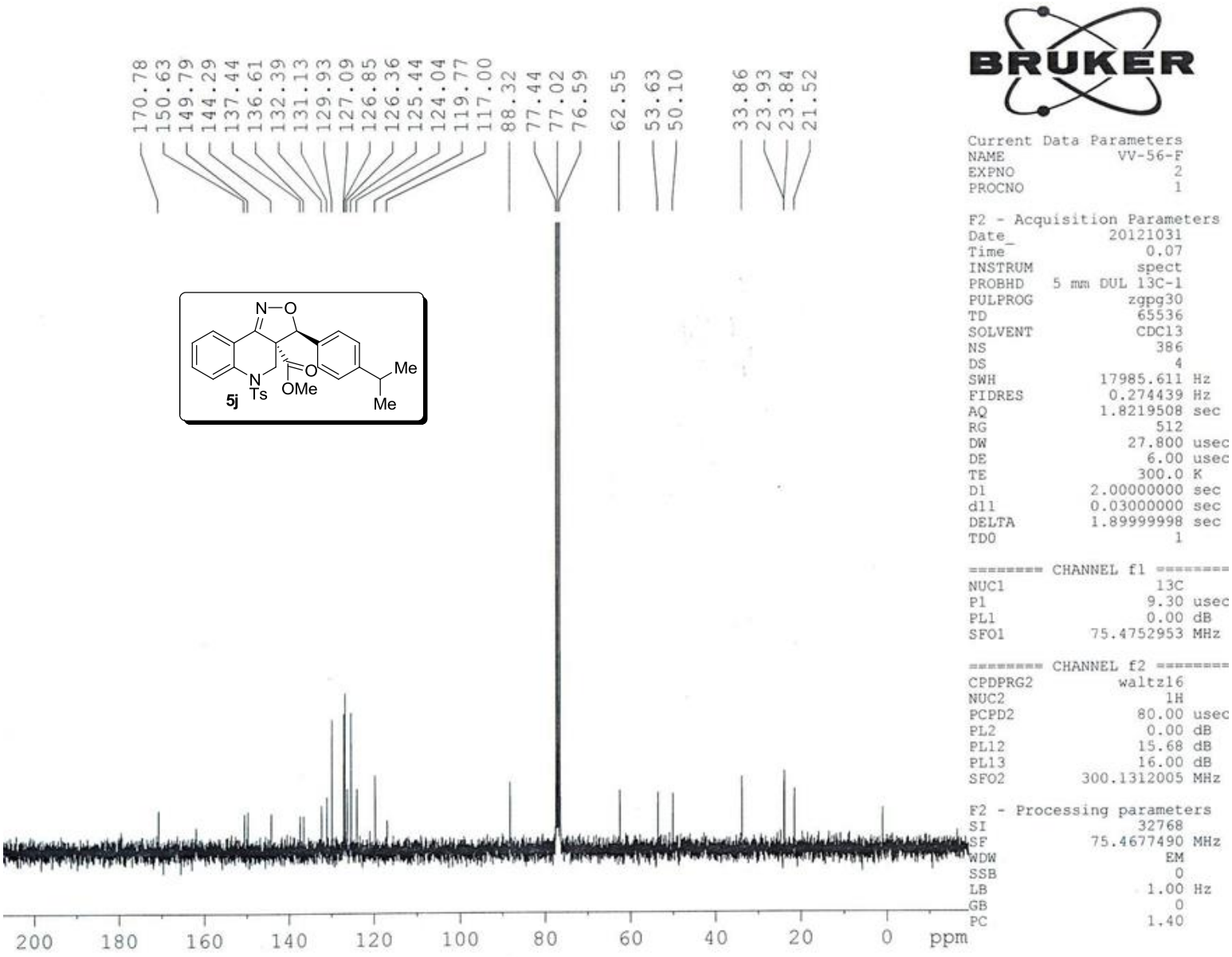






BRUKER

```
Current Data Parameters
NAME                  VV-56-F
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20121031
Time                    0.01
INSTRUM                spect
PROBHD    5 mm DUL 13C-1
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                        9
DS                        2
SWH                6172.839 Hz
FIDRES            0.094190 Hz
AQ                5.3084660 sec
RG                    322.5
DW                 81.000 usec
DE                  6.00 usec
TE                  300.0 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                 13.15 usec
PL1                 0.00 dB
SFO1          300.1318534 MHz

F2 - Processing parameters
SI                    32768
SF            300.1300274 MHz
WDW                      EM
SSB                       0
LB                 0.30 Hz
GB                        0
PC                     1.00
```



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Current Data Parameters
NAME VV-56-F
EXPNO 2
PROCNO 1

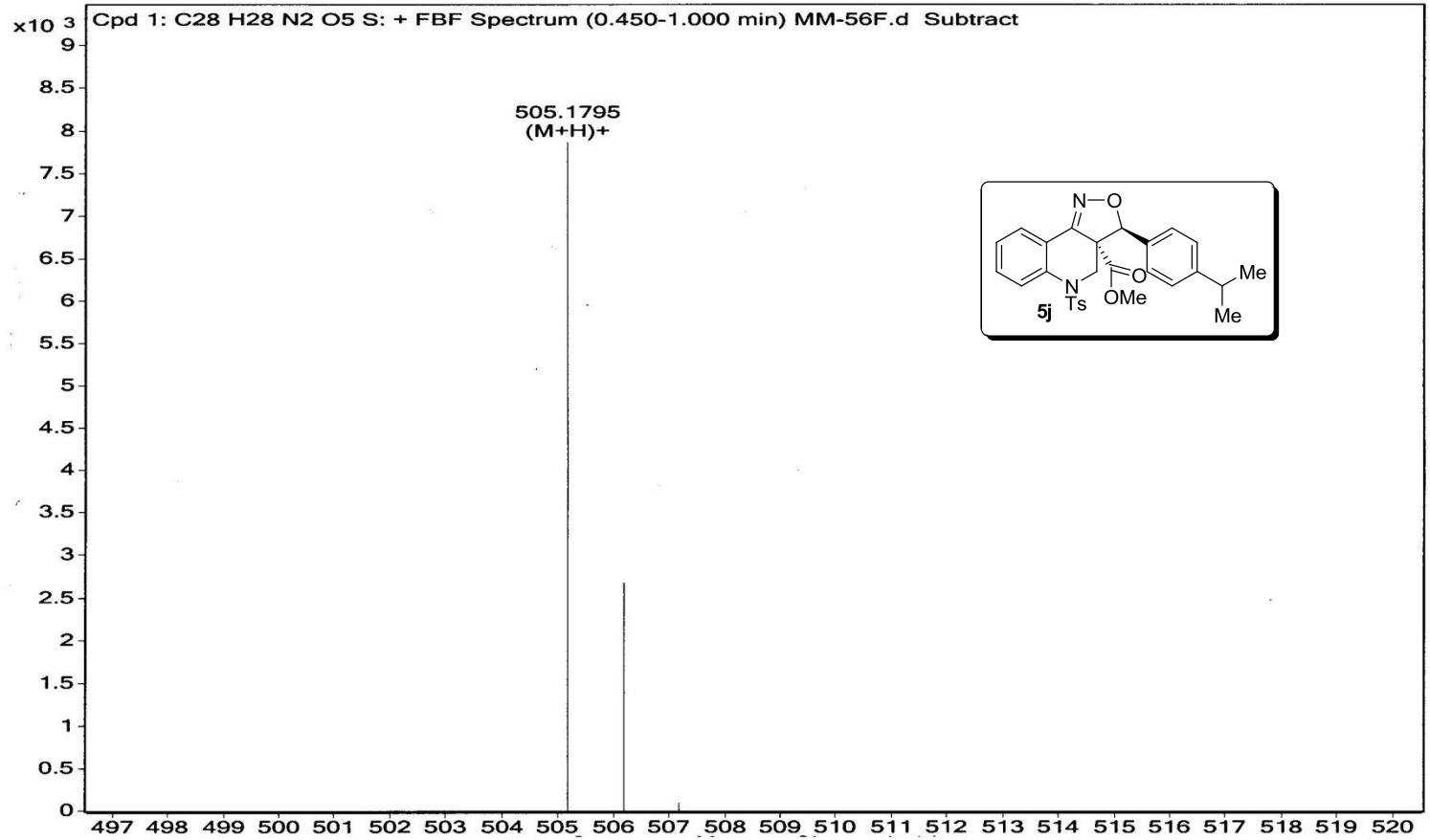
F2 - Acquisition Parameters
Date_ 20121031
Time 0.07
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 386
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 512
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

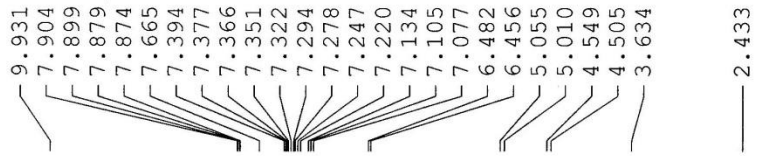
======== CHANNEL f1 ========
NUC1 13C
P1 9.30 usec
PL1 0.00 dB
SFO1 75.4752953 MHz

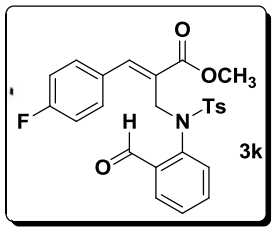
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.68 dB
PL13 16.00 dB
SFO2 300.1312005 MHz

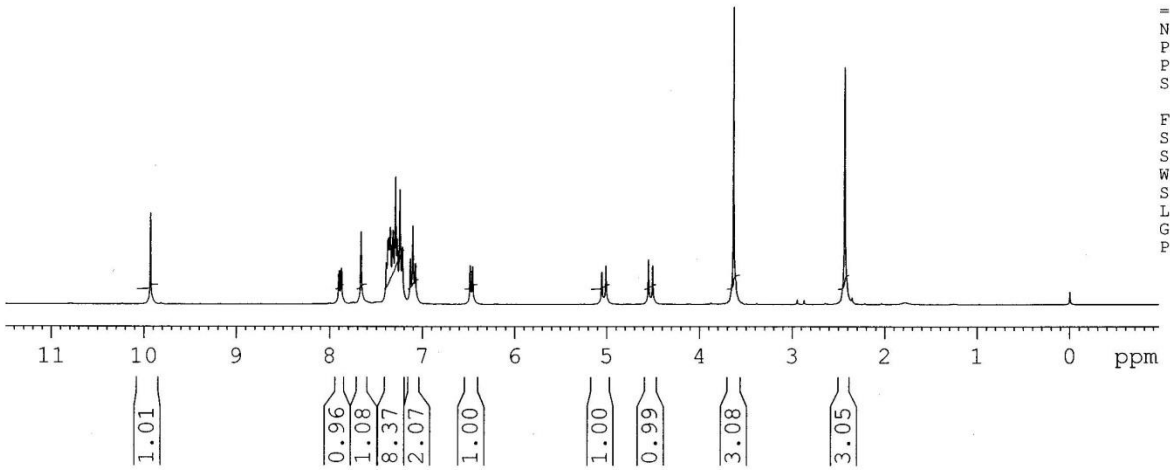
F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Sample Name	MM-56F	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	MM-56F.d	**ACQ Method**	Pondicherry Universi	**Comment**	MSK-MB-504.1718	**Acquired Time**	05-06-2015 12:47:15







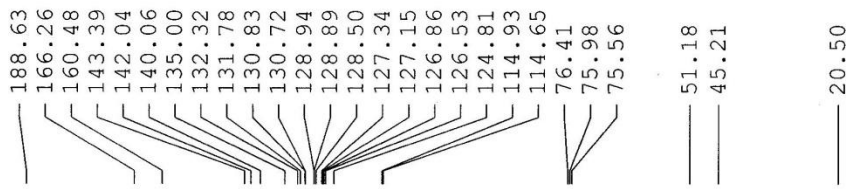


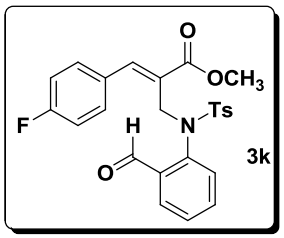
Current Data Parameters
NAME DK-V-4-F-EST-CHO
EXPNO 1
PROCNO 1

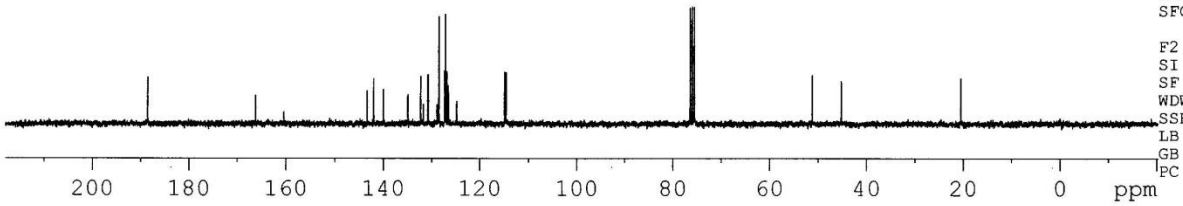
F2 - Acquisition Parameters
Date_ 20130303
Time 23.11
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 57
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 13.15 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300019 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00







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Current Data Parameters
NAME DK-V-4-F-EST-CHO
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_	20130303
Time	23.19
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	39
DS	4
SWH	17985.611 Hz
FIDRES	0.274439 Hz
AQ	1.8219508 sec
RG	1024
DW	27.800 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1

======== CHANNEL f1 ========

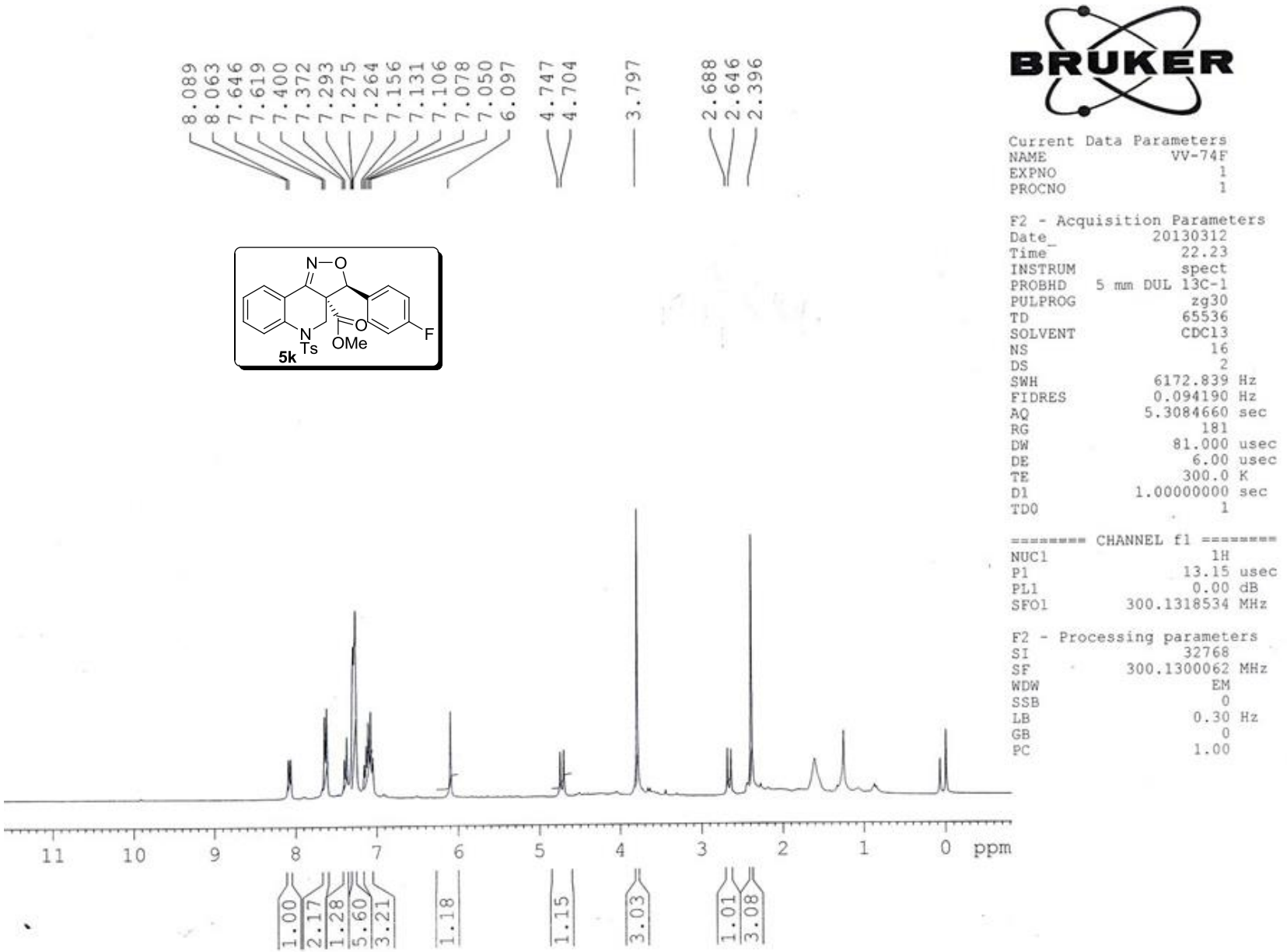
NUC1	13C
P1	9.30 usec
PL1	0.00 dB
SFO1	75.4752953 MHz

======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.00 dB
PL12	15.68 dB
PL13	16.00 dB
SFO2	300.1312005 MHz

F2 - Processing parameters

SI	32768
SF	75.4678335 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



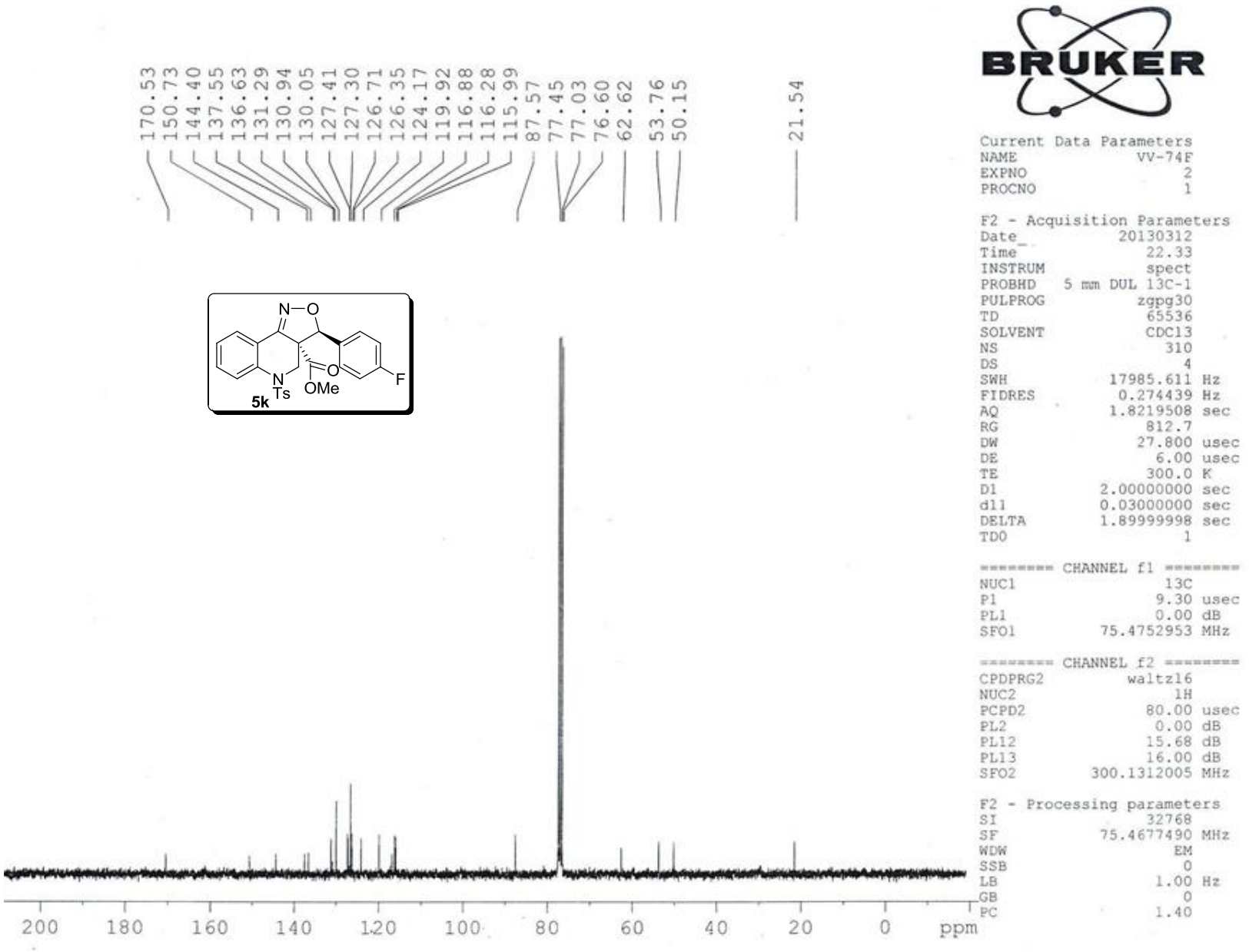
BRUKER

Current Data Parameters
NAME VV-74F
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130312
Time 22.23
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 181
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 13.15 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

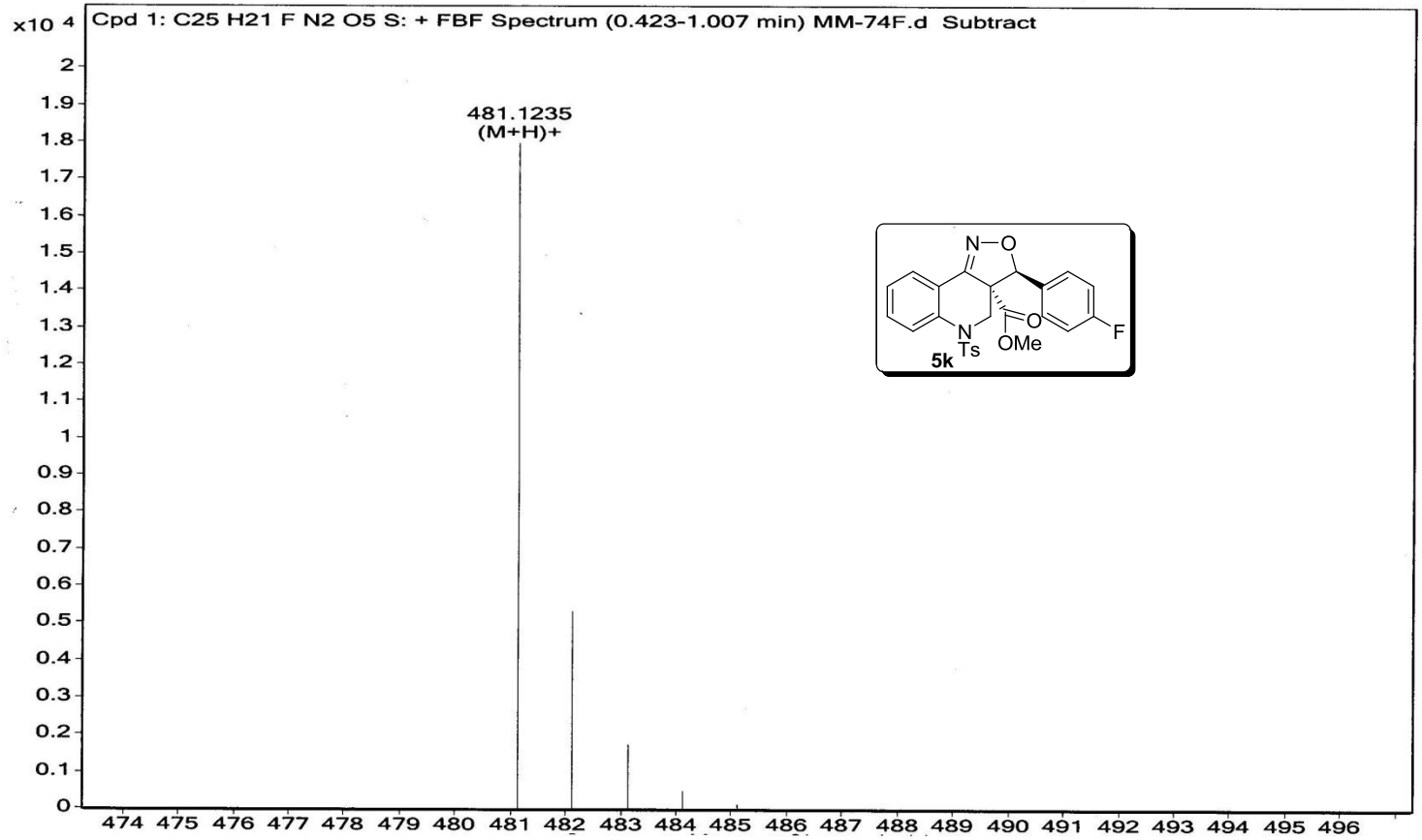
F2 - Processing parameters
SI 32768
SF 300.1300062 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

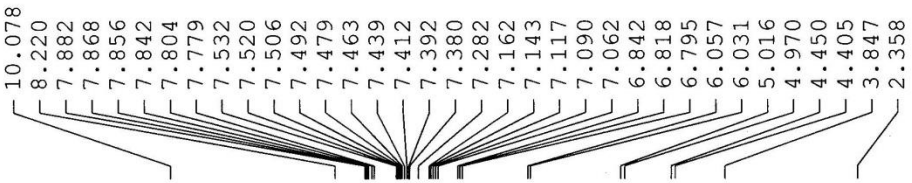


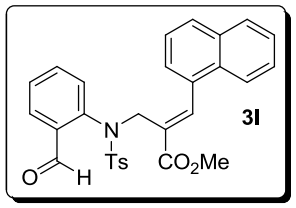
BRUKER

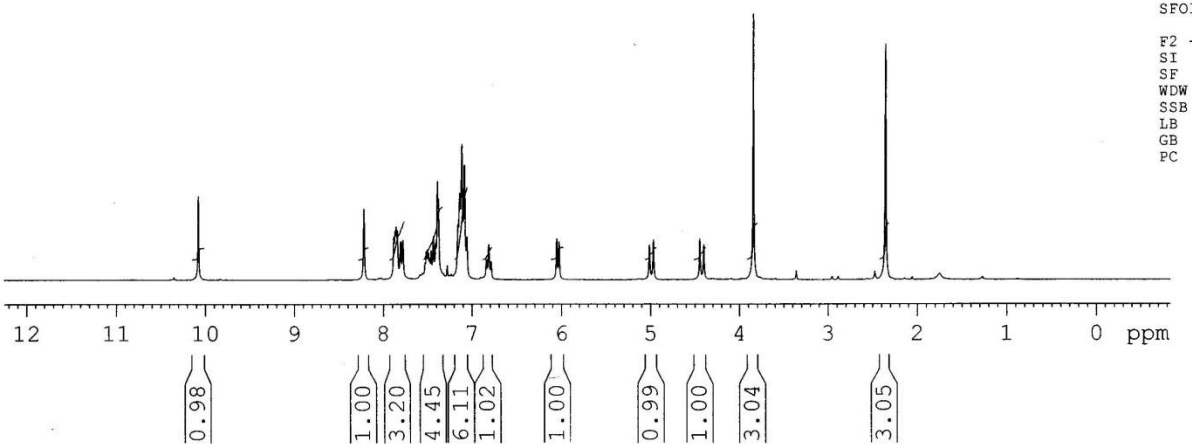
```
Current Data Parameters
NAME                  VV-74F
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20130312
Time                  22.33
INSTRUM               spect
PROBHD   5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT              CDC13
NS                     310
DS                       4
SWH             17985.611 Hz
FIDRES          0.274439 Hz
AQ              1.8219508 sec
RG                   812.7
DW                27.800 usec
DE                 6.00 usec
TE                 300.0 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                  9.30 usec
PL1                 0.00 dB
SFO1          75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                   1H
PCPD2              80.00 usec
PL2                 0.00 dB
PL12               15.68 dB
PL13               16.00 dB
SFO2         300.1312005 MHz

F2 - Processing parameters
SI                     32768
SF            75.4677490 MHz
WDW                    EM
SSB                     0
LB                  1.00 Hz
GB                      0
PC                  1.40
```

Sample Name	MM-74F	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	MM-74F.d	**ACQ Method**	Pondicherry Universi	**Comment**	MSK-MB-480.1155	**Acquired Time**	05-06-2015 13:16:38



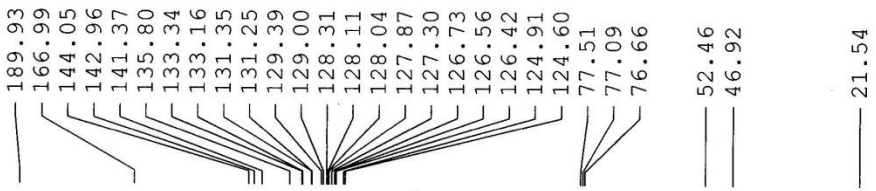


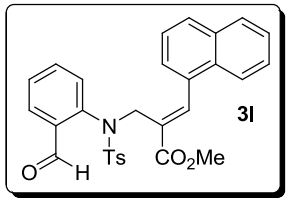


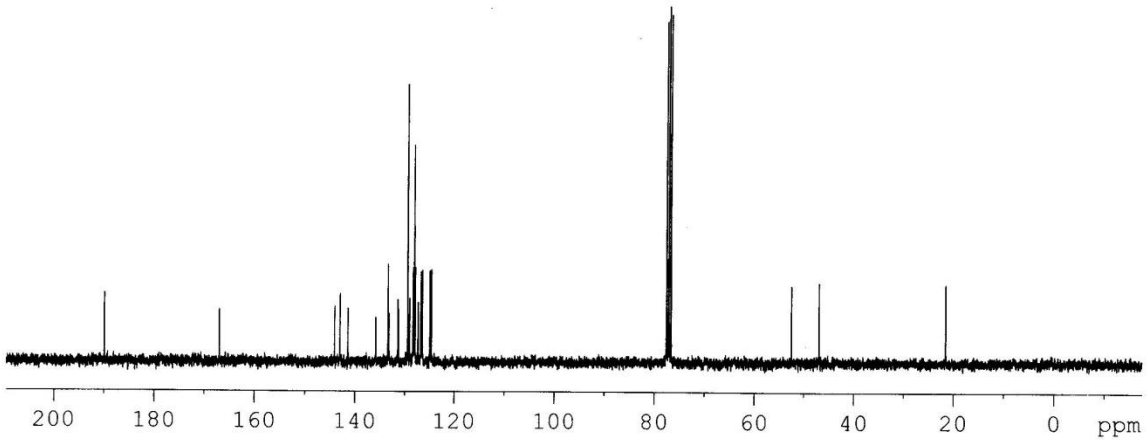


BRUKER

```
Current Data Parameters
NAME      DK-V-NAP-EST-Ts-CHO
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20111009
Time              16.19
INSTRUM           spect
PROBHD   5 mm DUL 13C-1
PULPROG             zg30
TD                65536
SOLVENT           CDCl3
NS                    7
DS                    2
SWH            6172.839 Hz
FIDRES         0.094190 Hz
AQ             5.3084660 sec
RG                   64
DW               81.000 usec
DE                6.00 usec
TE               300.0 K
D1            1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
P1                13.15 usec
PL1                0.00 dB
SFO1        300.1318534 MHz

F2 - Processing parameters
SI                32768
SF          300.1300000 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```

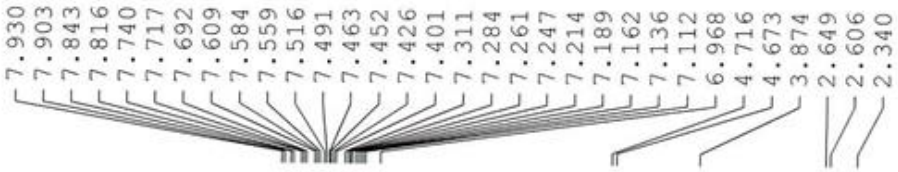


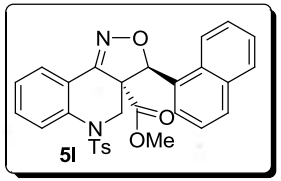


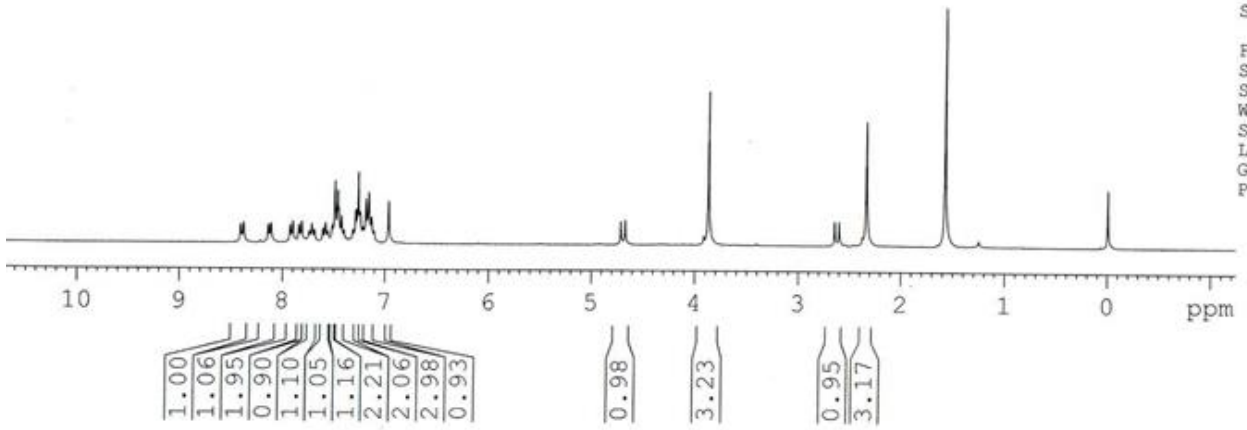


BRUKER

```
Current Data Parameters
NAME      DK-V-NAP-EST-Ts-CHO
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_              20111009
Time                  16.23
INSTRUM               spect
PROBHD   5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     106
DS                       4
SWH             17985.611 Hz
FIDRES              0.274439 Hz
AQ                1.8219508 sec
RG                   2580.3
DW                   27.800 usec
DE                    6.00 usec
TE                   300.0 K
D1               2.00000000 sec
d11              0.03000000 sec
DELTA            1.89999998 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                    13C
P1                     9.30 usec
PL1                    0.00 dB
SFO1           75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                    0.00 dB
PL12                  15.68 dB
PL13                  16.00 dB
SFO2          300.1312005 MHz

F2 - Processing parameters
SI                      32768
SF             75.4677490 MHz
WDW                        EM
SSB                         0
LB                     1.00 Hz
GB                          0
PC                     1.40
```

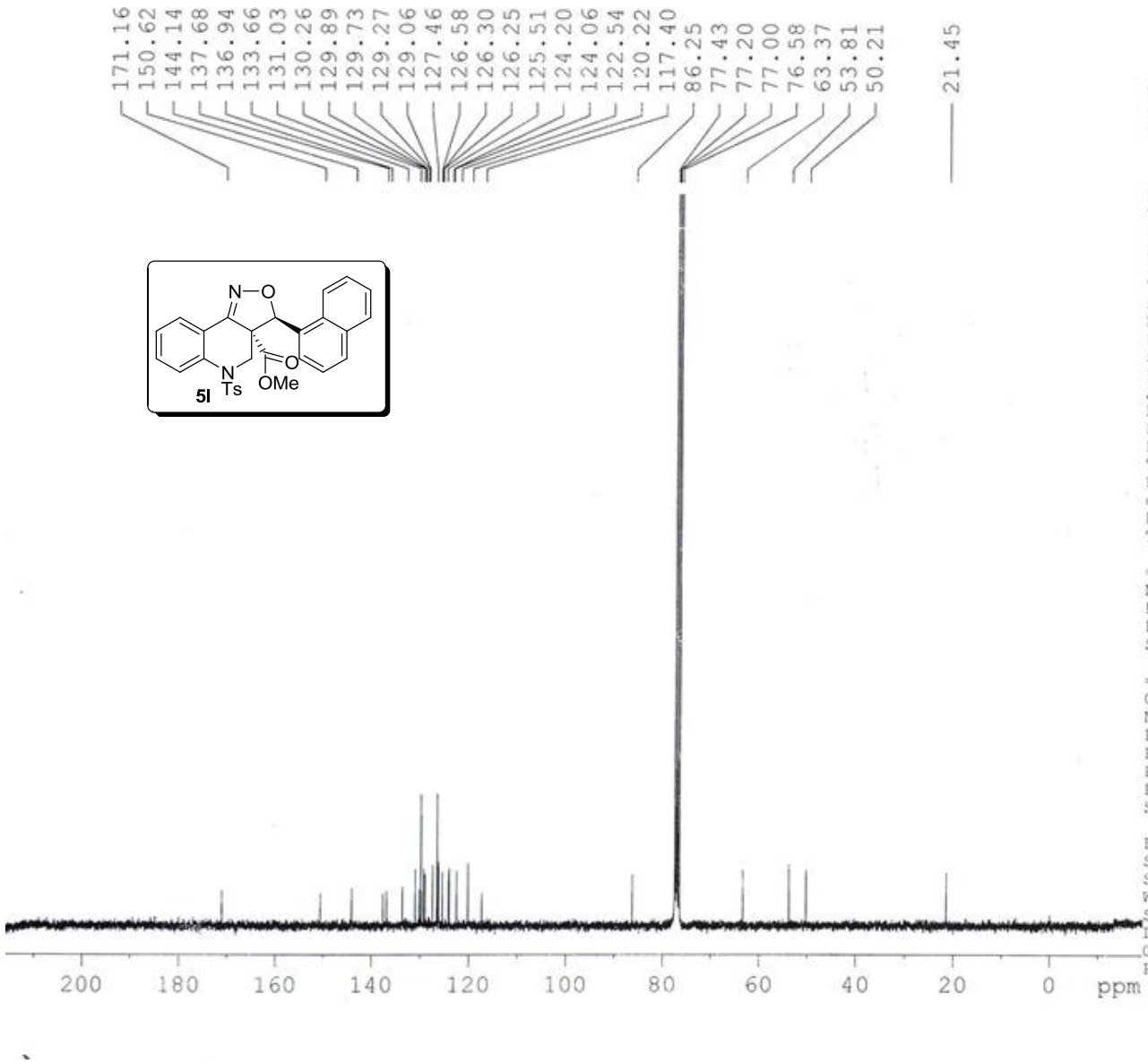






BRUKER

```
Current Data Parameters
NAME                  VV-73F
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20130516
Time                  18.11
INSTRUM               spect
PROBHD    5 mm DUL 13C-1
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH               6172.839 Hz
FIDRES               0.094190 Hz
AQ                5.3084660 sec
RG                    322.5
DW                  81.000 usec
DE                    6.00 usec
TE                   300.0 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                  13.15 usec
PL1                   0.00 dB
SFO1          300.1318534 MHz

F2 - Processing parameters
SI                    32768
SF            300.1300071 MHz
WDW                      EM
SSB                       0
LB                    0.30 Hz
GB                        0
PC                     1.00
```



BRUKER

Current Data Parameters
NAME VV-73F
EXPNO 3
PROCNO 1

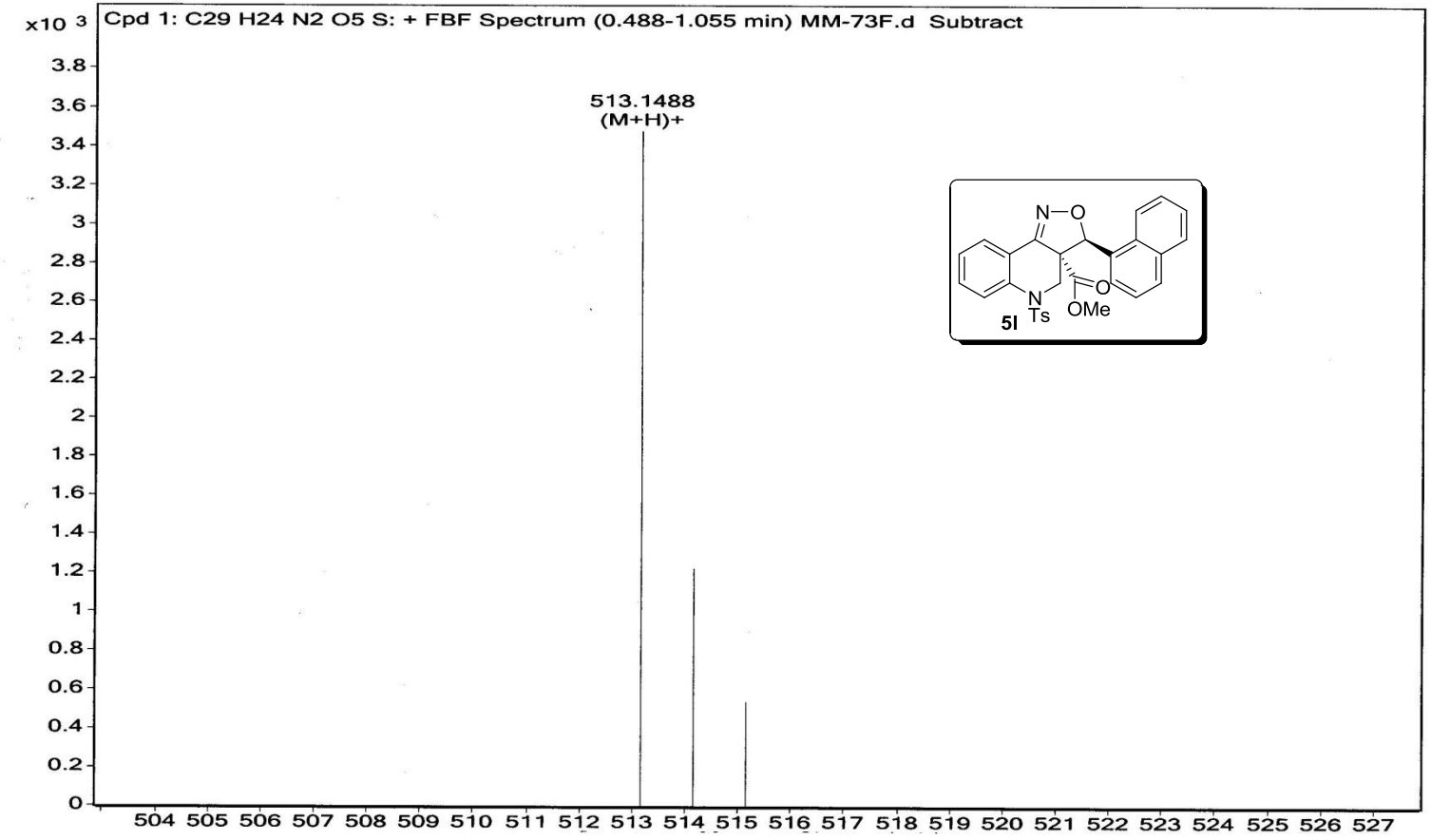
F2 - Acquisition Parameters
Date_ 20130523
Time 20.22
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2155
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 456.1
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

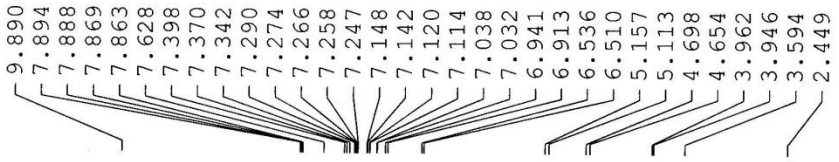
======== CHANNEL f1 ========
NUC1 13C
P1 9.30 usec
PL1 0.00 dB
SFO1 75.4752953 MHz

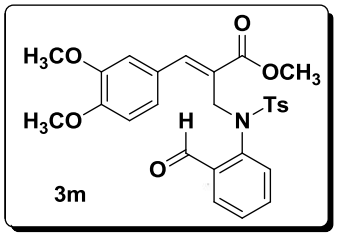
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.68 dB
PL13 16.00 dB
SFO2 300.1312005 MHz

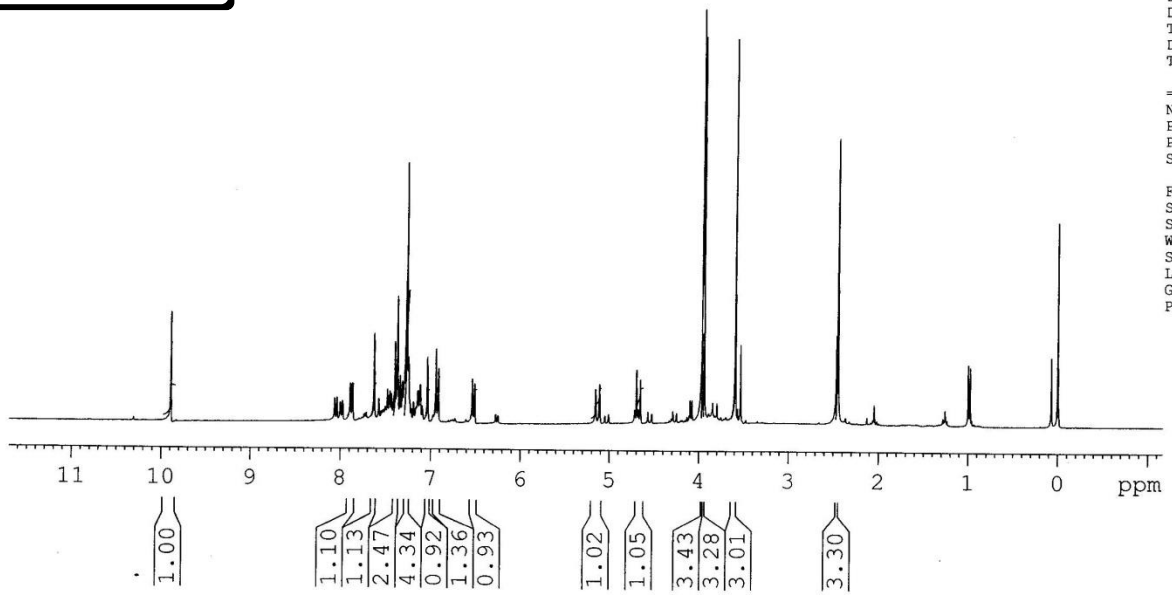
F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Sample Name	MM-73F	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	MM-73F.d	**ACQ Method**	Pondicherry Universi	**Comment**	MSK-MB-512.1406	**Acquired Time**	05-06-2015 12:50:52



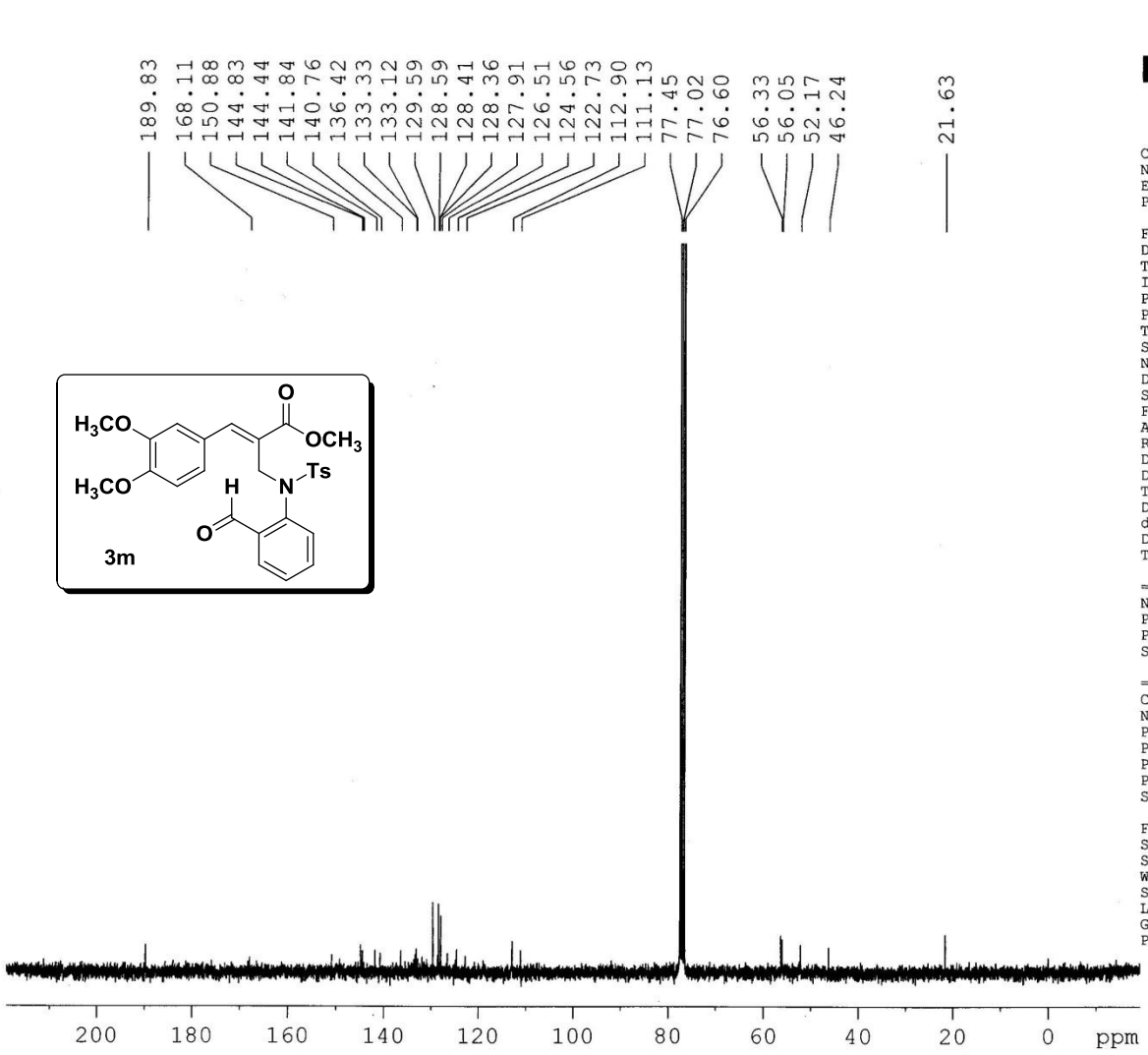






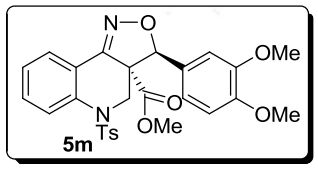
BRUKER

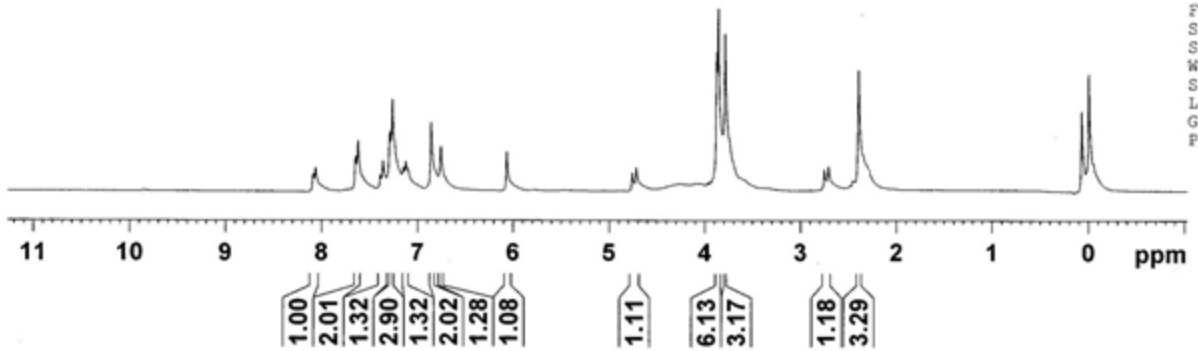
```
Current Data Parameters
NAME      DK-V-DI-OME-EST-TS-CHO
EXPNO                          1
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20130305
Time                       20.57
INSTRUM                    spect
PROBHD   5 mm DUL 13C-1
PULPROG                     zg30
TD                         65536
SOLVENT                    CDCl3
NS                            16
DS                             2
SWH                     6172.839 Hz
FIDRES                  0.094190 Hz
AQ                      5.3084660 sec
RG                         203.2
DW                        81.000 usec
DE                         6.00 usec
TE                        300.0 K
D1                      1.00000000 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                          1H
P1                         13.15 usec
PL1                         0.00 dB
SFO1                300.1318534 MHz

F2 - Processing parameters
SI                         32768
SF                  300.1300050 MHz
WDW                           EM
SSB                            0
LB                          0.30 Hz
GB                             0
PC                          1.00
```



BRUKER

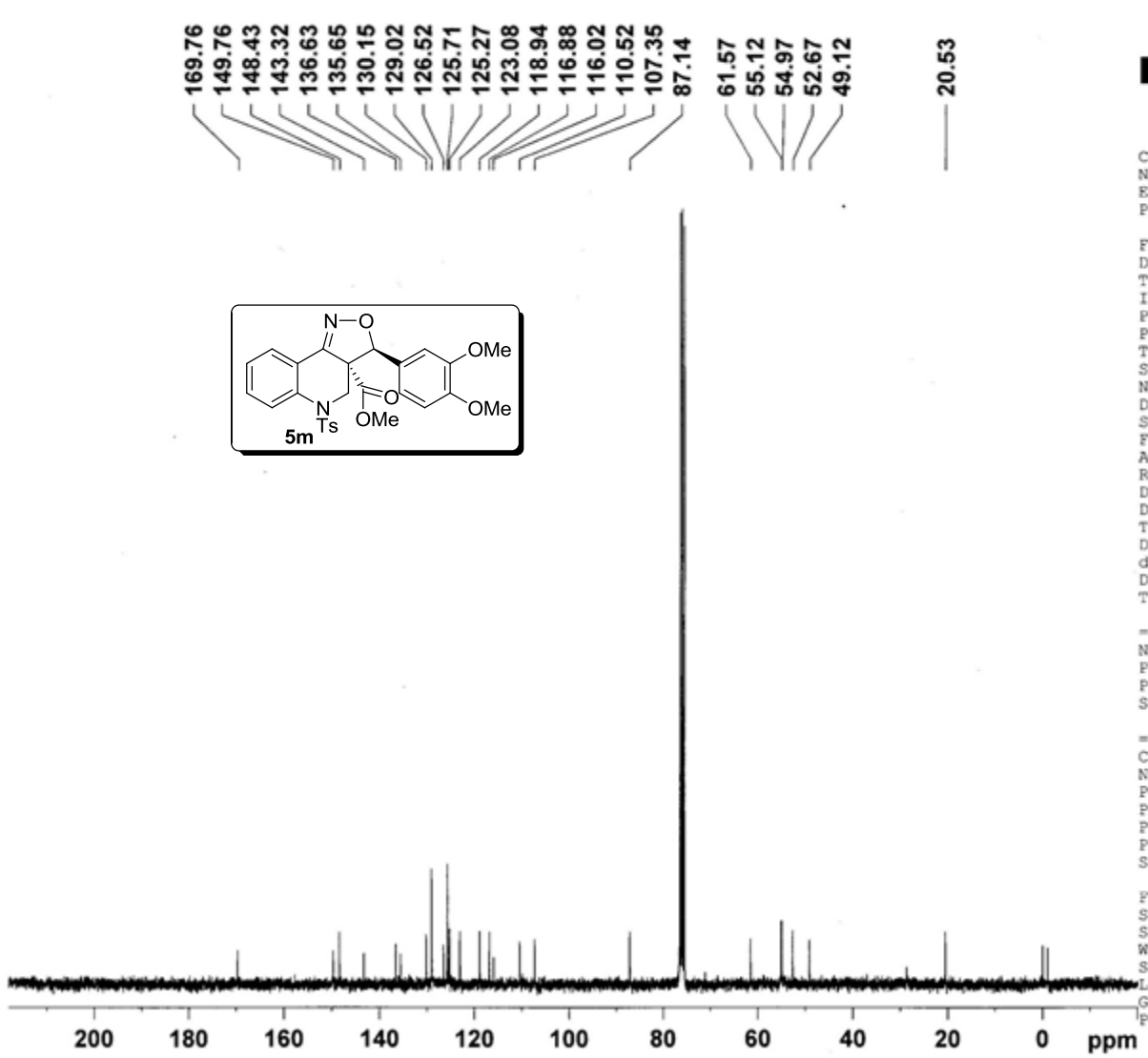
```
Current Data Parameters
NAME      DK-V-DI-OME-EST-TS-CHO
EXPNO                          2
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20130305
Time                       21.16
INSTRUM                    spect
PROBHD   5 mm DUL 13C-1
PULPROG                  zgpg30
TD                        65536
SOLVENT                   CDCl3
NS                          277
DS                            4
SWH                   17985.611 Hz
FIDRES                 0.274439 Hz
AQ                    1.8219508 sec
RG                        645.1
DW                       27.800 usec
DE                        6.00 usec
TE                       300.0 K
D1                  2.00000000 sec
d11                 0.03000000 sec
DELTA               1.89999998 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                        13C
P1                         9.30 usec
PL1                        0.00 dB
SFO1                75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                        1H
PCPD2                     80.00 usec
PL2                        0.00 dB
PL12                      15.68 dB
PL13                      16.00 dB
SFO2               300.1312005 MHz

F2 - Processing parameters
SI                         32768
SF                  75.4677490 MHz
WDW                           EM
SSB                            0
LB                          1.00 Hz
GB                             0
PC                          1.40
```





BRUKER

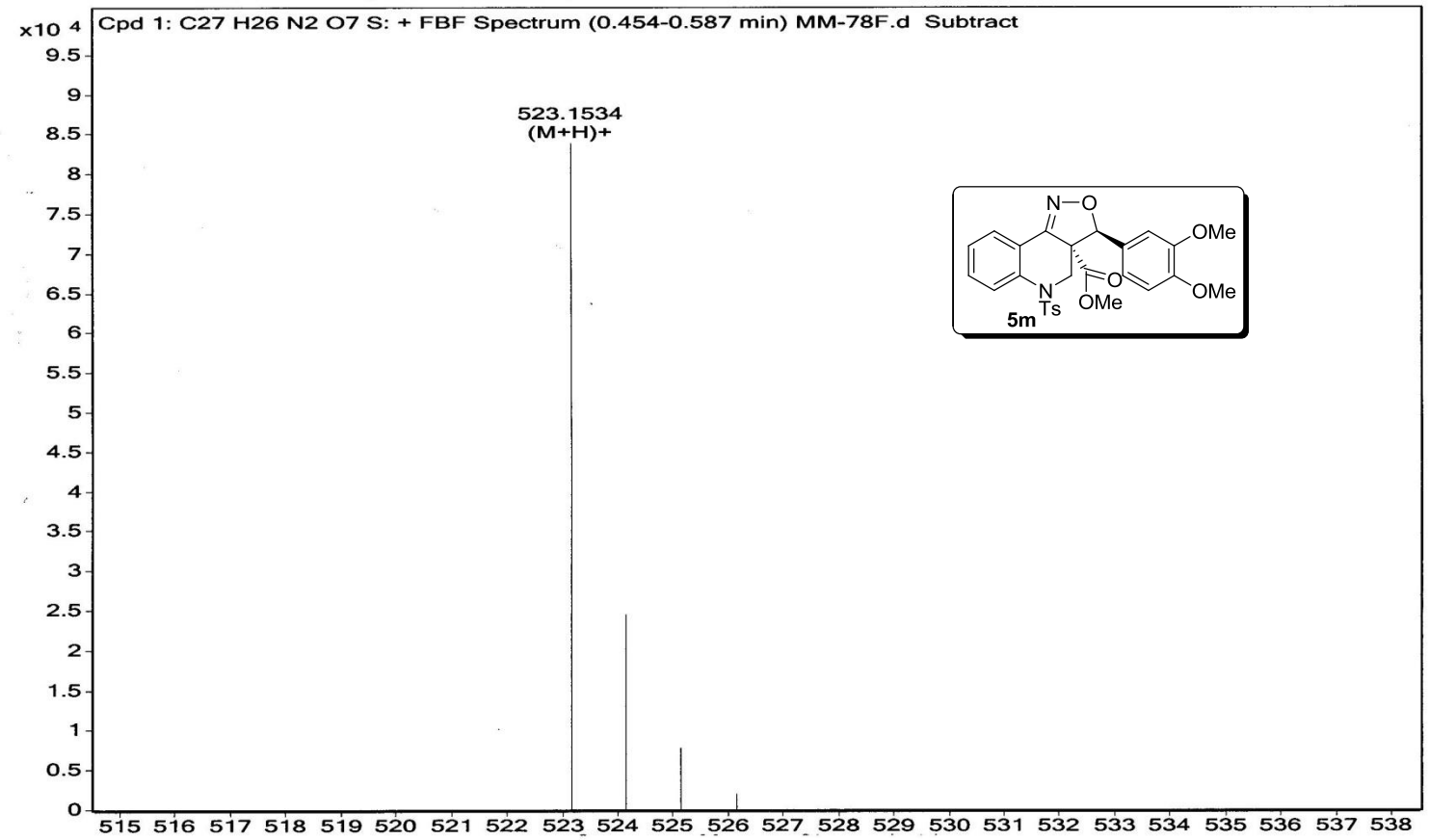
```
Current Data Parameters
NAME                  VV-78
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20130409
Time                 21.38
INSTRUM              spect
PROBHD   5 mm DUL 13C-1
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH                6172.839 Hz
FIDRES             0.094190 Hz
AQ                 5.3084660 sec
RG                      90.5
DW                    81.000 usec
DE                     6.00 usec
TE                    300.0 K
D1                 1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     1H
P1                    13.15 usec
PL1                    0.00 dB
SFO1           300.1318534 MHz

F2 - Processing parameters
SI                    32768
SF             300.1300078 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```

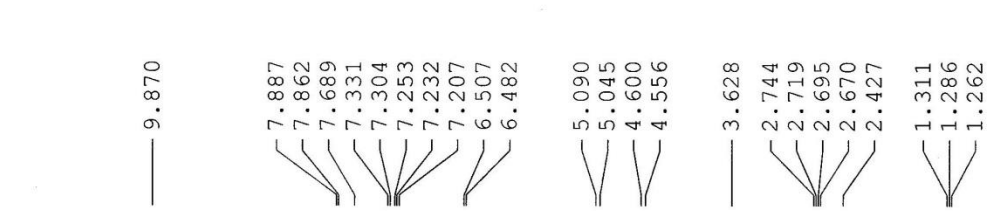


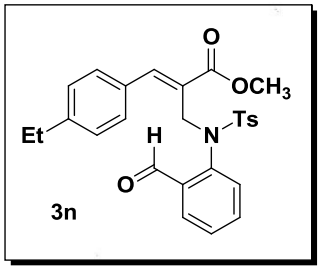
BRUKER

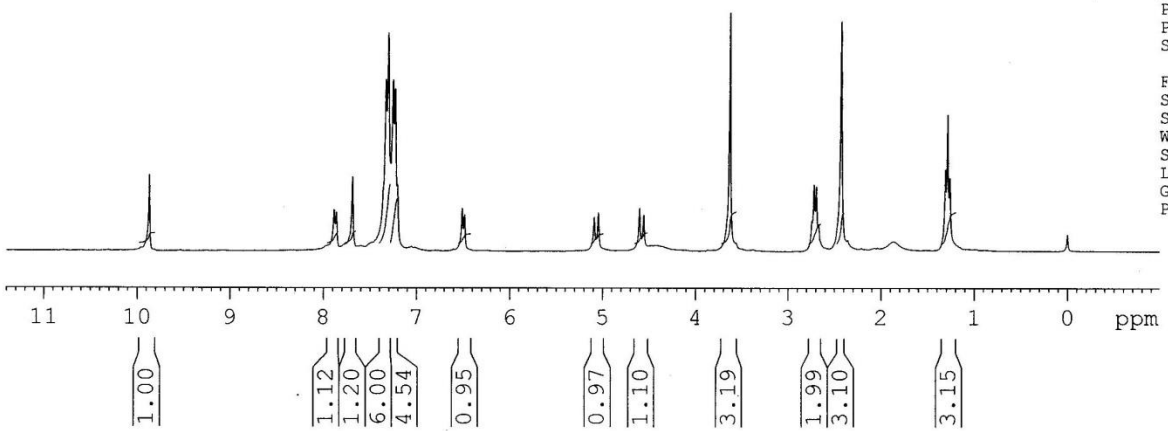
```
Current Data Parameters
NAME                  VV-78
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_              20130409
Time                  22.17
INSTRUM               spect
PROBHD    5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     600
DS                       4
SWH              17985.611 Hz
FIDRES           0.274439 Hz
AQ               1.8219508 sec
RG                  1824.6
DW                  27.800 usec
DE                   6.00 usec
TE                  300.0 K
D1               2.00000000 sec
d11              0.03000000 sec
DELTA            1.89999998 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                    9.30 usec
PL1                   0.00 dB
SFO1           75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                   1H
PCPD2                80.00 usec
PL2                   0.00 dB
PL12                 15.68 dB
PL13                 16.00 dB
SFO2          300.1312005 MHz

F2 - Processing parameters
SI                    32768
SF             75.4678256 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```

Sample Name	MM-78F	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	MM-78F.d	**ACQ Method**	Pondicherry Universi	**Comment**	MSK-MB-522.1460	**Acquired Time**	05-06-2015 14:45:06



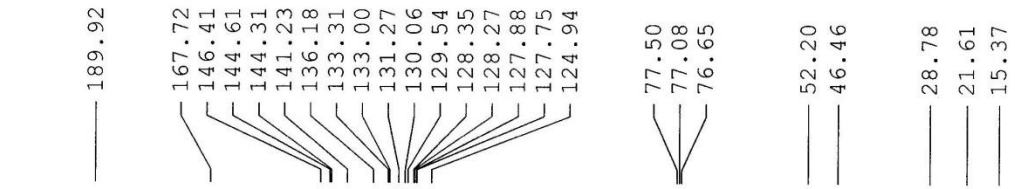


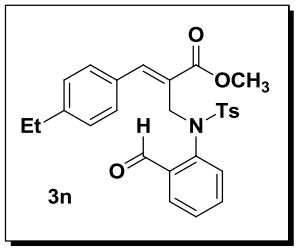


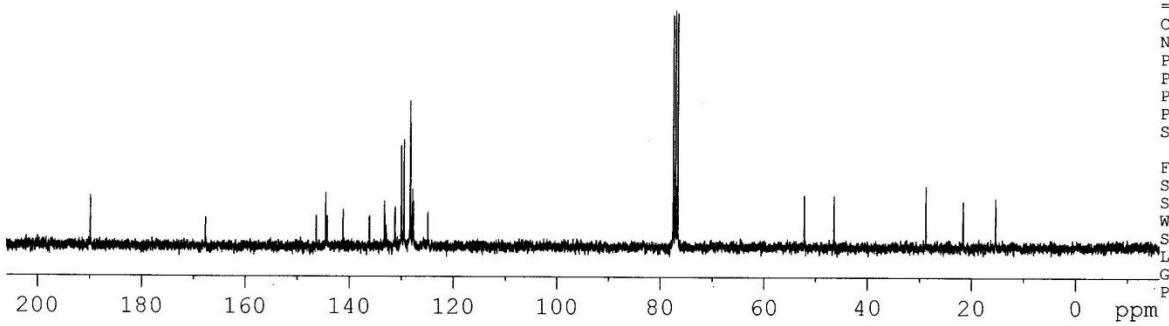


BRUKER

```
Current Data Parameters
NAME      DK-V-4-ET-EST-CHO
EXPNO                    3
PROCNO                   1

F2 - Acquisition Parameters
Date_              20130303
Time                 23.49
INSTRUM              spect
PROBHD   5 mm DUL 13C-1
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                      9
DS                      2
SWH             6172.839 Hz
FIDRES          0.094190 Hz
AQ              5.3084660 sec
RG                     64
DW                81.000 usec
DE                 6.00 usec
TE                300.0 K
D1             1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                 13.15 usec
PL1                 0.00 dB
SFO1         300.1318534 MHz

F2 - Processing parameters
SI                  32768
SF          300.1300041 MHz
WDW                    EM
SSB                     0
LB                 0.30 Hz
GB                      0
PC                   1.00
```







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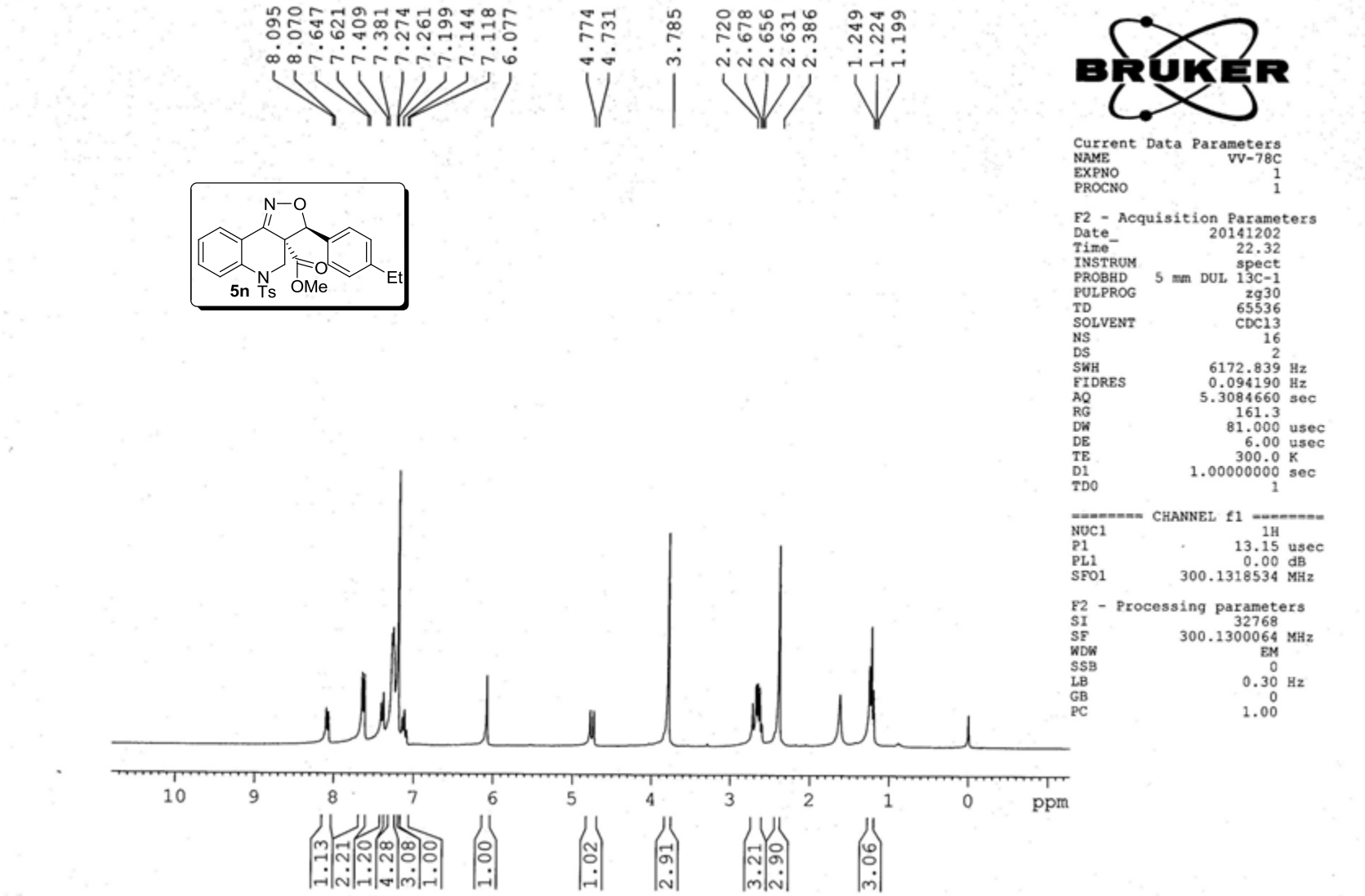
Current Data Parameters
NAME DK-V-4-ET-EST-CHO
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130303
Time 23.43
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 90
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 912.3
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.30 usec
PL1 0.00 dB
SFO1 75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.68 dB
PL13 16.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



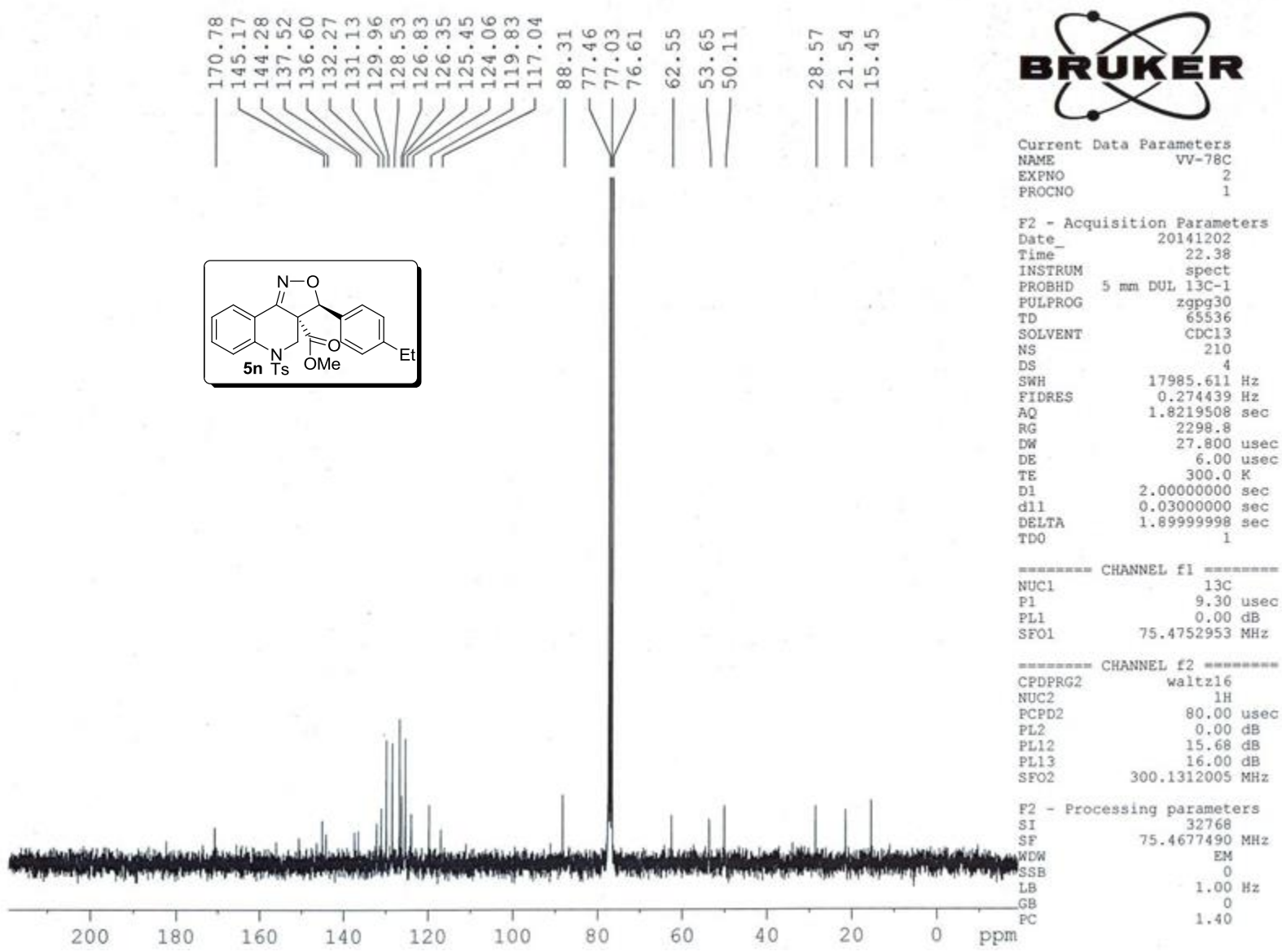
BRUKER

Current Data Parameters
NAME VV-78C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141202
Time 22.32
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 161.3
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 13.15 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

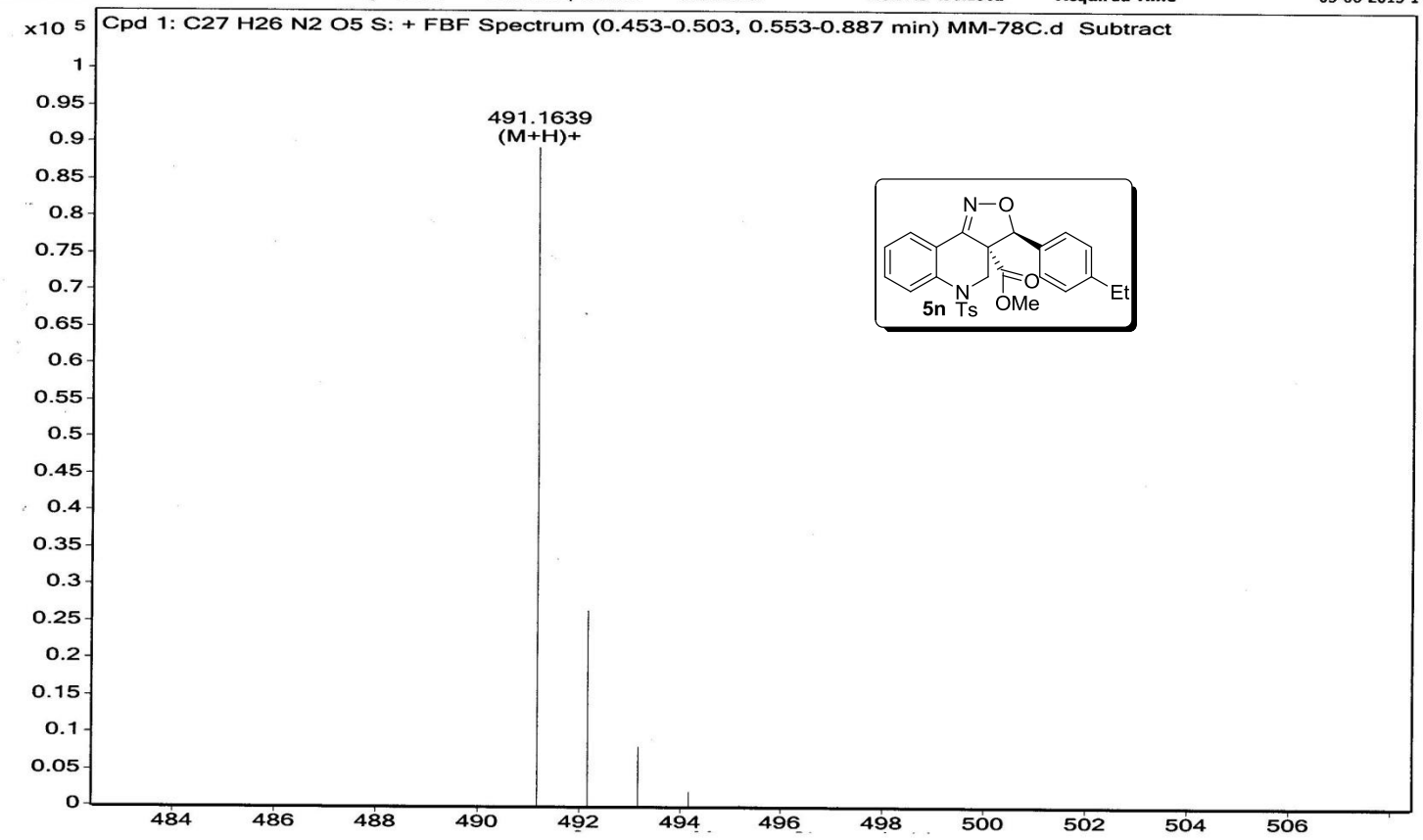
F2 - Processing parameters
SI 32768
SF 300.1300064 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

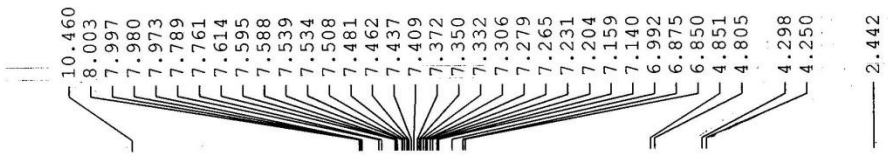


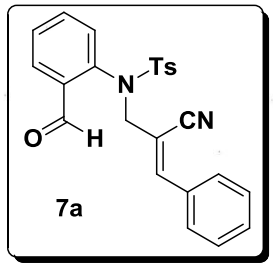
BRUKER

```
Current Data Parameters
NAME                  VV-78C
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20141202
Time                  22.38
INSTRUM               spect
PROBHD    5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     210
DS                       4
SWH               17985.611 Hz
FIDRES            0.274439 Hz
AQ                1.8219508 sec
RG                   2298.8
DW                   27.800 usec
DE                    6.00 usec
TE                   300.0 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                    13C
P1                    9.30 usec
PL1                   0.00 dB
SFO1           75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                   0.00 dB
PL12                 15.68 dB
PL13                 16.00 dB
SFO2          300.1312005 MHz

F2 - Processing parameters
SI                     32768
SF            75.4677490 MHz
WDW                       EM
SSB                        0
LB                    1.00 Hz
GB                         0
PC                    1.40
```

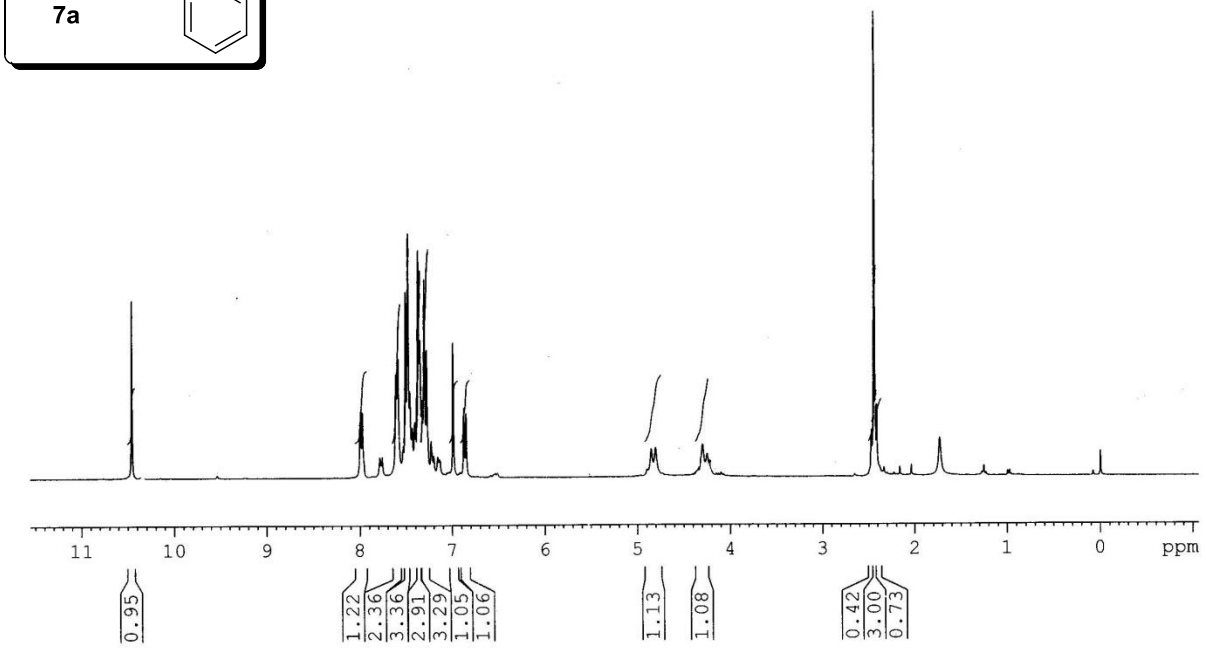
Sample Name	MM-78C	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	MM-78C.d	**ACQ Method**	Pondicherry Universi	**Comment**	MSK-MB-490.1562	**Acquired Time**	05-06-2015 14:24:55







7a

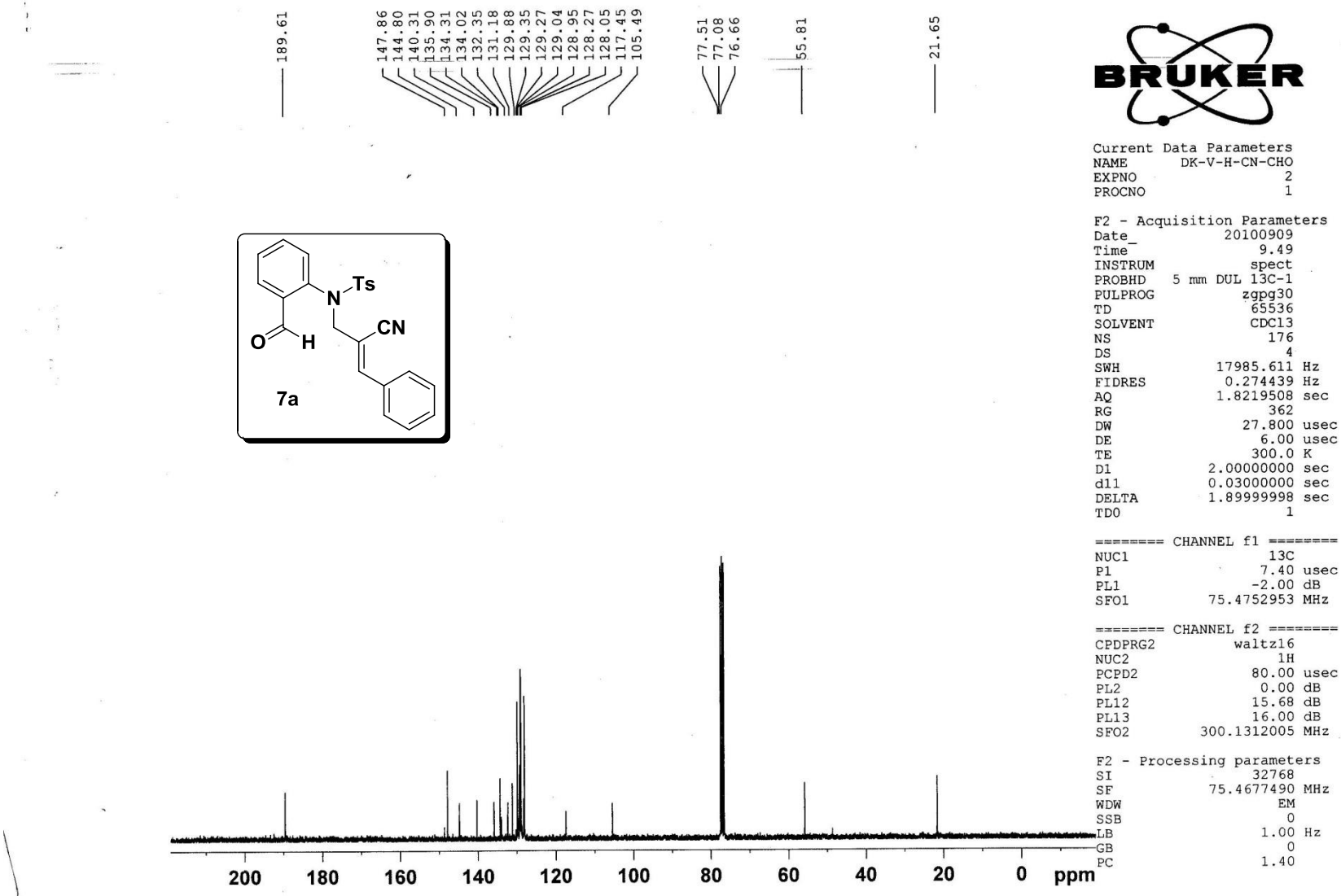


Current Data Parameters
NAME DK-V-H-CN-CHO
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100909
Time 9.37
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 7
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 71.8
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 13.15 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300051 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



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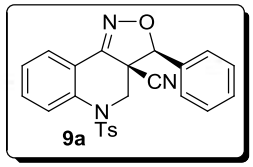
Current Data Parameters
NAME DK-V-H-CN-CHO
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100909
Time 9.49
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 176
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 362
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 7.40 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz

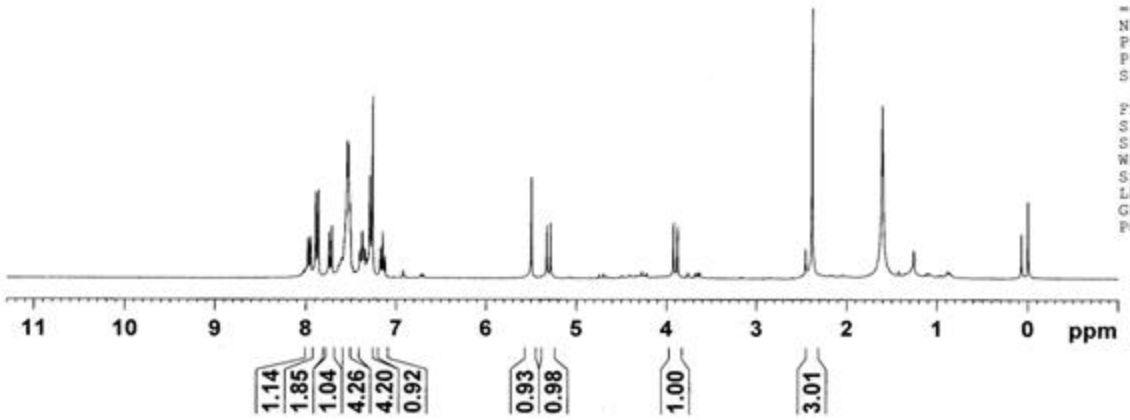
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.68 dB
PL13 16.00 dB
SFO2 300.1312005 MHz

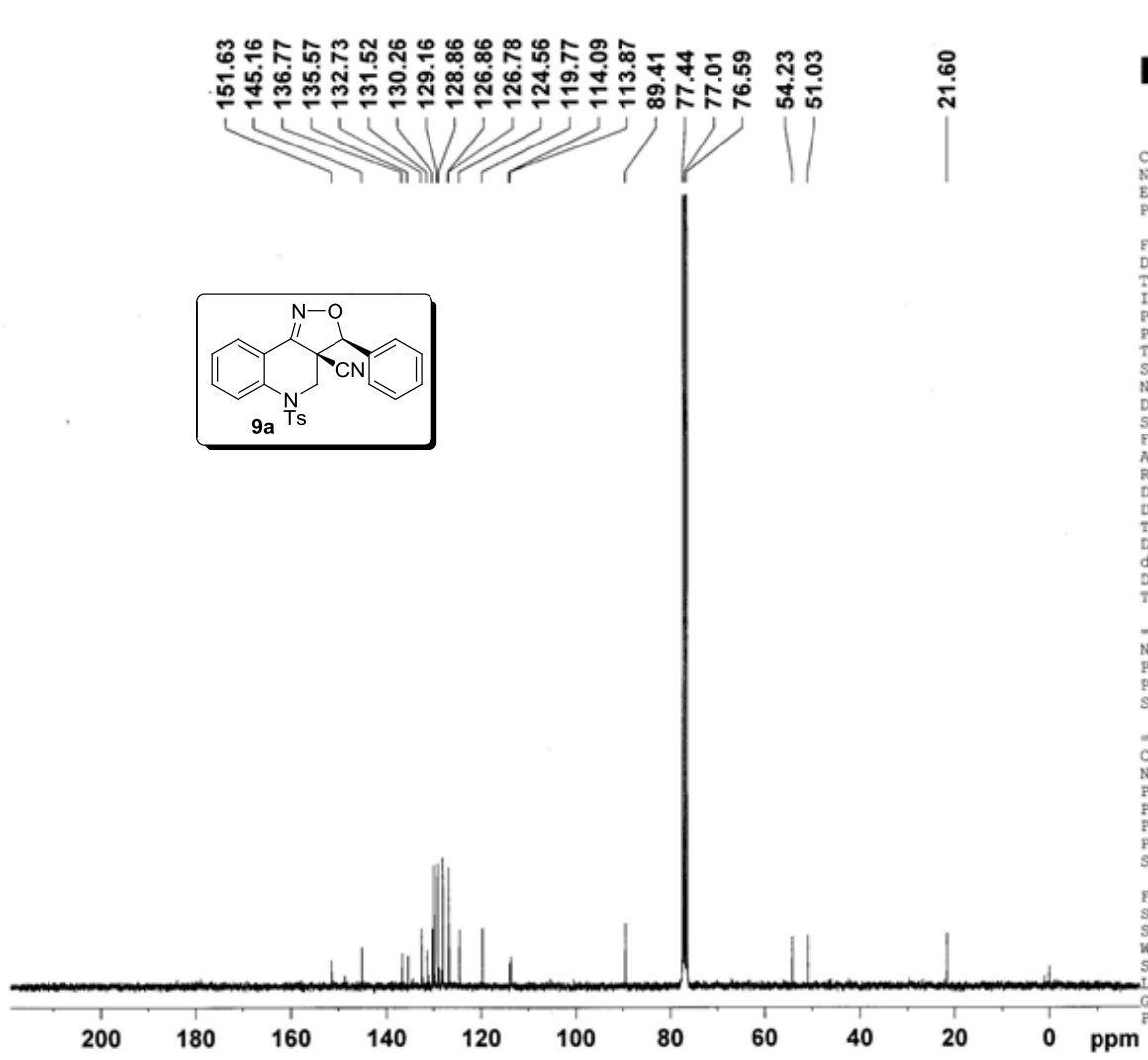
F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



BRUKER

```
Current Data Parameters
NAME                  VV-66
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20121204
Time                  23.04
INSTRUM               spect
PROBHD   5 mm DUL 13C-1
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       10
DS                        2
SWH                6172.839 Hz
FIDRES             0.094190 Hz
AQ                 5.3084660 sec
RG                     287.4
DW                    81.000 usec
DE                     6.00 usec
TE                    300.0 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                     13.15 usec
PL1                     0.00 dB
SFO1           300.1318534 MHz

F2 - Processing parameters
SI                        32768
SF             300.1300059 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00
```

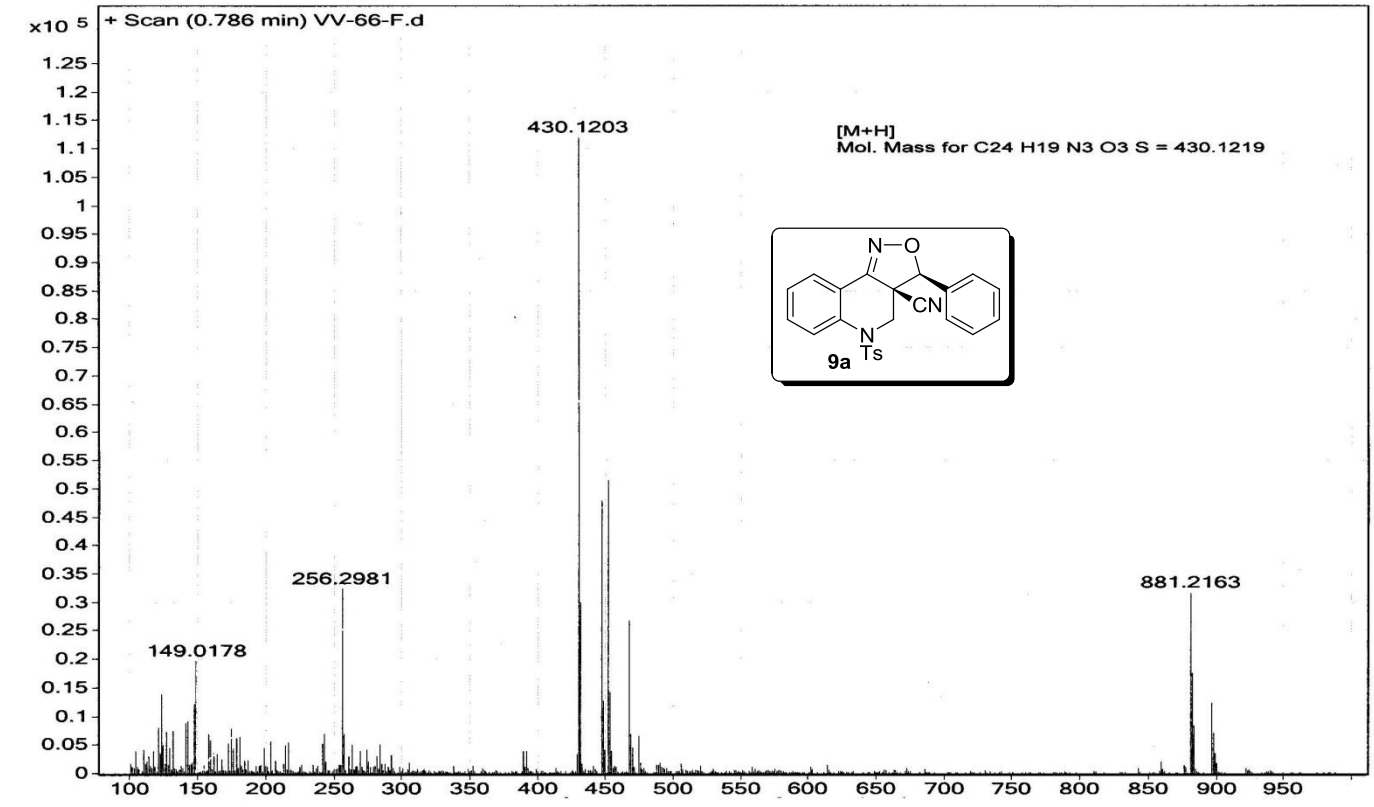


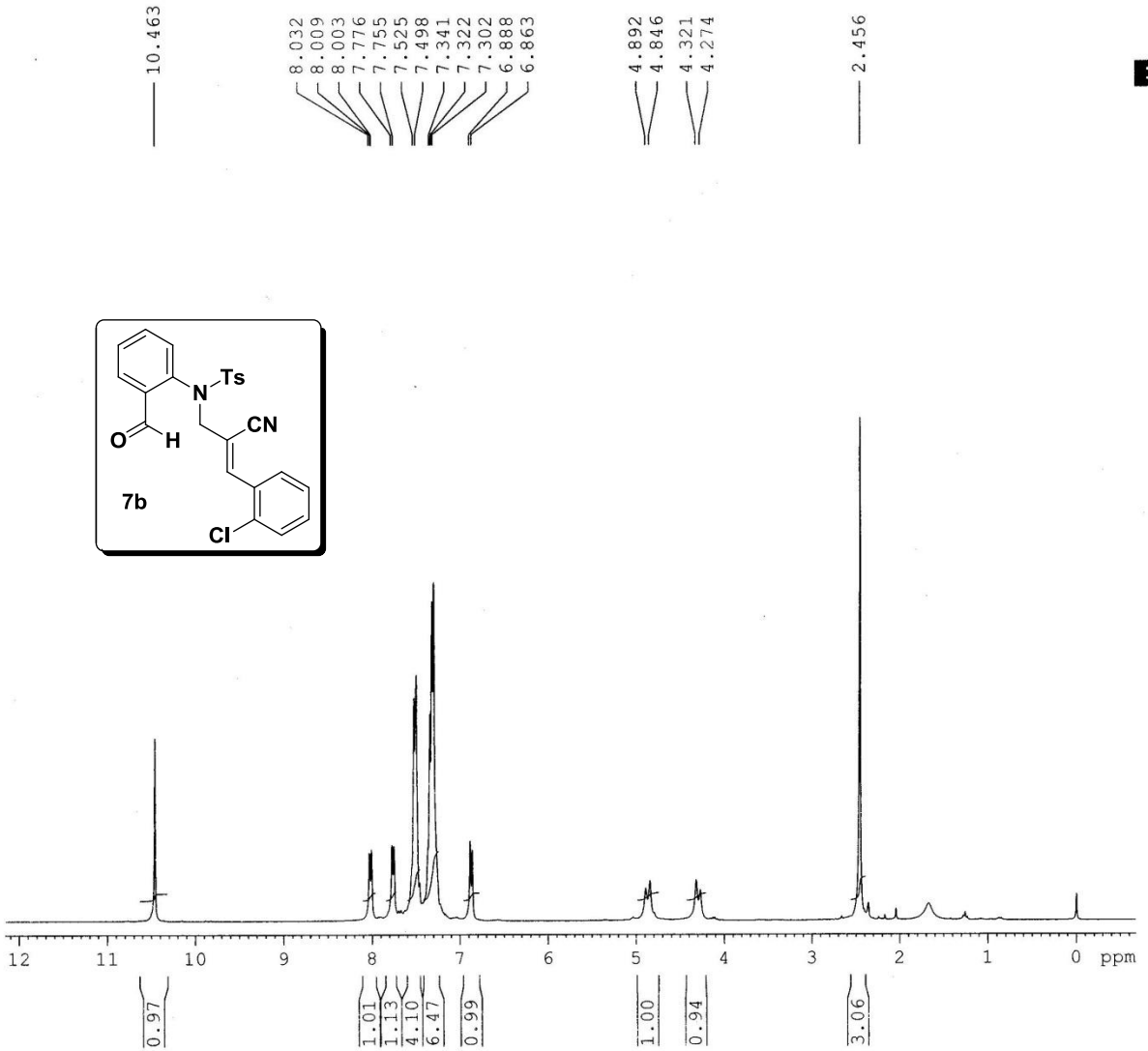


BRUKER

```
Current Data Parameters
NAME                  VV-66F
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20130123
Time                 21.35
INSTRUM              spect
PROBHD    5 mm DUL 13C-1
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                   2653
DS                      4
SWH              17985.611 Hz
FIDRES           0.274439 Hz
AQ               1.8219508 sec
RG                  912.3
DW                 27.800 usec
DE                  6.00 usec
TE                 300.0 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                    13C
P1                     9.30 usec
PL1                    0.00 dB
SFO1           75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                   0.00 dB
PL12                 15.68 dB
PL13                 16.00 dB
SFO2          300.1312005 MHz

F2 - Processing parameters
SI                     32768
SF             75.4677490 MHz
WDW                       EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.40
```

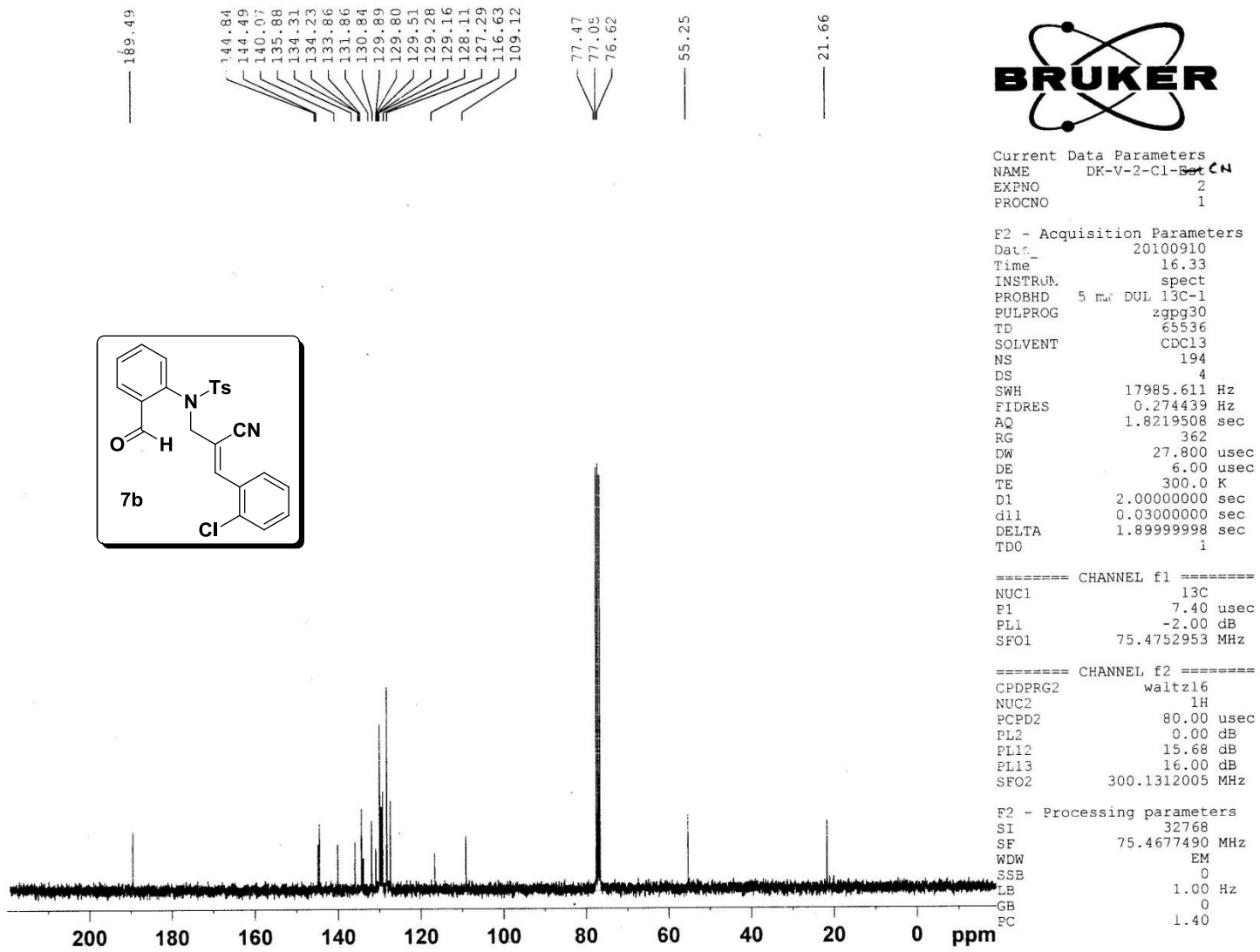
Sample Name	VV-66-F	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	VV-66-F.d	**ACQ Method**	Pondicherry Universi	**Comment**	MM-MB-429.1147	**Acquired Time**	18-11-2014 15:00:55





BRUKER

```
Current Data Parameters
NAME        DK-V-2-Cl-Est-CN
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20100910
Time                16.26
INSTRUM             spect
PROBHD   5 mm DUL 13C-1
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH              6172.839 Hz
FIDRES           0.094190 Hz
AQ               5.3084660 sec
RG                 143.7
DW                81.000 usec
DE                 6.00 usec
TE                300.0 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 13.15 usec
PL1                0.00 dB
SFO1         300.1318534 MHz

F2 - Processing parameters
SI                 32768
SF           300.1300049 MHz
WDW                   EM
SSB                    0
LB                 0.30 Hz
GB                     0
PC                 1.00
```



BRUKER

Current Data Parameters
NAME DK-V-2-Cl-Bat CN
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_	20100910
Time	16.33
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	194
DS	4
SWH	17985.611 Hz
FIDRES	0.274439 Hz
AQ	1.8219508 sec
RG	362
DW	27.800 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1

======== CHANNEL f1 ========

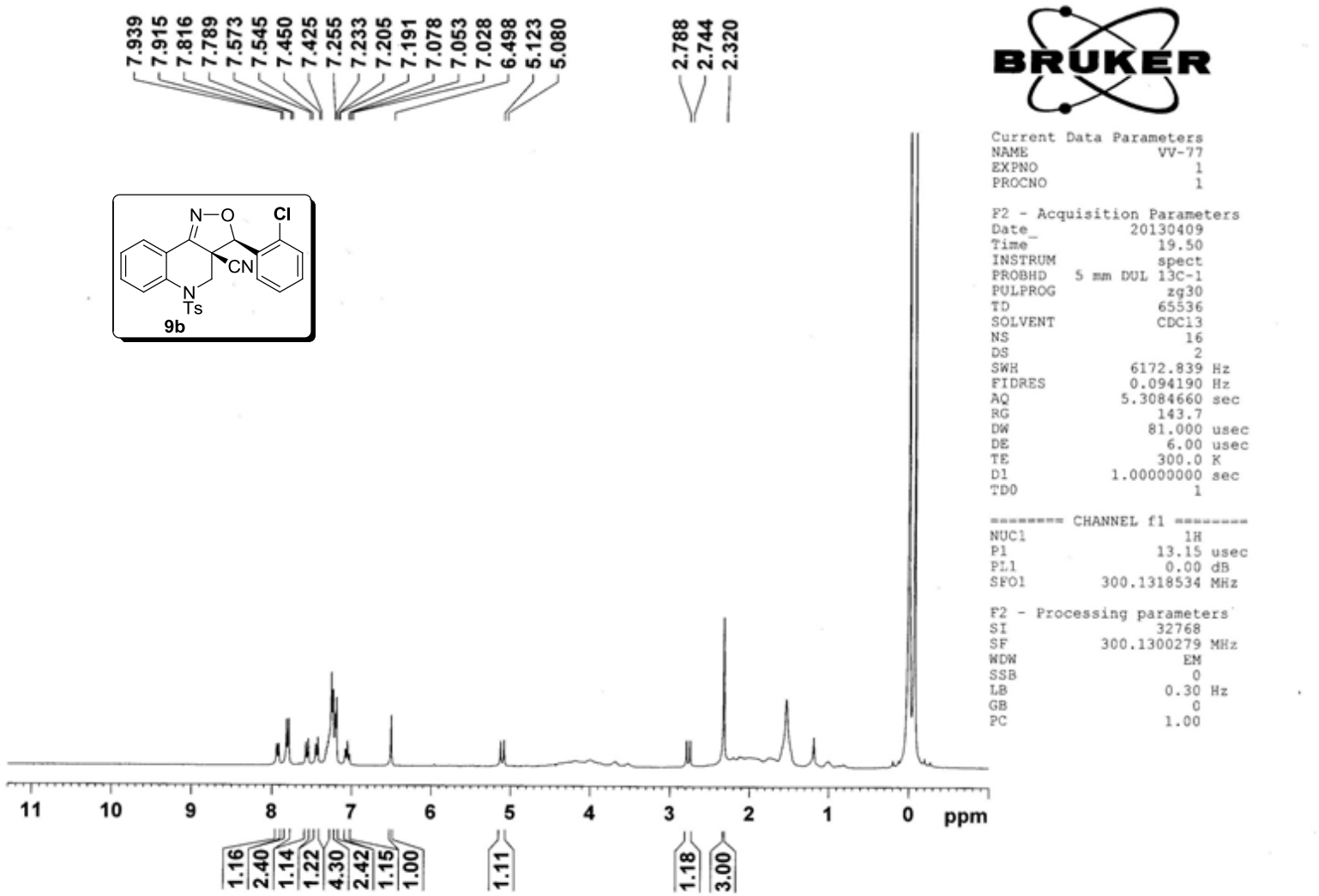
NUC1	13C
P1	7.40 usec
PL1	-2.00 dB
SFO1	75.4752953 MHz

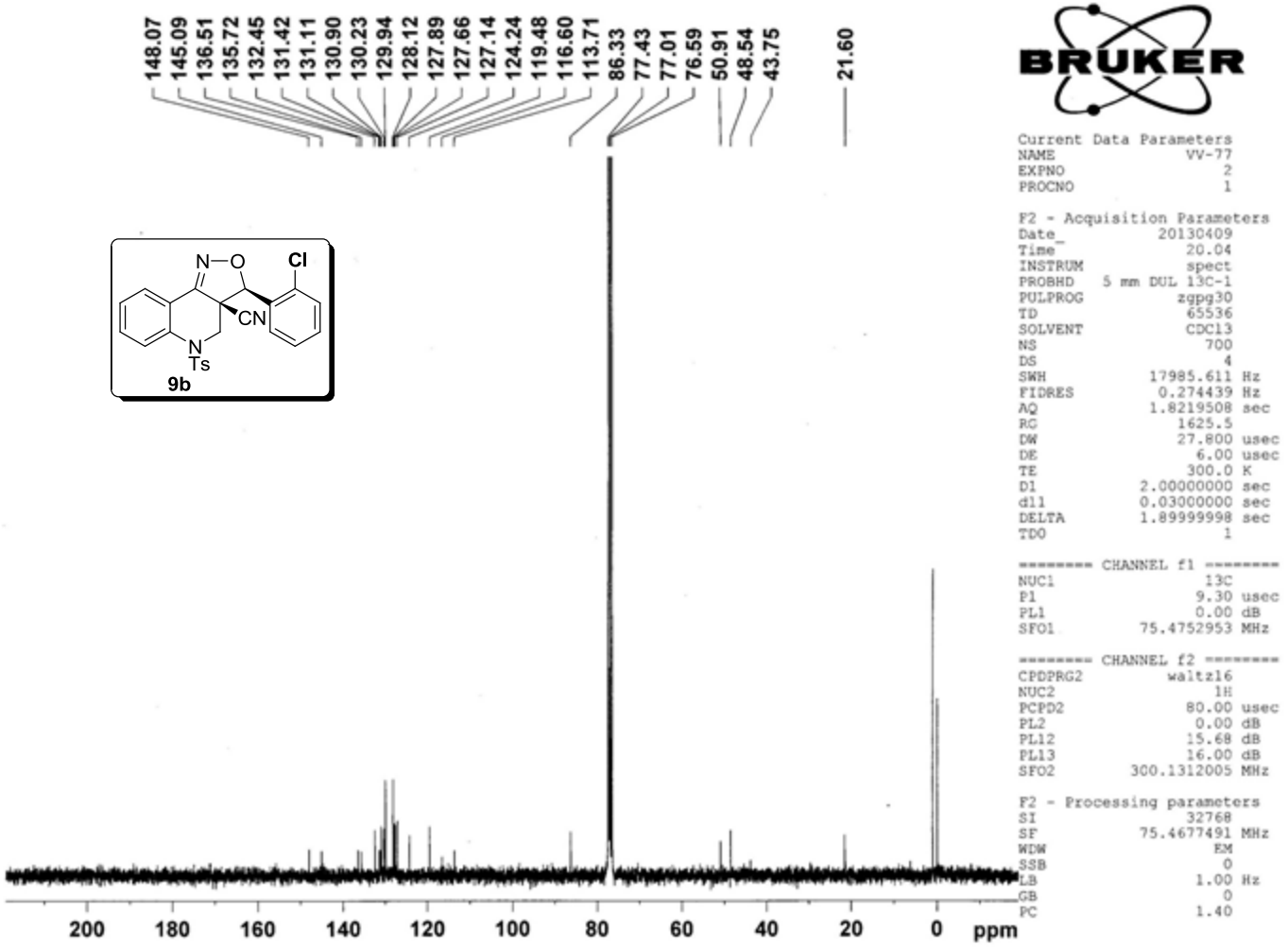
======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.00 dB
PL12	15.68 dB
PL13	16.00 dB
SFO2	300.1312005 MHz

F2 - Processing parameters

SI	32768
SF	75.4677490 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40


7.939
7.915
7.816
7.789
7.573
7.545
7.450
7.425
7.255
7.233
7.205
7.191
7.078
7.053
7.028
6.498
5.123
5.080
2.788
2.744
2.320
N—O
Cl
CN
N
Ts
9b
BRUKER
Current Data Parameters
NAME VV-77
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130409
Time 19.50
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 143.7
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.15 usec
PL1 0.00 dB
SFO1 300.1318534 MHz
F2 - Processing parameters
SI 32768
SF 300.1300279 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.16
2.40
1.14
1.22
4.30
2.42
1.15
1.00
1.11
1.18
3.00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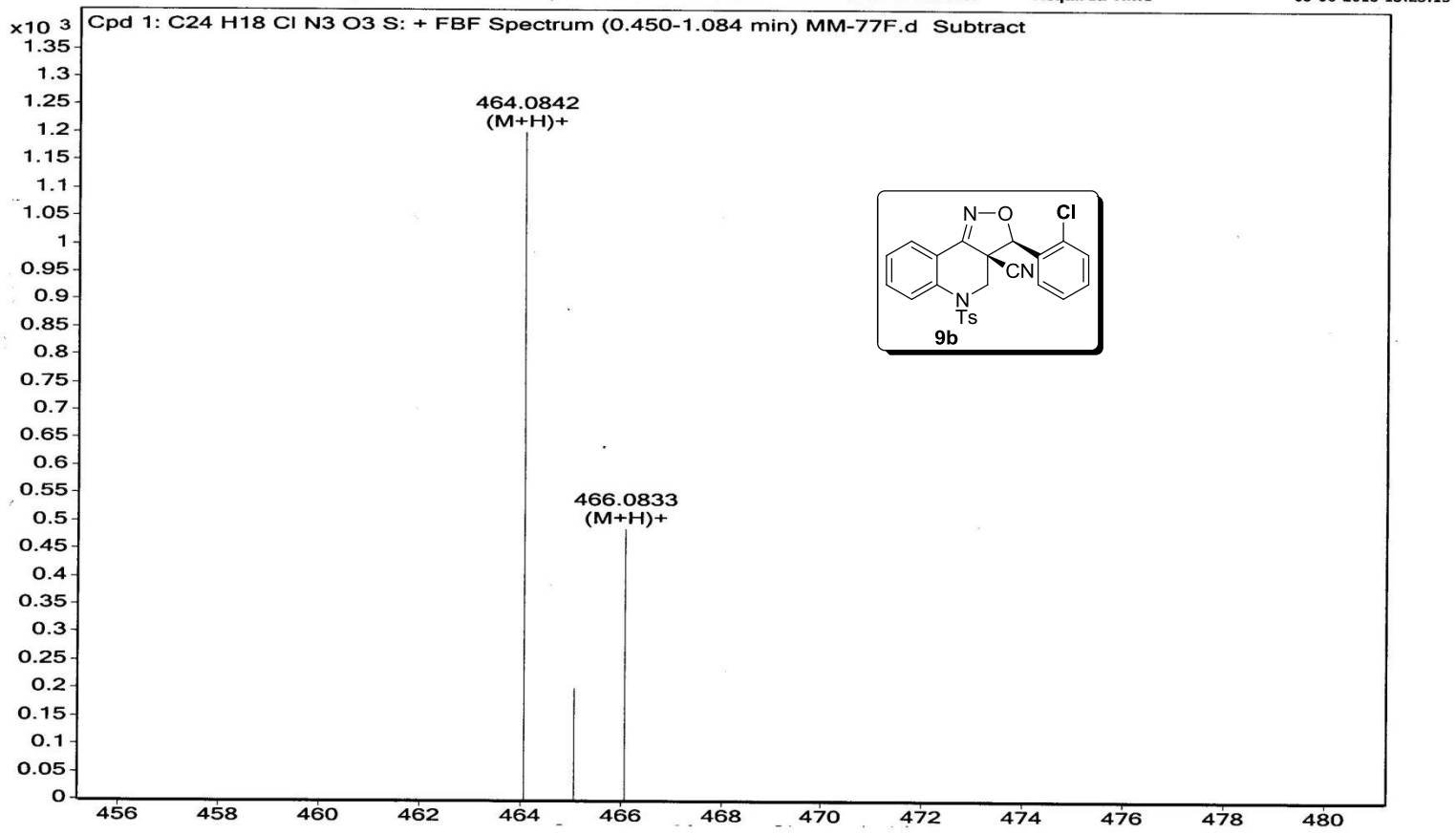
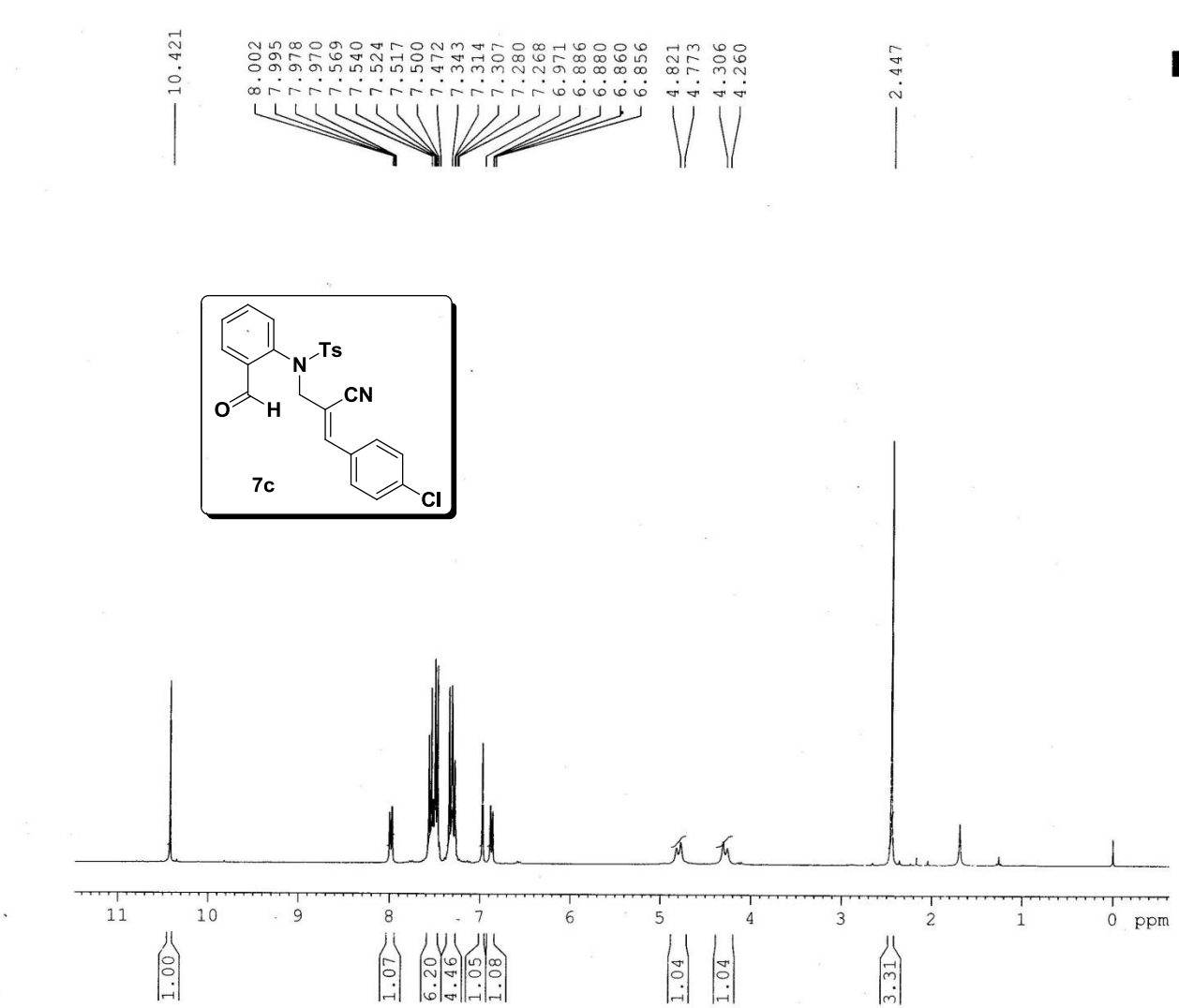
145.09
136.51
135.72
132.45
131.42
131.11
130.90
130.23
129.94
128.12
127.89
127.66
127.14
124.24
119.48
116.60
113.71
86.33
77.43
77.01
76.59
50.91
48.54
43.75
21.60
N—O
Cl
CN
N
Ts
9b
200
180
160
140
120
100
80
60
40
20
0
ppm
BRUKER
Current Data Parameters
NAME VV-77
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130409
Time 20.04
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 700
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 1625.5
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.30 usec
PL1 0.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.68 dB
PL13 16.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677491 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

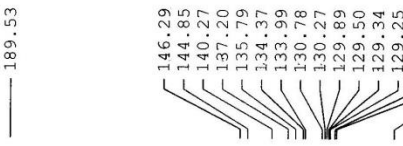
Sample Name	MM-77F	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	MM-77F.d	**ACQ Method**	Pondicherry Universi	**Comment**	MSK-MB-463.0757	**Acquired Time**	05-06-2015 13:23:15

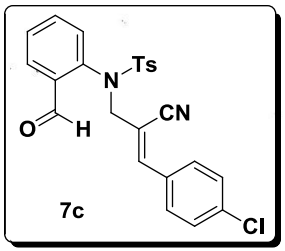


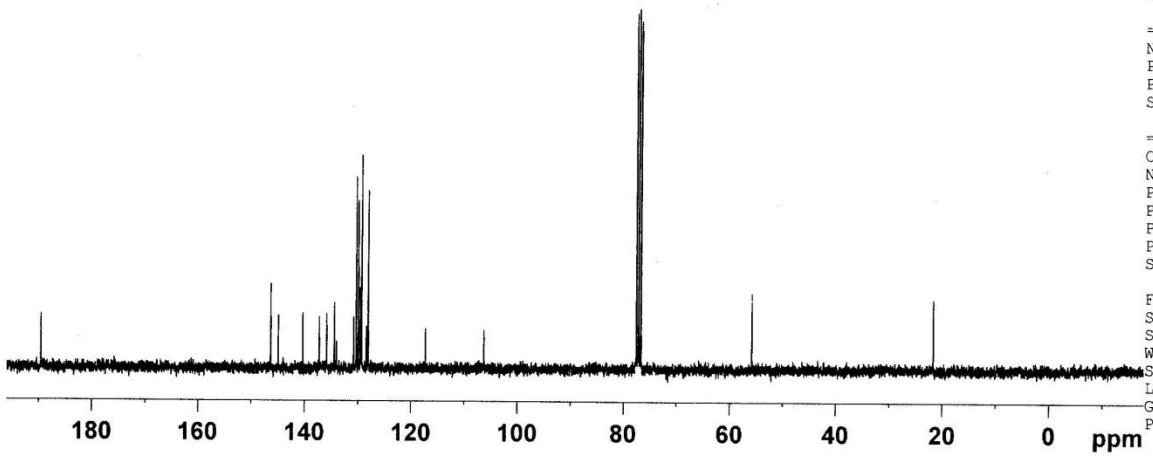


BRUKER

```
Current Data Parameters
NAME      DK-V-4-Cl-CN-CHO
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20100909
Time                 10.13
INSTRUM              spect
PROBHD   5 mm DUL 13C-1
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH               6172.839 Hz
FIDRES               0.094190 Hz
AQ                5.3084660 sec
RG                     101.6
DW                  81.000 usec
DE                   6.00 usec
TE                   300.0 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                  13.15 usec
PL1                  0.00 dB
SFO1          300.1318534 MHz

F2 - Processing parameters
SI                   32768
SF            300.1300042 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```







BRUKER

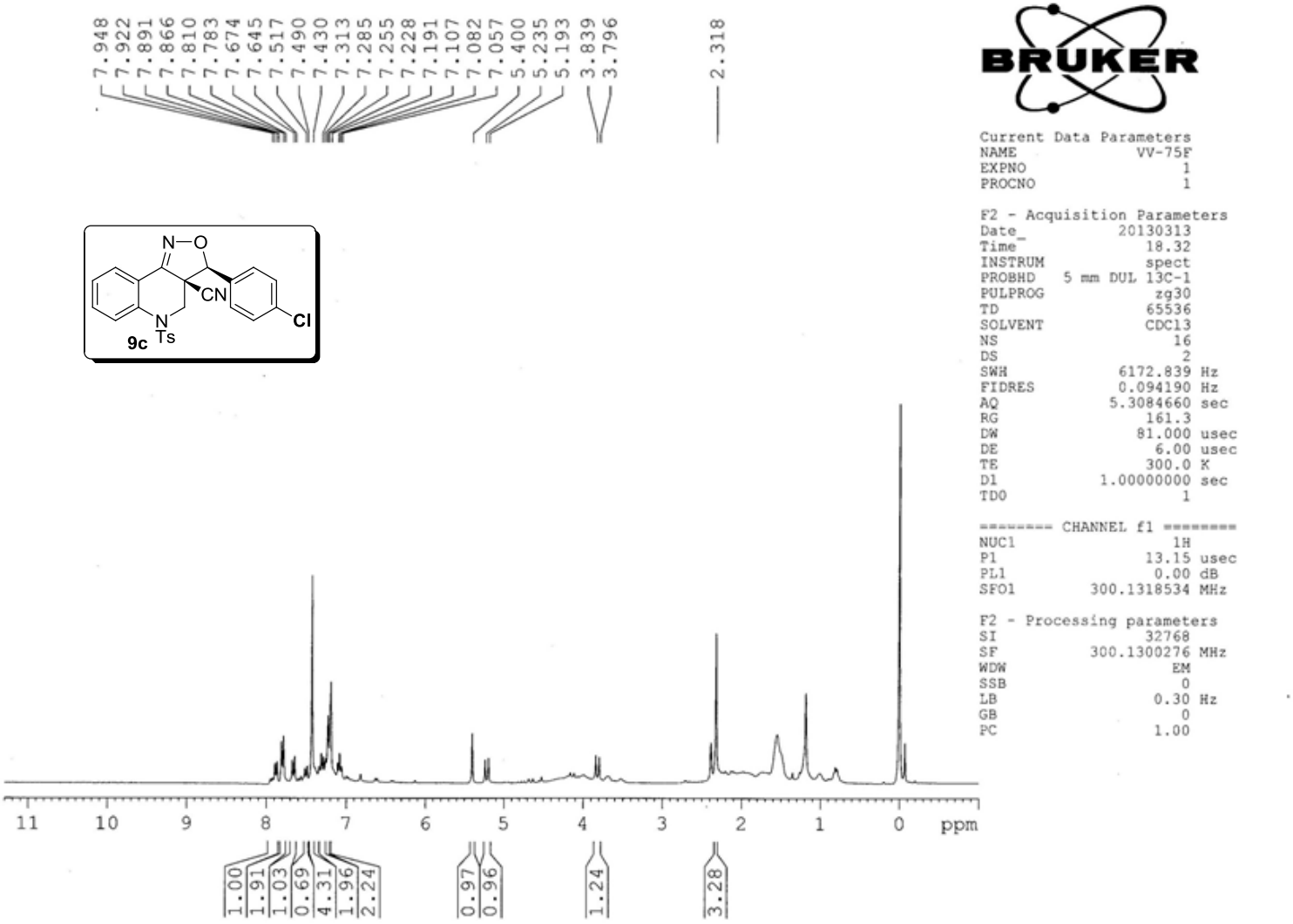
Current Data Parameters
NAME DK-V-4-Cl-CN-CHO
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100909
Time 10.24
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 72
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 362
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 7.40 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.68 dB
PL13 16.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40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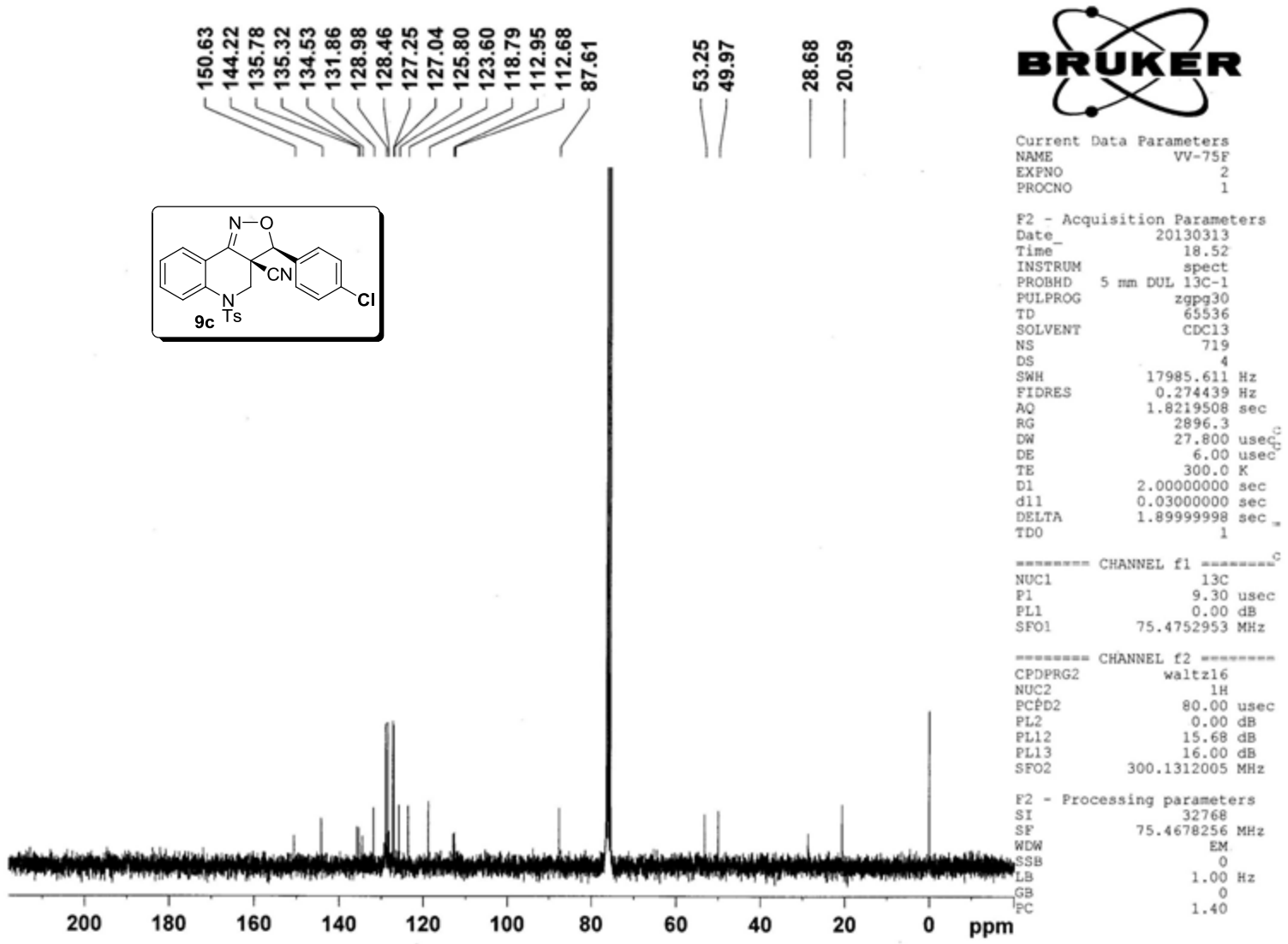
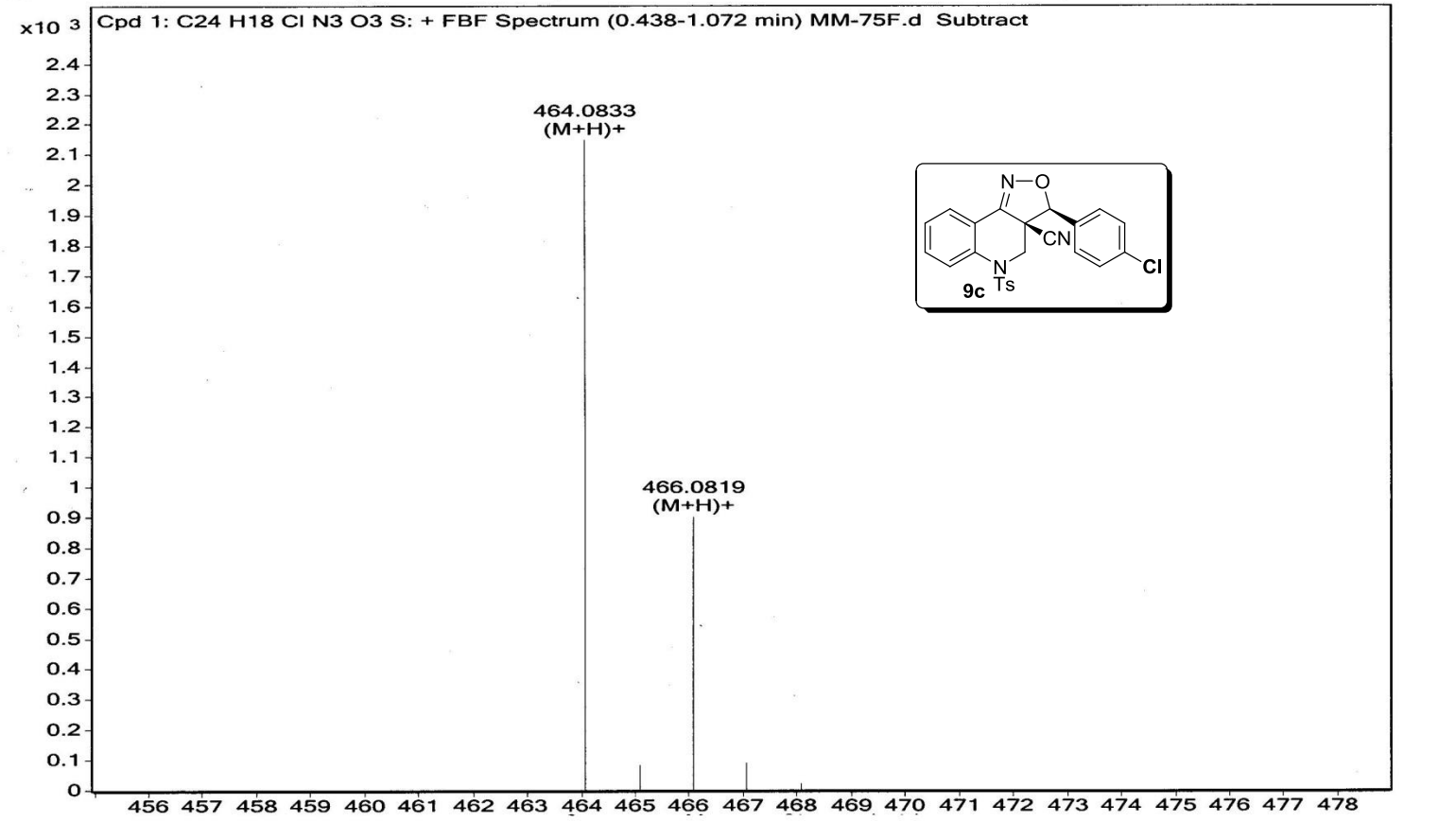
7.891
7.866
7.810
7.783
7.674
7.645
7.517
7.490
7.430
7.313
7.285
7.255
7.228
7.191
7.107
7.082
7.057
5.400
5.235
5.193
3.839
3.796
2.318
N
O
CN
Cl
N
Ts
9c
BRUKER
Current Data Parameters
NAME VV-75F
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130313
Time 18.32
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 161.3
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.15 usec
PL1 0.00 dB
SFO1 300.1318534 MHz
F2 - Processing parameters
SI 32768
SF 300.1300276 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.91
1.03
0.69
4.31
1.96
2.24
0.97
0.96
1.24
3.28

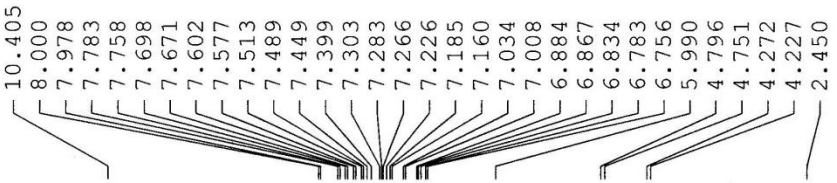


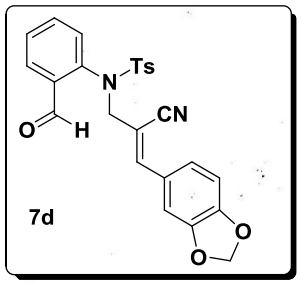
BRUKER

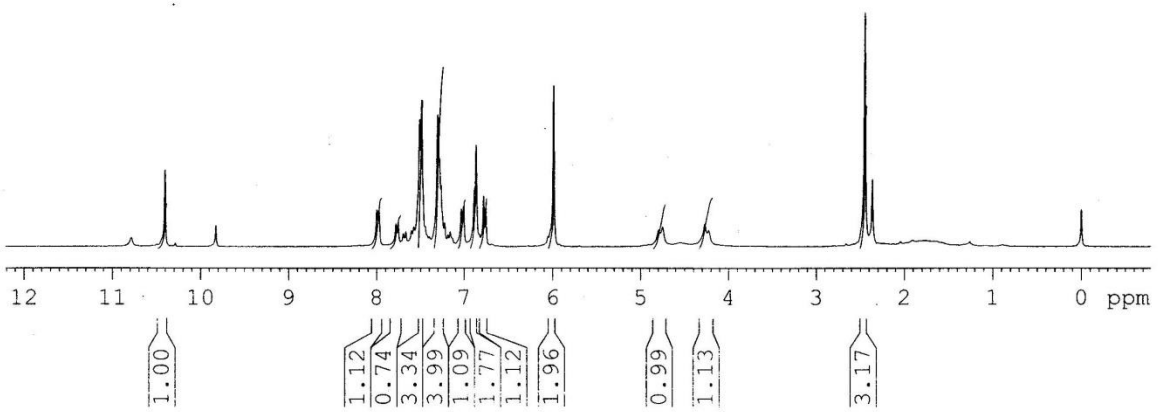
```
Current Data Parameters
NAME                  VV-75F
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20130313
Time                  18.52
INSTRUM               spect
PROBHD   5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     719
DS                       4
SWH               17985.611 Hz
FIDRES             0.274439 Hz
AQ                 1.8219508 sec
RG                    2896.3
DW                   27.800 usec
DE                    6.00 usec
TE                   300.0 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                    13C
P1                    9.30 usec
PL1                   0.00 dB
SFO1           75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                   0.00 dB
PL12                 15.68 dB
PL13                 16.00 dB
SFO2          300.1312005 MHz

F2 - Processing parameters
SI                     32768
SF             75.4678256 MHz
WDW                       EM
SSB                        0
LB                    1.00 Hz
GB                         0
PC                    1.40
```

Sample Name	MM-75F	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	MM-75F.d	**ACQ Method**	Pondicherry Universi	**Comment**	MSK-MB-463.0758	**Acquired Time**	05-06-2015 13:40:22

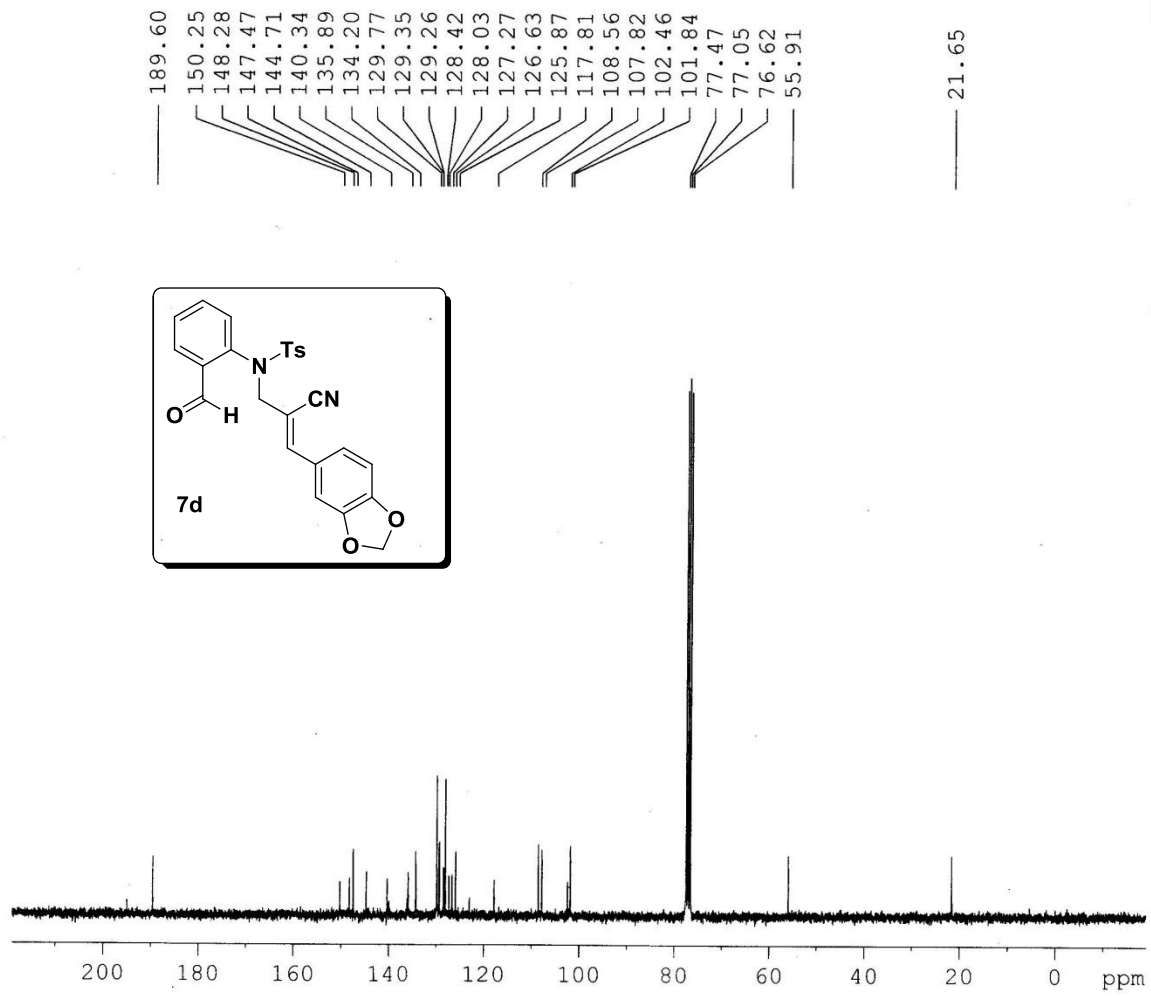






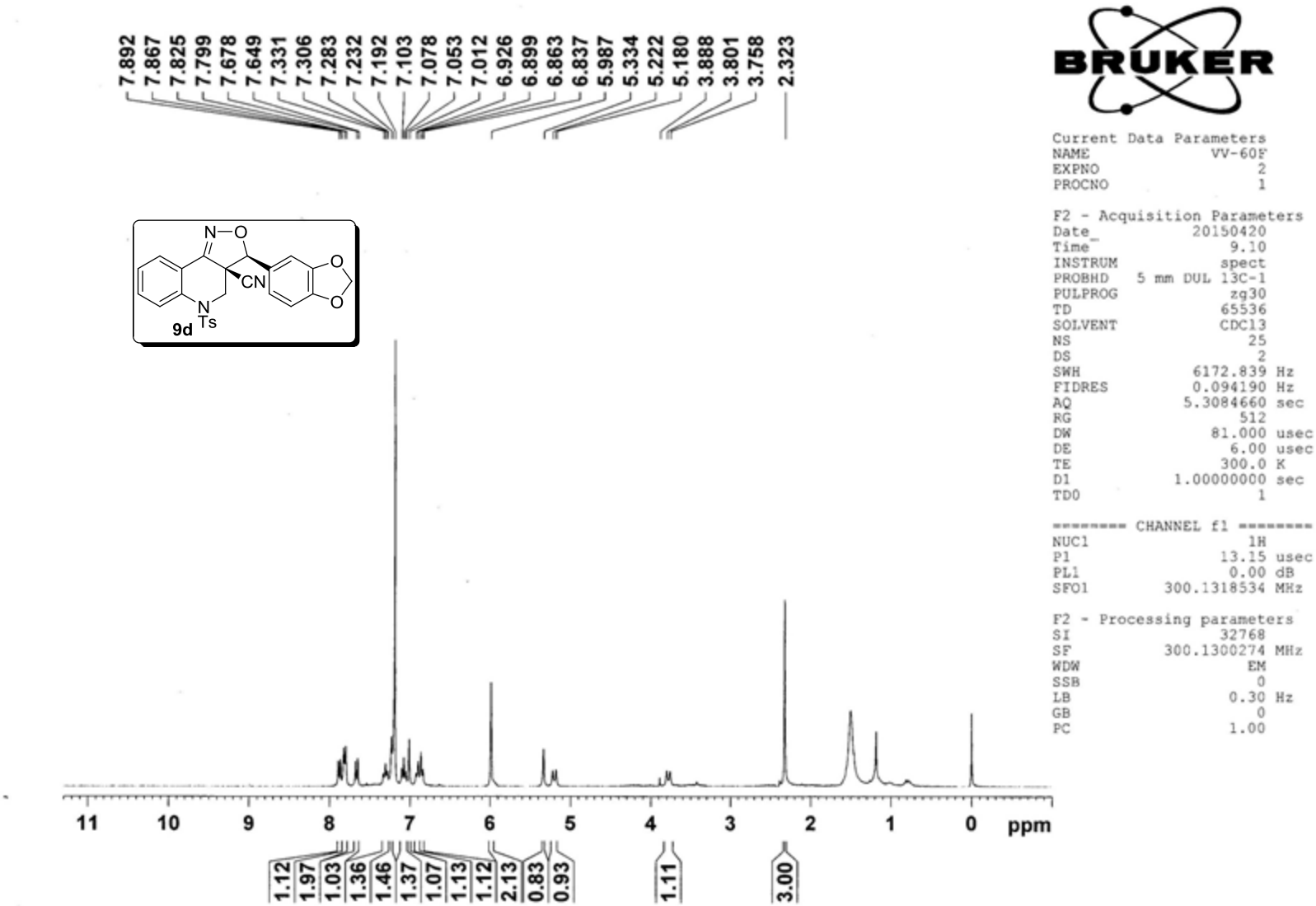



```
Current Data Parameters
NAME      DK-V-PIP-CN-Ts-PYZ
EXPNO                      3
PROCNO                     1

F2 - Acquisition Parameters
Date_            20111210
Time                17.50
INSTRUM             spect
PROBHD   5 mm DUL 13C-1
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     5
DS                     2
SWH              6172.839 Hz
FIDRES           0.094190 Hz
AQ               5.3084660 sec
RG                 143.7
DW                81.000 usec
DE                 6.00 usec
TE                300.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                   1H
P1                 13.15 usec
PL1                 0.00 dB
SFO1         300.1318534 MHz

F2 - Processing parameters
SI                 32768
SF           300.1300050 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



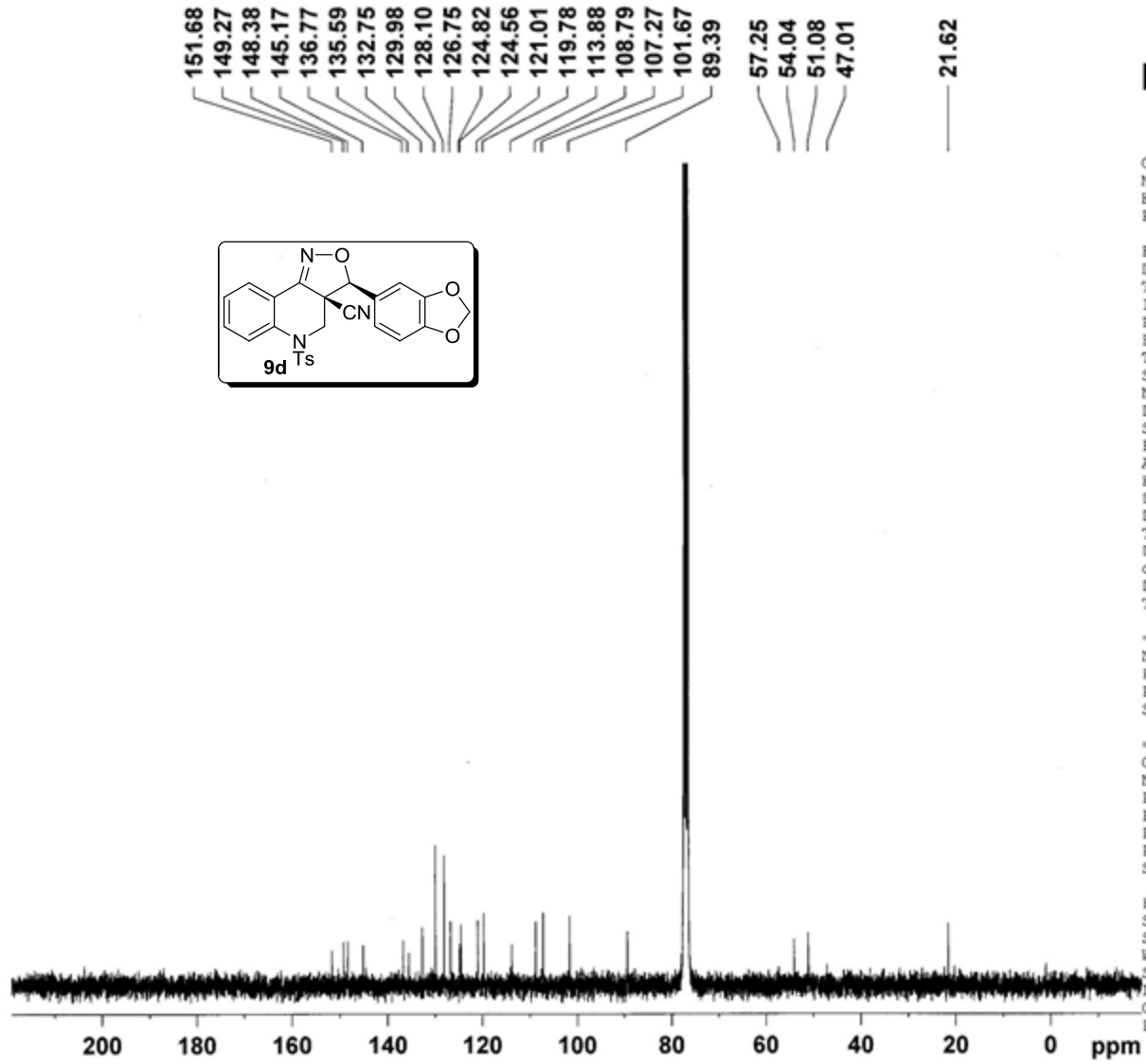
BRUKER

```
Current Data Parameters
NAME      DK-V-PIP-CN-Ts-PYZ
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_              20111210
Time                 17.49
INSTRUM              spect
PROBHD    5 mm DUL 13C-1
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                    500
DS                      4
SWH             17985.611 Hz
FIDRES              0.274439 Hz
AQ                1.8219508 sec
RG                  20642.5
DW                   27.800 usec
DE                    6.00 usec
TE                   300.0 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   13C
P1                    9.30 usec
PL1                   0.00 dB
SFO1           75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                   1H
PCPD2                80.00 usec
PL2                   0.00 dB
PL12                 15.68 dB
PL13                 16.00 dB
SFO2          300.1312005 MHz

F2 - Processing parameters
SI                    32768
SF             75.4677490 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```



BRUKER

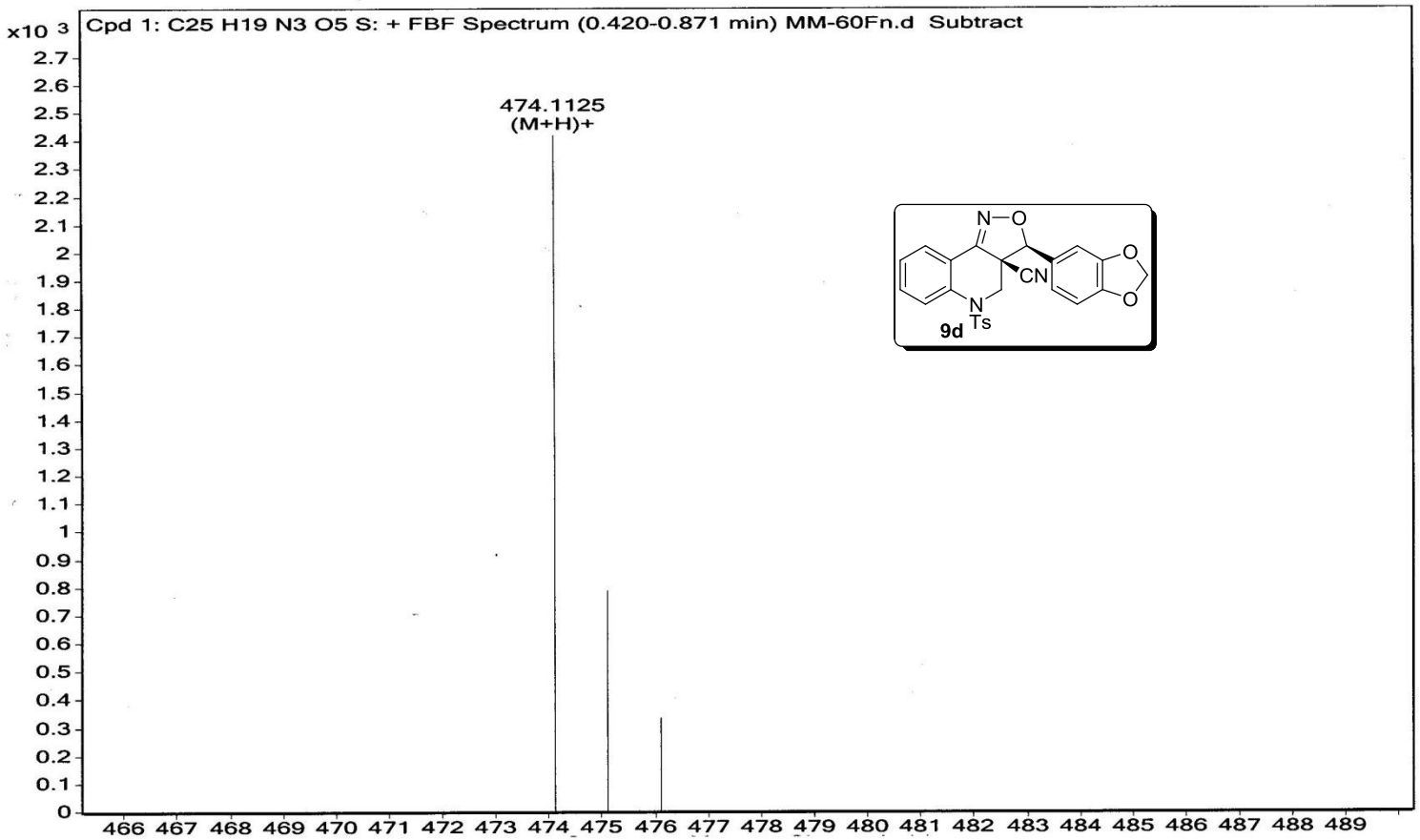
```
Current Data Parameters
NAME                  VV-60F
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20150420
Time                   9.10
INSTRUM               spect
PROBHD   5 mm DUL 13C-1
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                        25
DS                         2
SWH                6172.839 Hz
FIDRES                0.094190 Hz
AQ                 5.3084660 sec
RG                       512
DW                    81.000 usec
DE                     6.00 usec
TE                     300.0 K
D1                1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     13.15 usec
PL1                     0.00 dB
SFO1           300.1318534 MHz

F2 - Processing parameters
SI                        32768
SF             300.1300274 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00
```

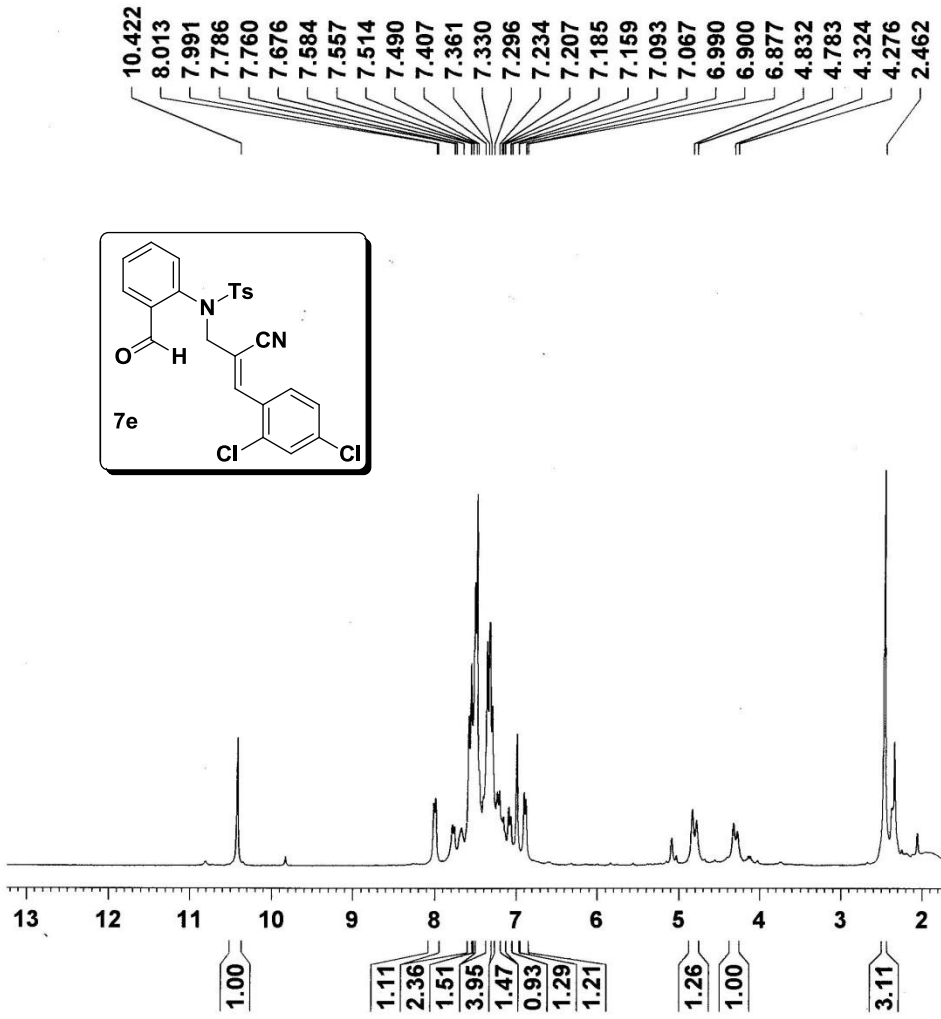


BRUKER

```
Current Data Parameters
NAME                  VV-60F
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20150420
Time                   8.56
INSTRUM               spect
PROBHD   5 mm DUL 13C-1
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     9615
DS                        4
SWH               17985.611 Hz
FIDRES            0.274439 Hz
AQ                1.8219508 sec
RG                   1290.2
DW                  27.800 usec
DE                   6.00 usec
TE                   300.0 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                    13C
P1                    9.30 usec
PL1                   0.00 dB
SFO1           75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                   0.00 dB
PL12                 15.68 dB
PL13                 16.00 dB
SFO2          300.1312005 MHz

F2 - Processing parameters
SI                     32768
SF             75.4677490 MHz
WDW                       EM
SSB                        0
LB                    1.00 Hz
GB                         0
PC                     1.40
```

Sample Name	MM-60F	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	MM-60Fn.d	**ACQ Method**	Pondicherry Universi	**Comment**	MSK-MB-473.1045	**Acquired Time**	05-06-2015 12:26:32





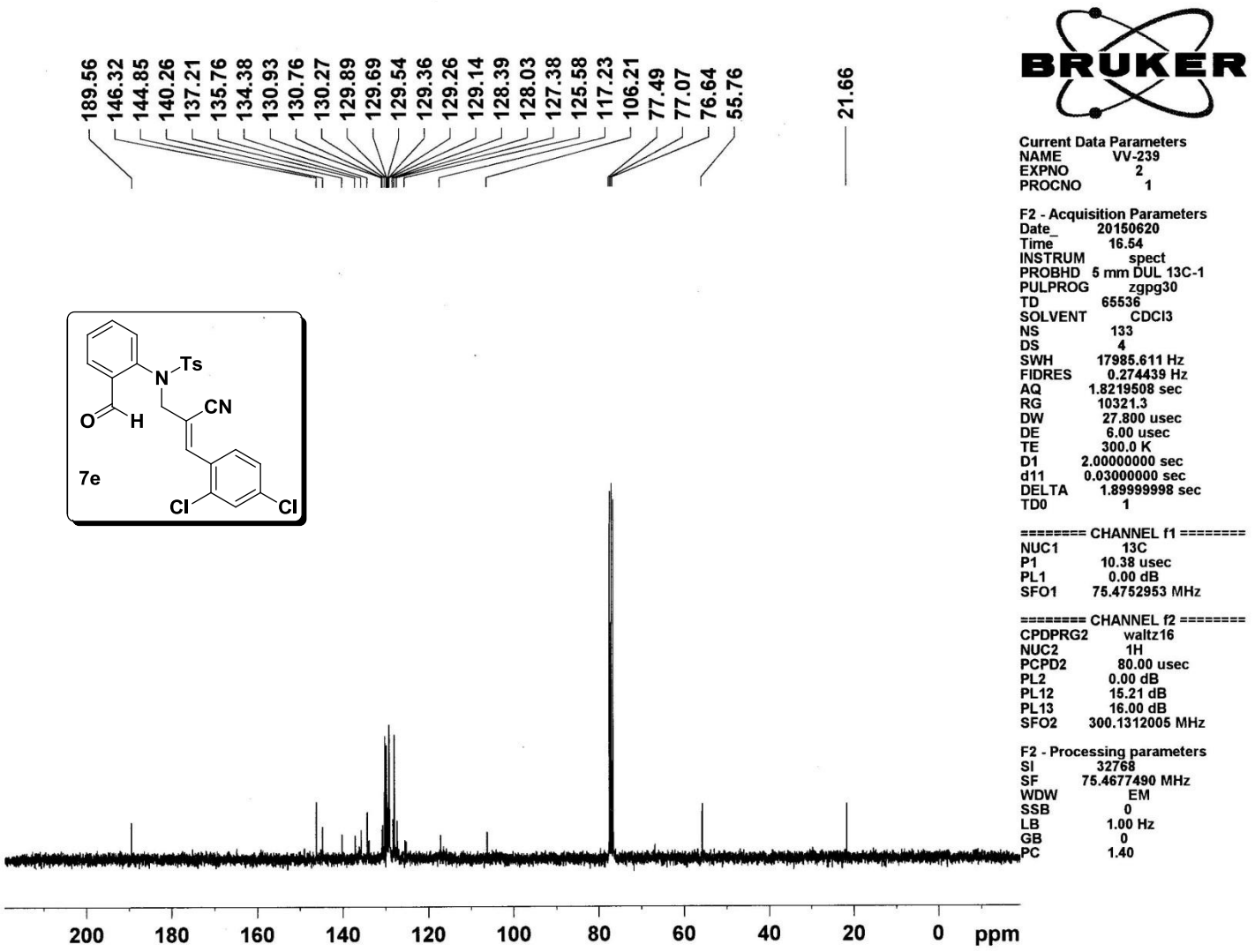
BRUKER

Current Data Parameters
NAME VV-239
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150620
Time 16.50
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 90.5
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 13.88 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



BRUKER

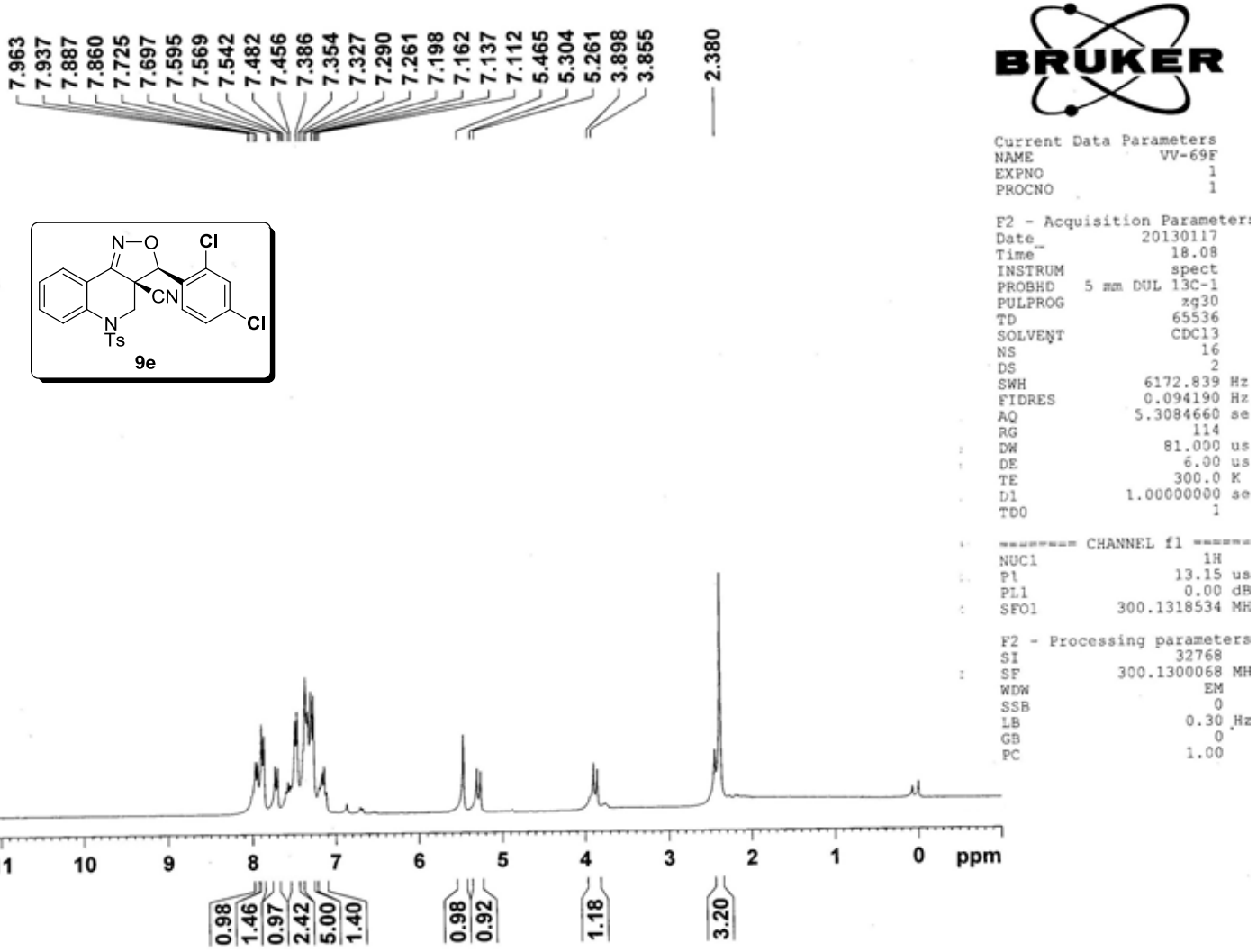
Current Data Parameters
NAME VV-239
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150620
Time 16.54
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 133
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 10321.3
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.38 usec
PL1 0.00 dB
SFO1 75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.21 dB
PL13 16.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40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7.937
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7.725
7.697
7.595
7.569
7.542
7.482
7.456
7.386
7.354
7.327
7.290
7.261
7.198
7.162
7.137
7.112
5.465
5.304
5.261
3.898
3.855
2.380
N—O
Cl
CN
N
Ts
Cl
9e
BRUKER
Current Data Parameters
NAME VV-69F
EXPNO 1
PROCNO 1
F2 - Acquisition Parameter
Date_ 20130117
Time 18.08
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 se
RG 114
DW 81.000 us
DE 6.00 us
TE 300.0 K
D1 1.00000000 se
TD0 1
======== CHANNEL f1 ======
NUC1 1H
P1 13.15 us
PL1 0.00 dB
SFO1 300.1318534 MH
F2 - Processing parameters
SI 32768
SF 300.1300068 MH
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.98
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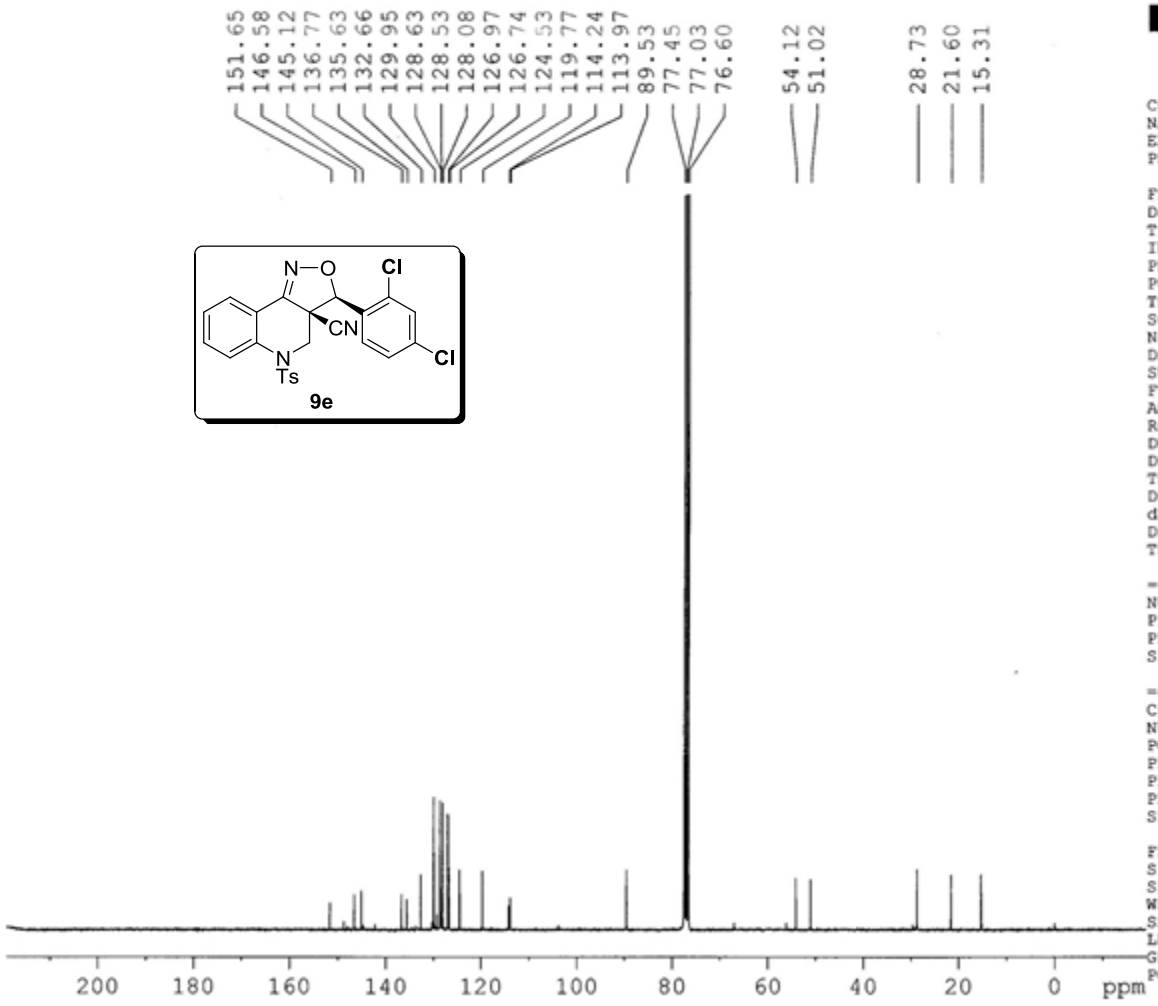
0.97
2.42
5.00
1.40
0.98
0.92
1.18
3.20

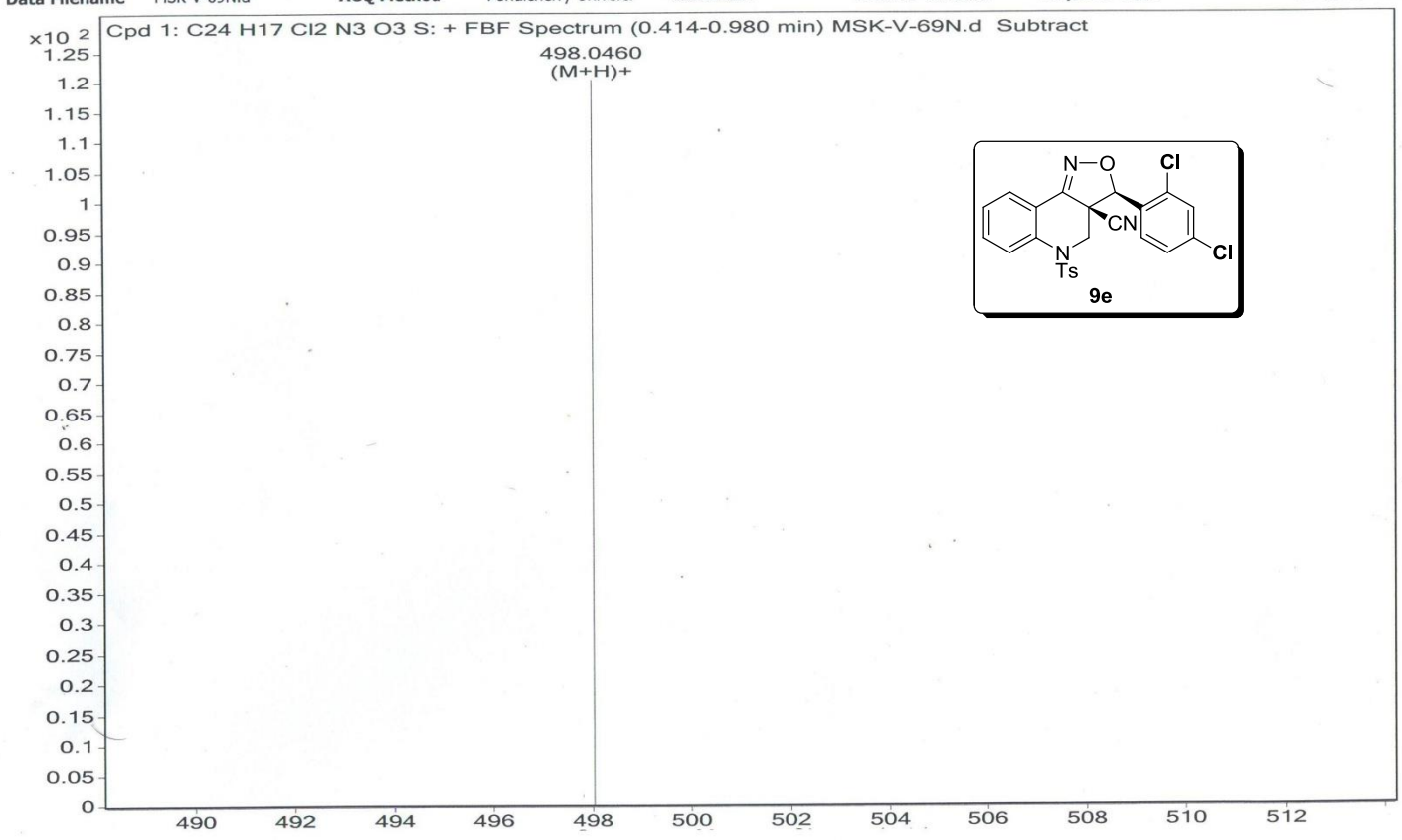
University of Madras

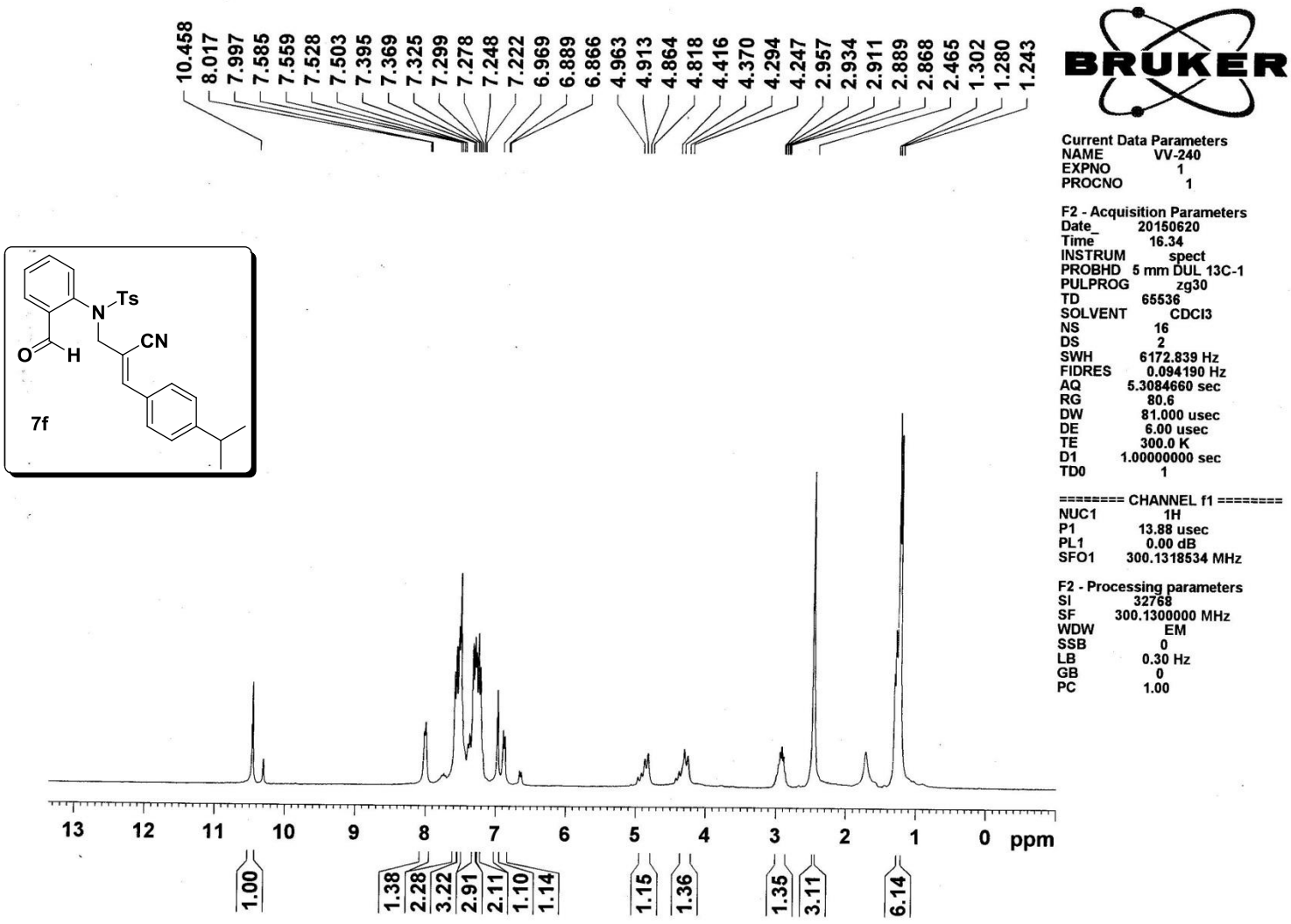


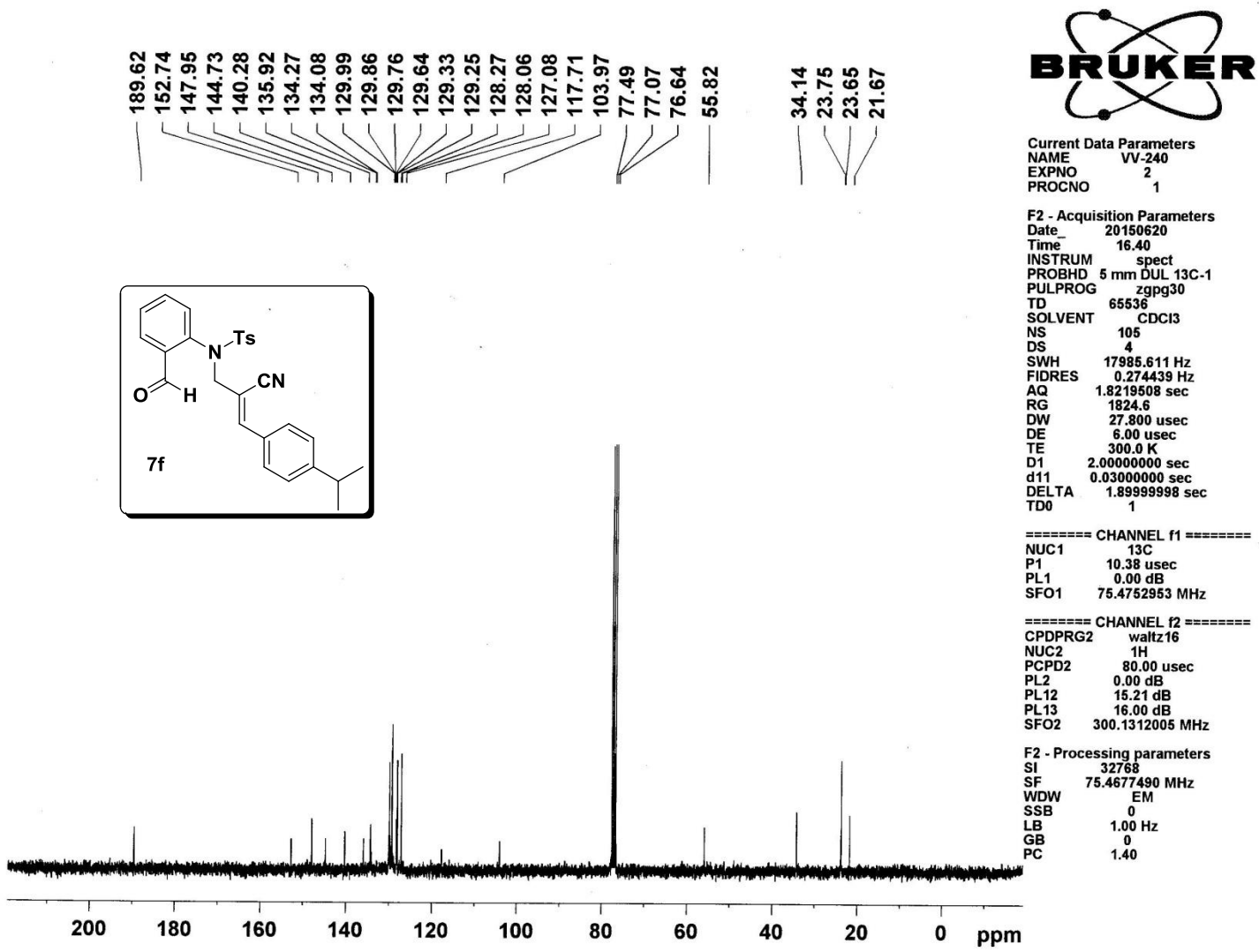
BRUKER

```
Current Data Parameters
NAME                  VV-69F
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20130123
Time                   8.35
INSTRUM               spect
PROBHD    5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    7645
DS                       4
SWH              17985.611 Hz
FIDRES           0.274439 Hz
AQ               1.8219508 sec
RG                  2580.3
DW                  27.800 usec
DE                   6.00 usec
TE                  300.0 K
D1               2.00000000 sec
d11              0.03000000 sec
DELTA            1.89999998 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                    13C
P1                     9.30 usec
PL1                    0.00 dB
SFO1            75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                    0.00 dB
PL12                  15.68 dB
PL13                  16.00 dB
SFO2           300.1312005 MHz

F2 - Processing parameters
SI                     32768
SF              75.4677490 MHz
WDW                       EM
SSB                        0
LB                    1.00 Hz
GB                         0
PC                      1.40
```

Sample Name	MSK-V-69	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	MSK-V-69N.d	**ACQ Method**	Pondicherry Universi	**Comment**	MSK-MB-497.0368	**Acquired Time**	23-06-2015 11:11:18




10.458
8.017
7.997
7.585
7.559
7.528
7.503
7.395
7.369
7.325
7.299
7.278
7.248
7.222
6.969
6.889
6.866
4.963
4.913
4.864
4.818
4.416
4.370
4.294
4.247
2.957
2.934
2.911
2.889
2.868
2.465
1.302
1.280
1.243
BRUKER
Current Data Parameters
NAME VV-240
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150620
Time 16.34
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 80.6
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.88 usec
PL1 0.00 dB
SFO1 300.1318534 MHz
F2 - Processing parameters
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
N
Ts
CN
O
H
7f
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.38
2.28
3.22
2.91
2.11
1.10
1.14
1.15
1.36
1.35
3.11
6.14



BRUKER

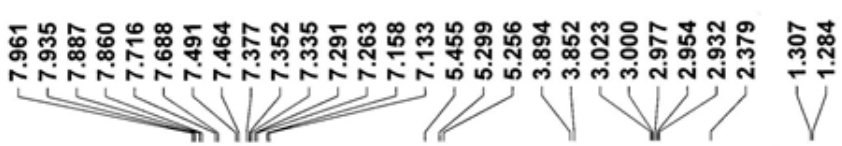
Current Data Parameters
NAME VV-240
EXPNO 2
PROCNO 1

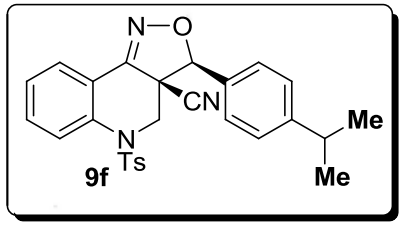
F2 - Acquisition Parameters
Date_ 20150620
Time 16.40
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 105
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 1824.6
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

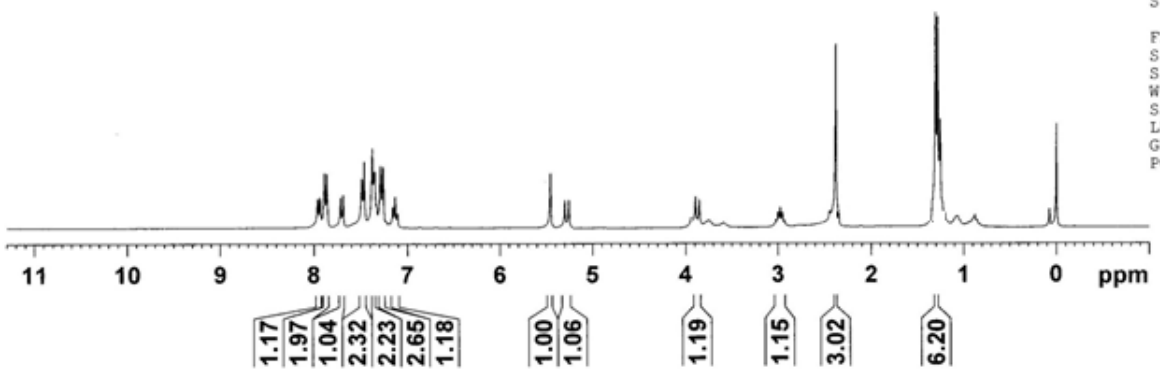
======== CHANNEL f1 ========
NUC1 13C
P1 10.38 usec
PL1 0.00 dB
SFO1 75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.21 dB
PL13 16.00 dB
SFO2 300.1312005 MHz

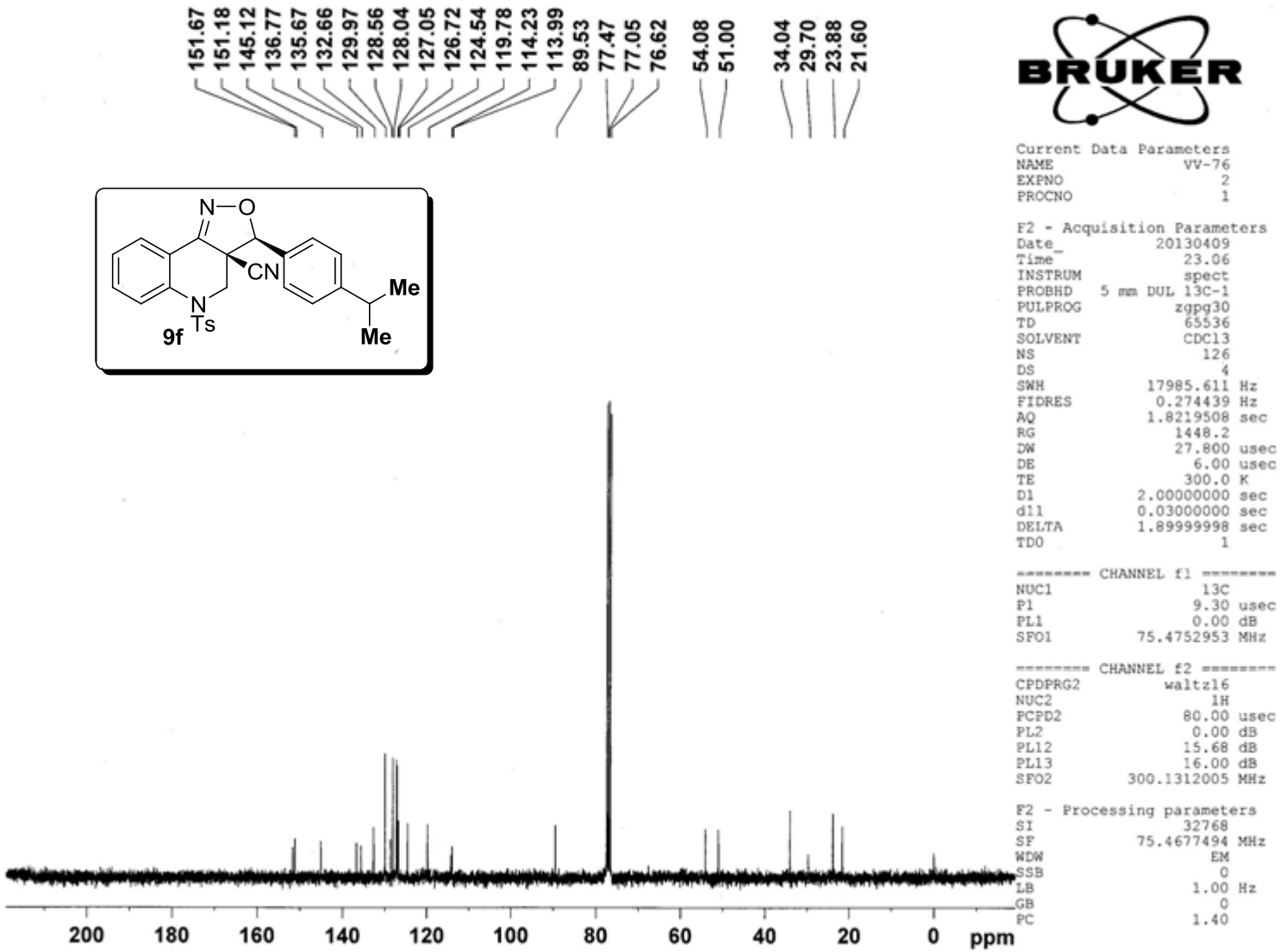
F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40








```
Current Data Parameters
NAME                  VV-76
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20130409
Time                 22.59
INSTRUM              spect
PROBHD   5 mm DUL 13C-1
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH                6172.839 Hz
FIDRES             0.094190 Hz
AQ                 5.3084660 sec
RG                    71.8
DW                   81.000 usec
DE                    6.00 usec
TE                   300.0 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     1H
P1                   13.15 usec
PL1                   0.00 dB
SFO1          300.1318534 MHz

F2 - Processing parameters
SI                    32768
SF            300.1300073 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```



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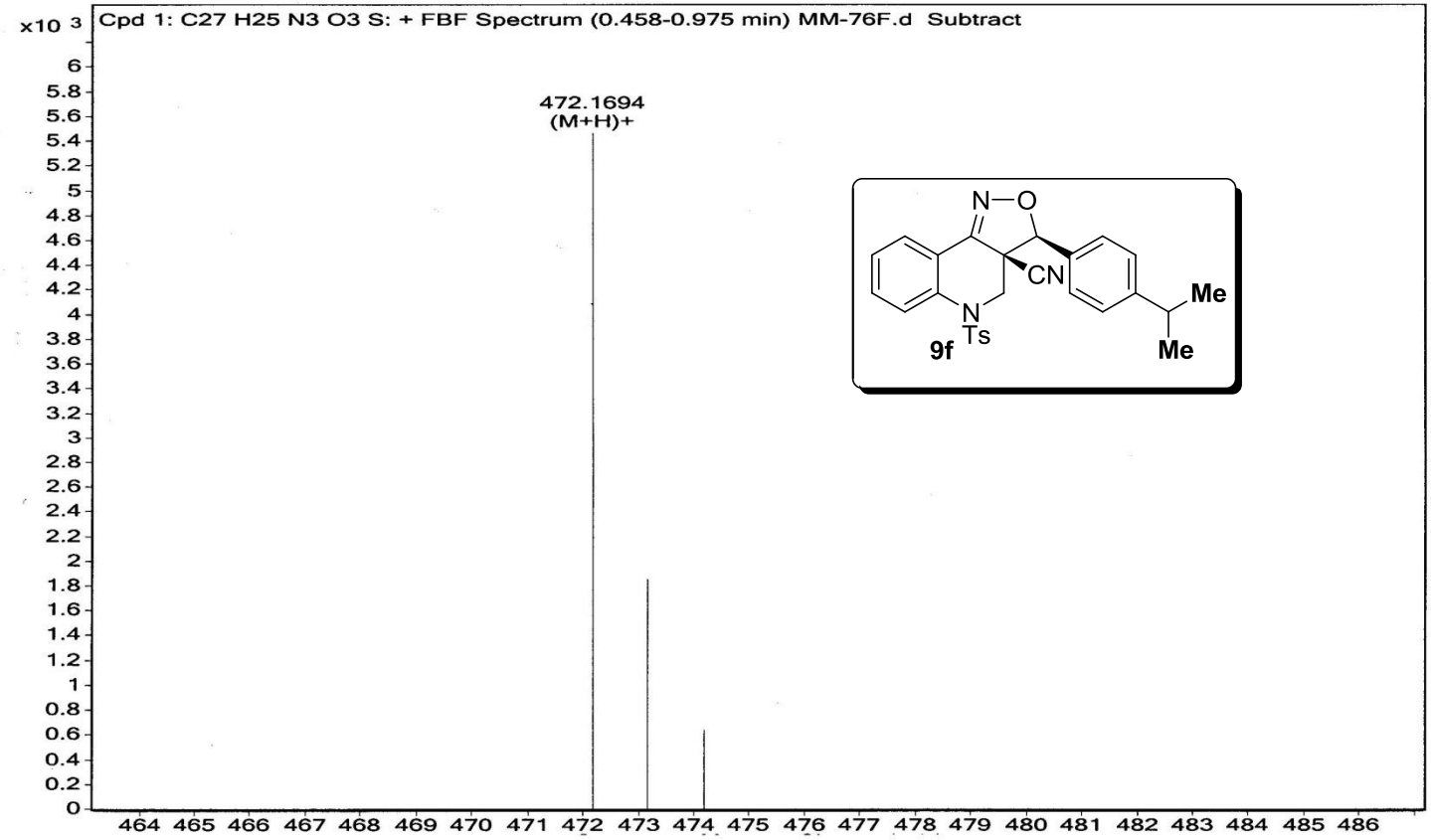
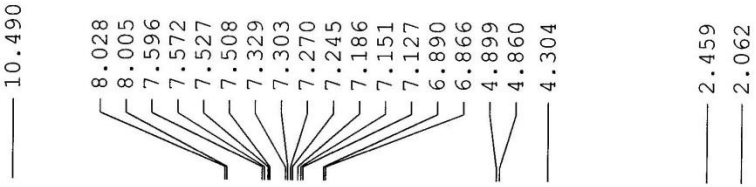
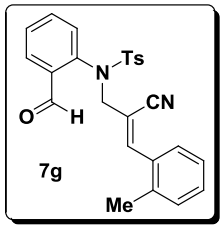
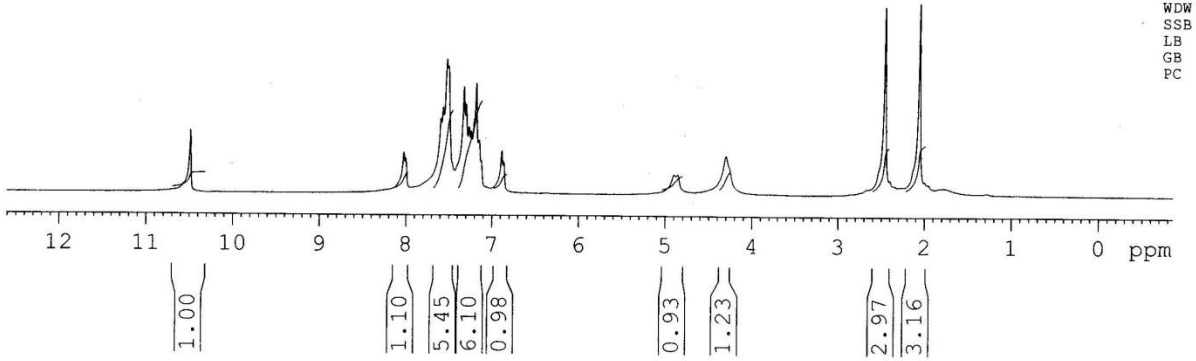
```
Current Data Parameters
NAME                  VV-76
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_              20130409
Time                 23.06
INSTRUM              spect
PROBHD   5 mm DUL 13C-1
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      126
DS                        4
SWH              17985.611 Hz
FIDRES            0.274439 Hz
AQ                1.8219508 sec
RG                   1448.2
DW                  27.800 usec
DE                   6.00 usec
TE                   300.0 K
D1               2.00000000 sec
d11              0.03000000 sec
DELTA            1.89999998 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                    13C
P1                    9.30 usec
PL1                   0.00 dB
SFO1           75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                   0.00 dB
PL12                 15.68 dB
PL13                 16.00 dB
SFO2          300.1312005 MHz

F2 - Processing parameters
SI                    32768
SF             75.4677494 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

Sample Name	MM-76-F	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	MM-76F.d	**ACQ Method**	Pondicherry Universi	**Comment**	MSK-MB-471.1617	**Acquired Time**	05-06-2015 12:30:32







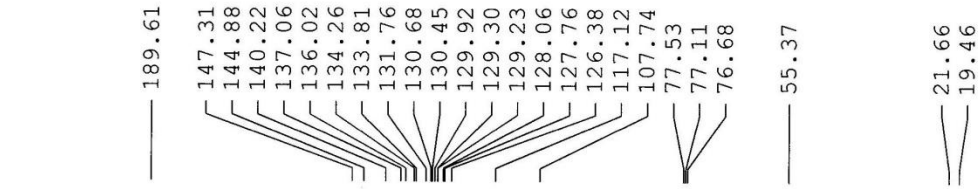


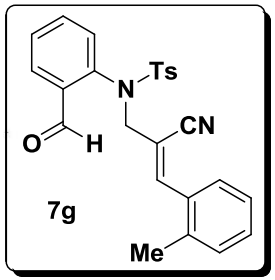
Current Data Parameters
NAME DK-V-2-Me-TS-CN-CHO
EXPNO 3
PROCNO 1

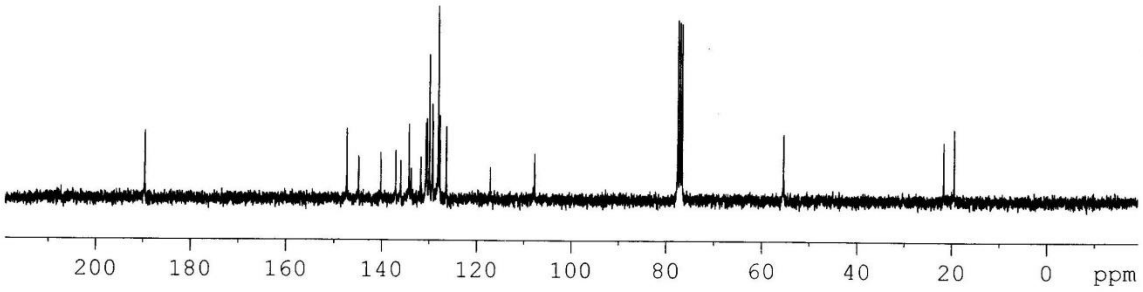
F2 - Acquisition Parameters
Date_ 20111024
Time 13.46
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 5
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 64
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 13.15 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00







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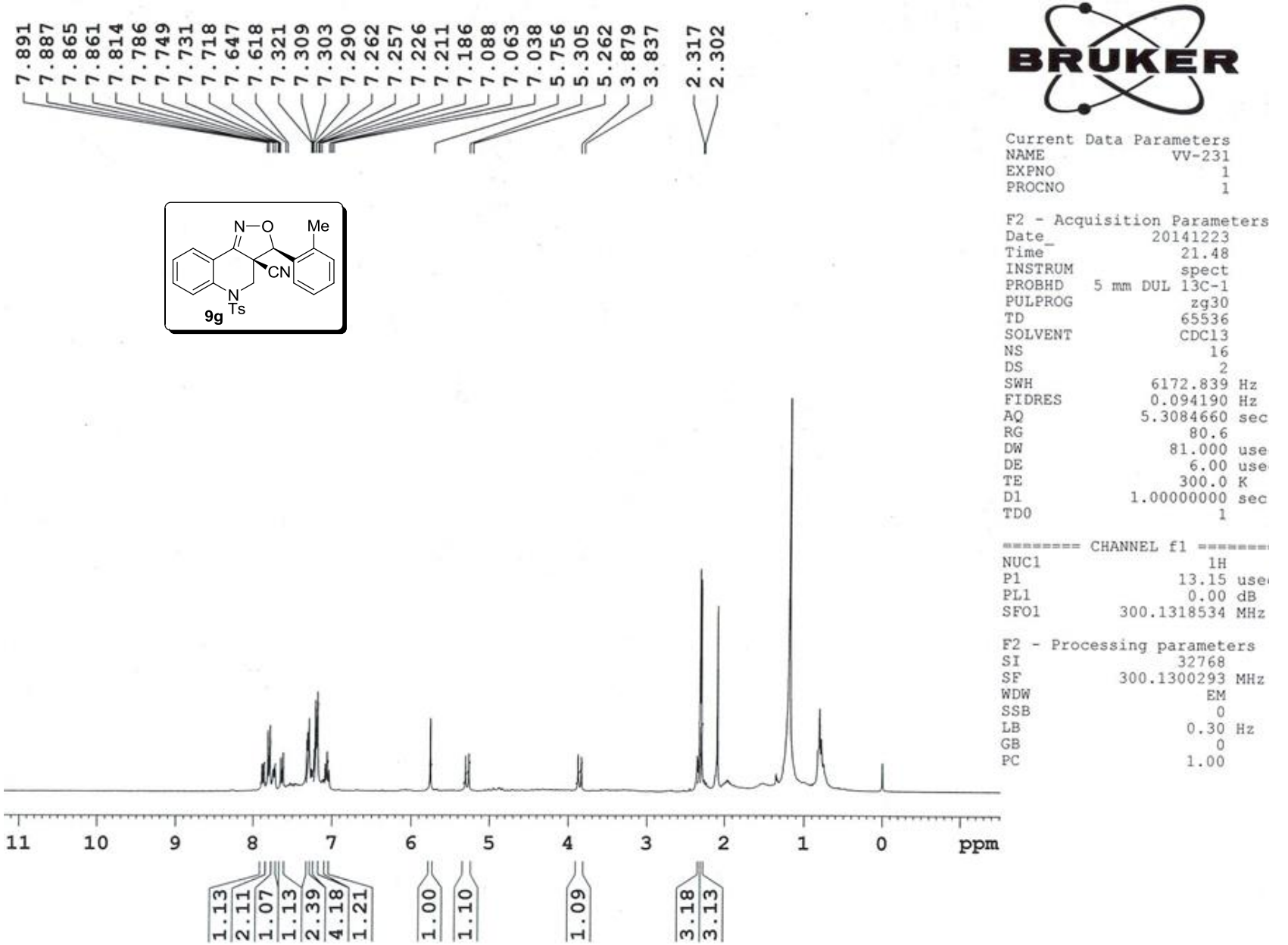
```
Current Data Parameters
NAME      DK-V-2-Me-TS-CN-CHO
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_              20111024
Time                 13.38
INSTRUM              spect
PROBHD   5 mm DUL 13C-1
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      146
DS                        4
SWH              17985.611 Hz
FIDRES           0.274439 Hz
AQ               1.8219508 sec
RG                 20642.5
DW                  27.800 usec
DE                   6.00 usec
TE                  300.0 K
D1               2.00000000 sec
d11              0.03000000 sec
DELTA            1.89999998 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                    13C
P1                     9.30 usec
PL1                    0.00 dB
SFO1           75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                    0.00 dB
PL12                  15.68 dB
PL13                  16.00 dB
SFO2          300.1312005 MHz

F2 - Processing parameters
SI                     32768
SF             75.4677490 MHz
WDW                       EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.40
```



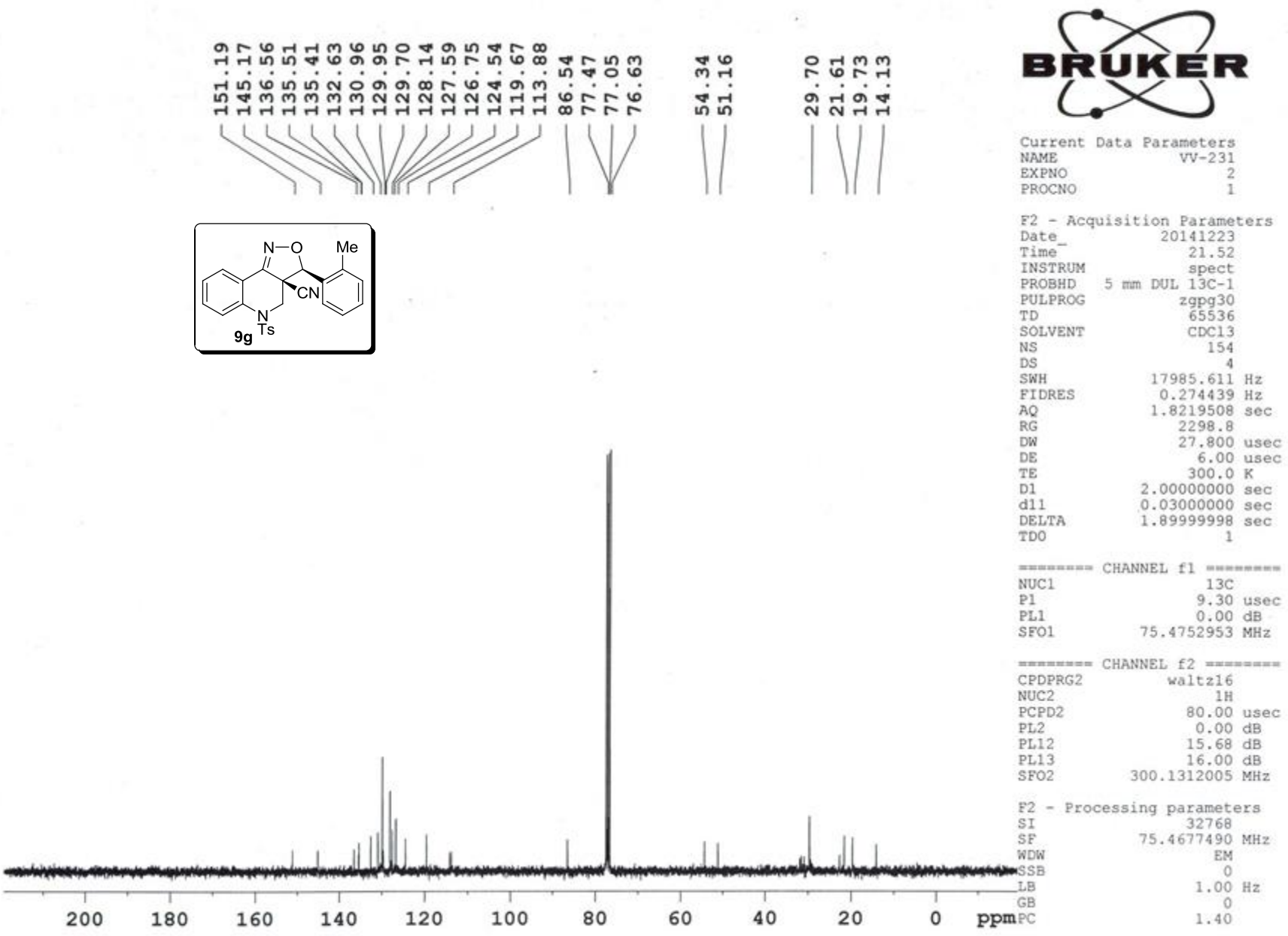
BRUKER

Current Data Parameters
NAME VV-231
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141223
Time 21.48
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 80.6
DW 81.000 use
DE 6.00 use
TE 300.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 13.15 use
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300293 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



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Current Data Parameters
NAME VV-231
EXPNO 2
PROCNO 1

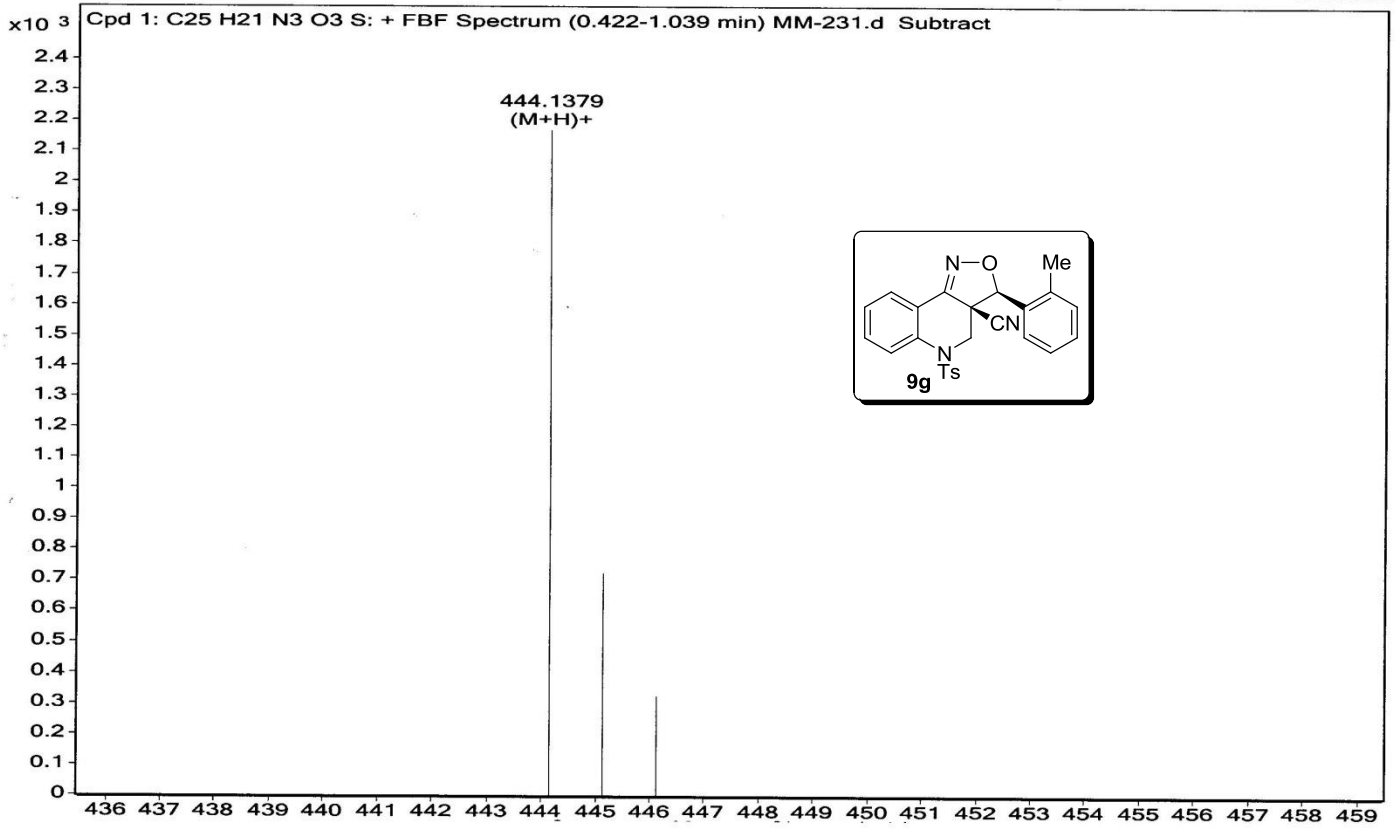
F2 - Acquisition Parameters
Date_ 20141223
Time 21.52
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 154
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 2298.8
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.30 usec
PL1 0.00 dB
SFO1 75.4752953 MHz

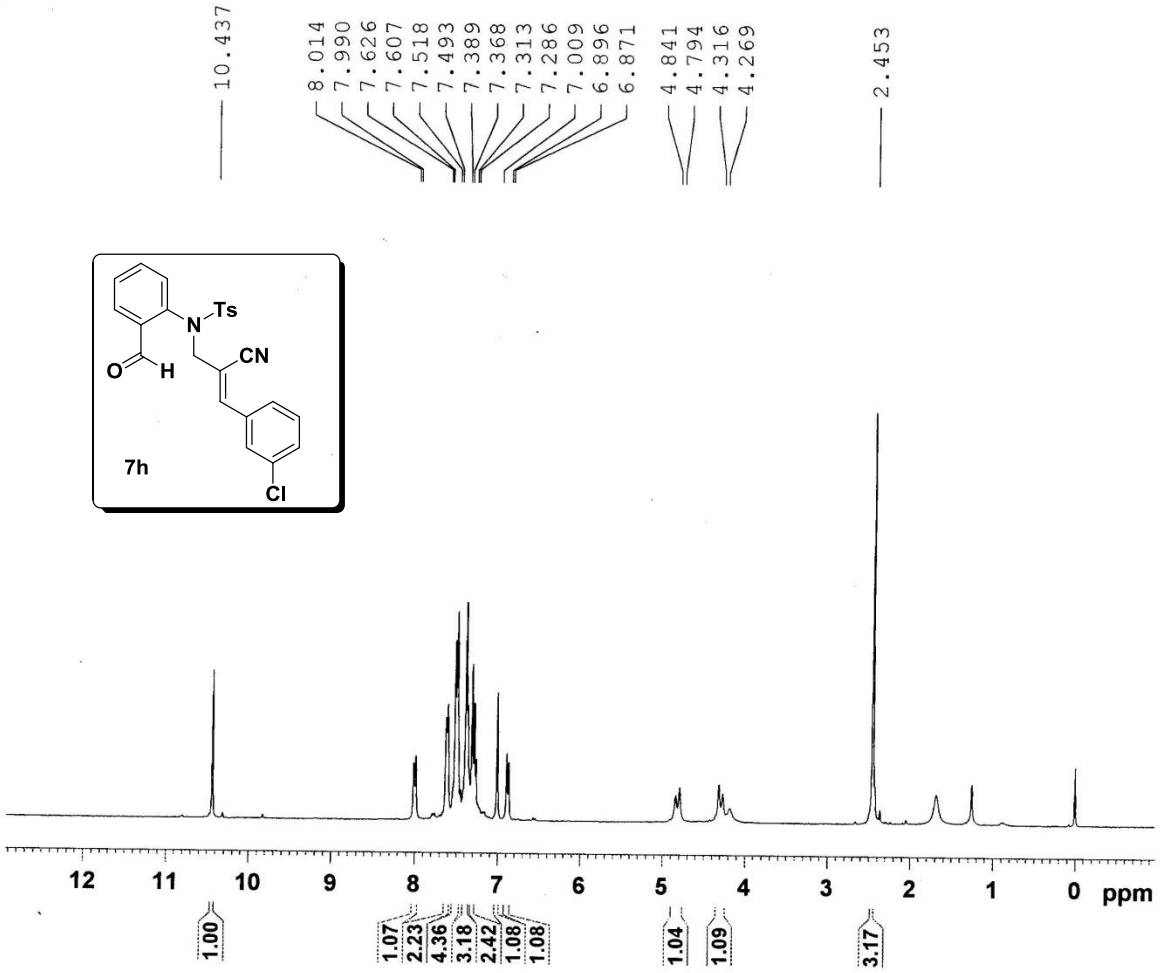
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.68 dB
PL13 16.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Sample Name	MM-231	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	MM-231.d	**ACQ Method**	Pondicherry Universi	**Comment**	MSK-MB-443.1304	**Acquired Time**	05-06-2015 14:21:13



UNIV. OF MADRAS



BRUKER

Current Data Parameters

NAME	V.V.-238
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20150622
Time	12.35
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	6172.839 Hz
FIDRES	0.094190 Hz
AQ	5.3084660 sec
RG	128
DW	81.000 usec
DE	6.00 usec
TE	300.0 K
D1	1.00000000 sec
TD0	1

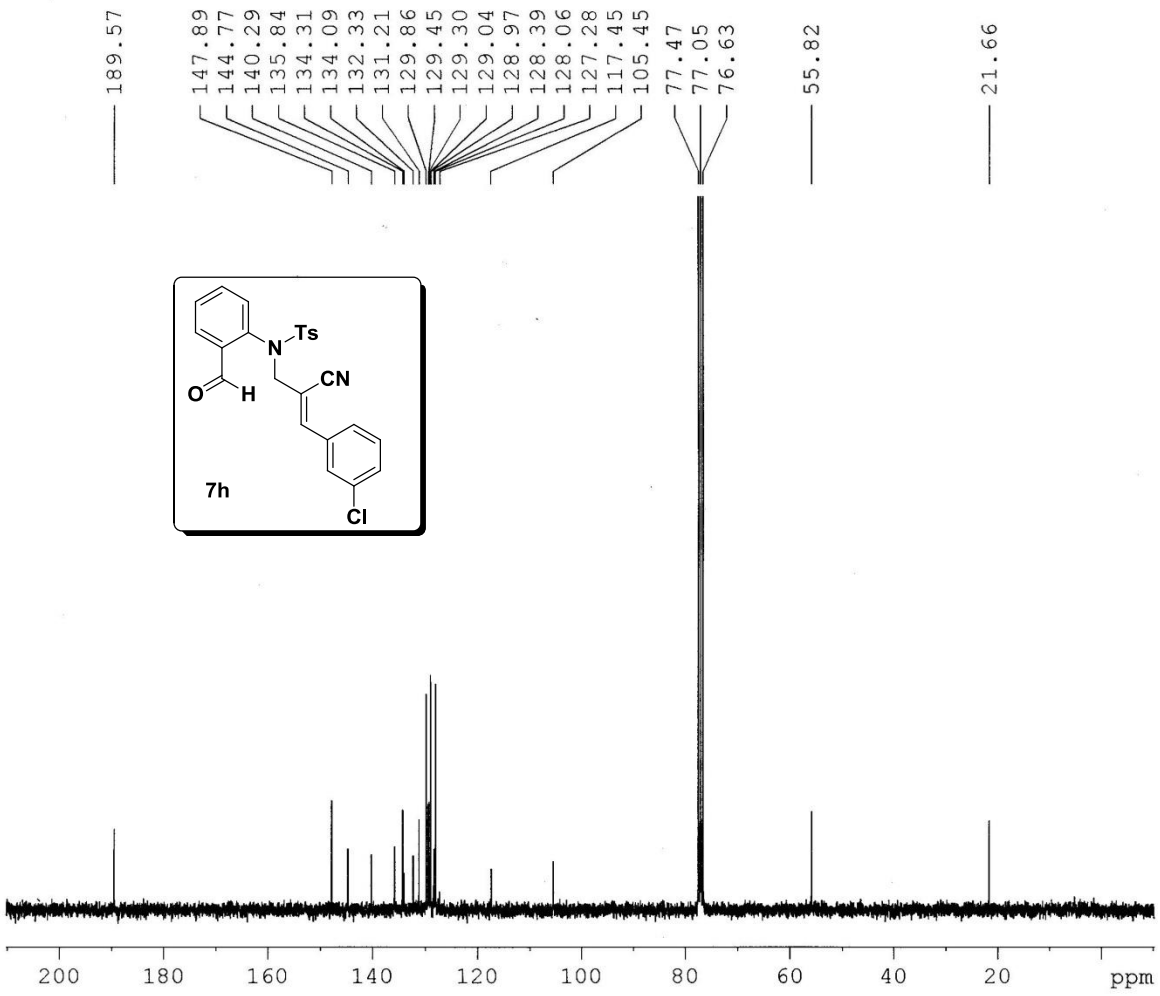
======== CHANNEL f1 ========

NUC1	1H
P1	13.88 usec
PL1	0.00 dB
SFO1	300.1318534 MHz

F2 - Processing parameters

SI	32768
SF	300.1300040 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

UNIV. OF MADRAS



BRUKER

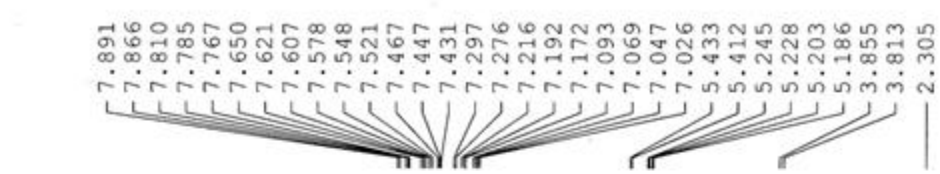
Current Data Parameters
NAME V.V. 238
EXPNO 2
PROCNO 1

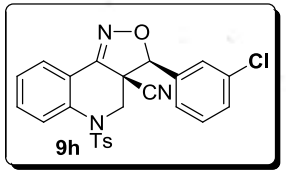
F2 - Acquisition Parameters
Date_ 20150622
Time 12.52
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 250
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 20642.5
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.38 usec
PL1 0.00 dB
SFO1 75.4752953 MHz

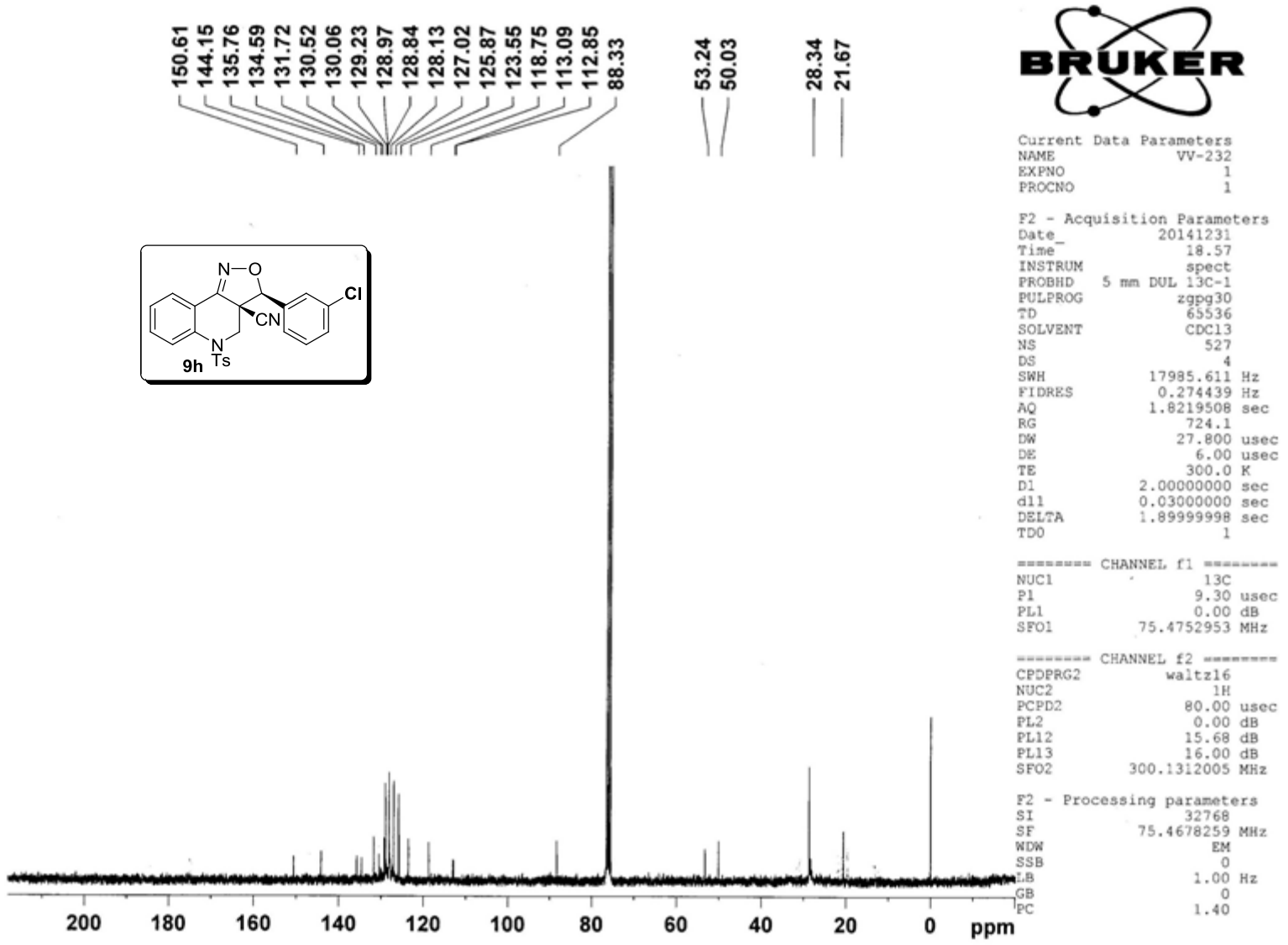
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.21 dB
PL13 16.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





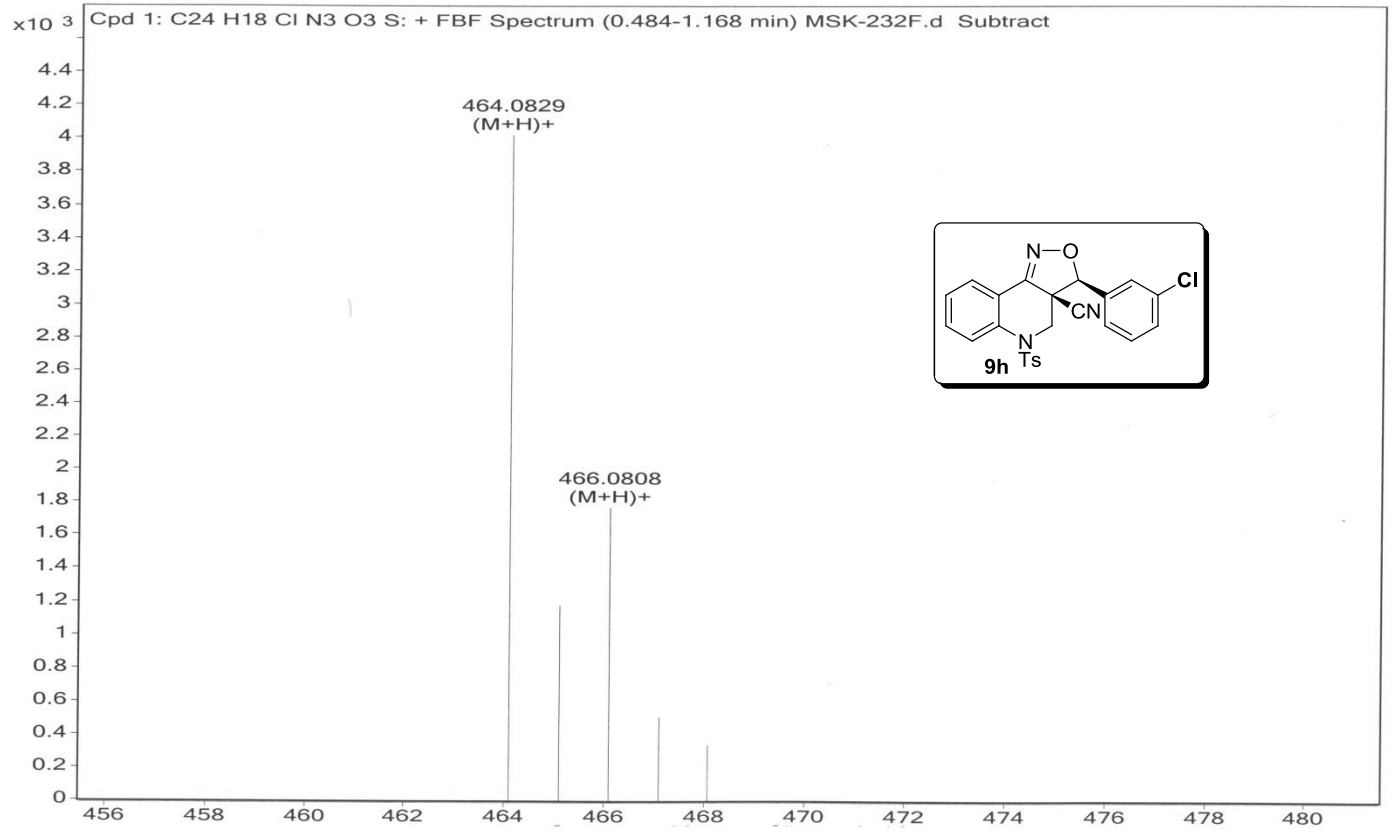

```
Current Data Parameters
NAME                  VV-232
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20141230
Time                 21.31
INSTRUM              spect
PROBHD    5 mm DUL 13C-1
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH               6172.839 Hz
FIDRES            0.094190 Hz
AQ                5.3084660 sec
RG                      64
DW                 81.000 usec
DE                  6.00 usec
TE                 300.0 K
D1              1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                   1H
P1                  13.15 usec
PL1                  0.00 dB
SFO1          300.1318534 MHz

F2 - Processing parameters
SI                     32768
SF            300.1300288 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

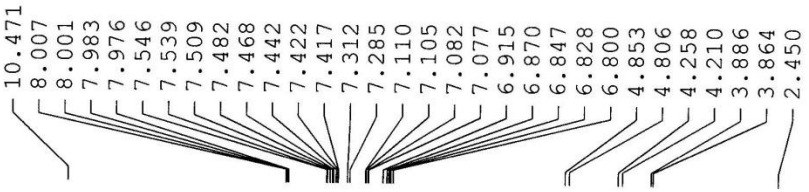


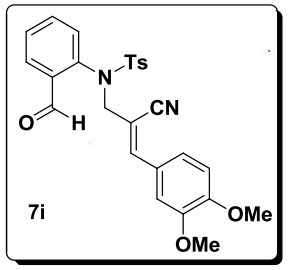
BRUKER

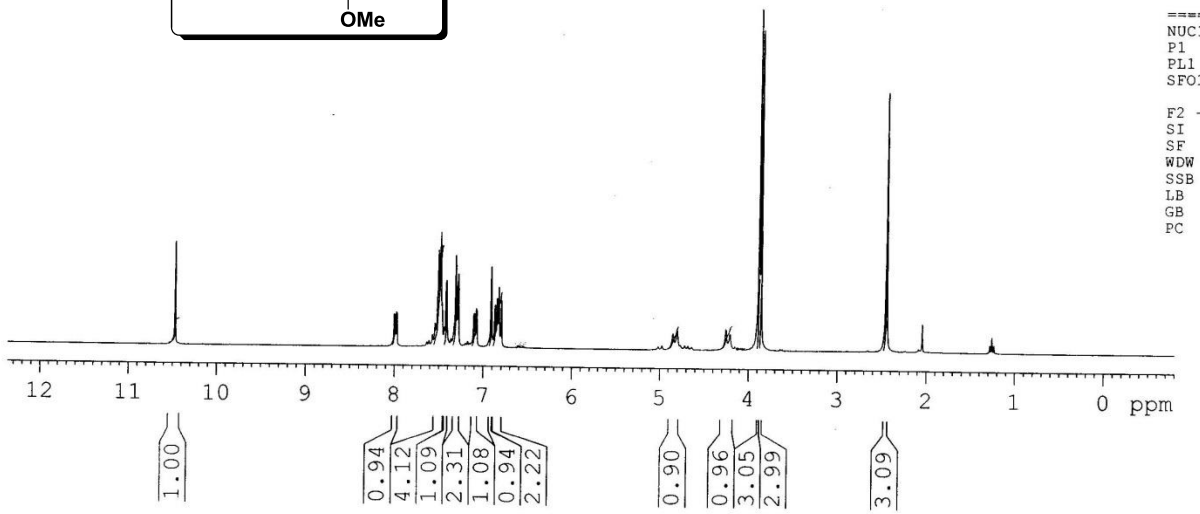
```
Current Data Parameters
NAME                  VV-232
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20141231
Time                  18.57
INSTRUM               spect
PROBHD    5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     527
DS                       4
SWH             17985.611 Hz
FIDRES           0.274439 Hz
AQ               1.8219508 sec
RG                   724.1
DW                  27.800 usec
DE                   6.00 usec
TE                  300.0 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                   13C
P1                    9.30 usec
PL1                   0.00 dB
SFO1           75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                   1H
PCPD2                80.00 usec
PL2                   0.00 dB
PL12                 15.68 dB
PL13                 16.00 dB
SFO2          300.1312005 MHz

F2 - Processing parameters
SI                     32768
SF             75.4678259 MHz
WDW                       EM
SSB                        0
LB                    1.00 Hz
GB                         0
PC                    1.40
```

Sample Name	MSK-232F	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	MSK-232F.d	**ACQ Method**	Pondicherry Universi	**Comment**	MSK-463.0757	**Acquired Time**	15-06-2015 14:36:02







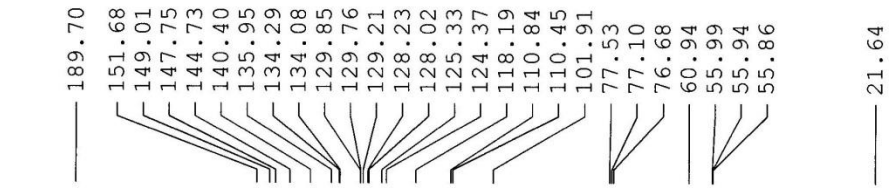


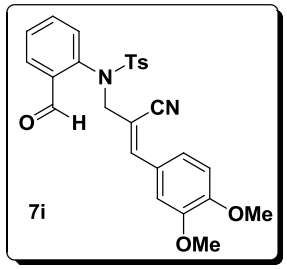
Current Data Parameters
NAME DK-V-OMe2 CN Ts-CHO
EXPNO 1
PROCNO 1

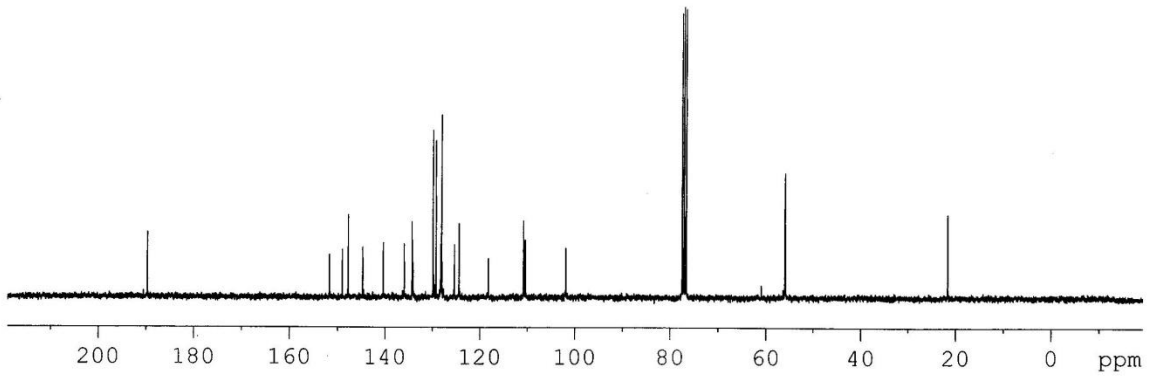
F2 - Acquisition Parameters
Date_ 20111009
Time 18.07
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 64
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 13.15 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

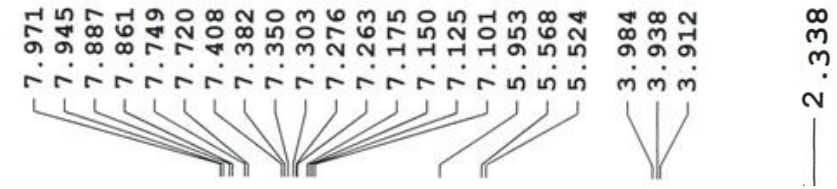


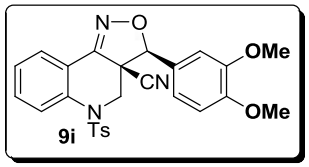


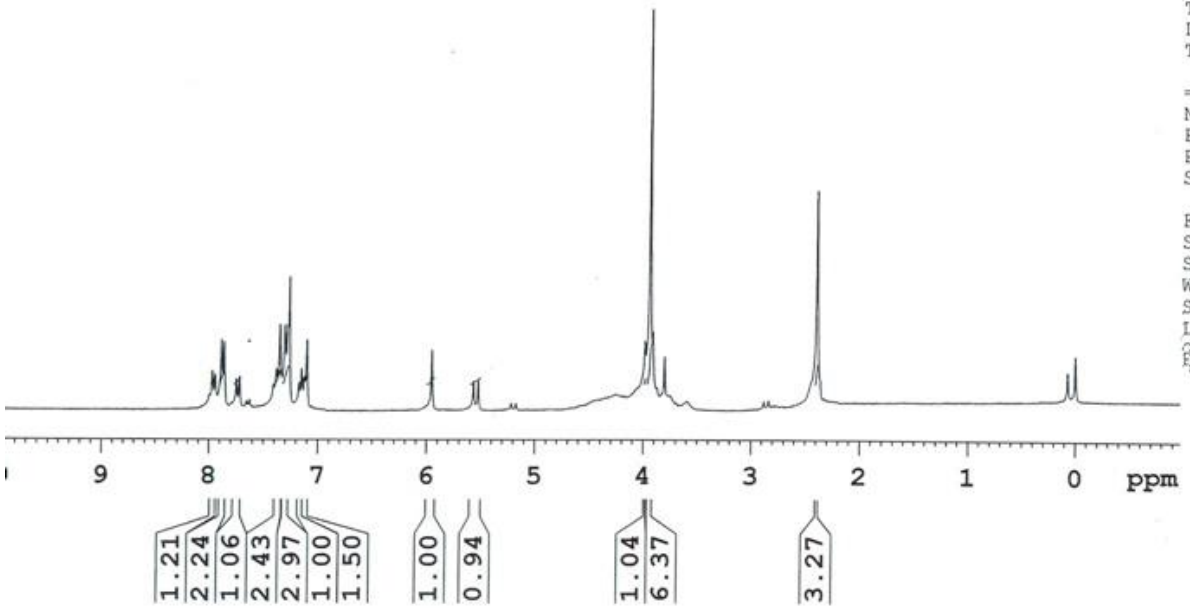


BRUKER

```
Current Data Parameters
NAME      DK-V-OMe2 CN Ts-CHO
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20111009
Time                  18.22
INSTRUM               spect
PROBHD    5 mm DUL 13C-1
PULPROG               zgpg30
TD                     65536
SOLVENT                CDCl3
NS                       219
DS                         4
SWH               17985.611 Hz
FIDRES             0.274439 Hz
AQ                 1.8219508 sec
RG                    5160.6
DW                    27.800 usec
DE                     6.00 usec
TE                    300.0 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                     13C
P1                      9.30 usec
PL1                     0.00 dB
SFO1            75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                     1H
PCPD2                 80.00 usec
PL2                     0.00 dB
PL12                   15.68 dB
PL13                   16.00 dB
SFO2           300.1312005 MHz

F2 - Processing parameters
SI                       32768
SF              75.4677490 MHz
WDW                         EM
SSB                          0
LB                      1.00 Hz
GB                           0
PC                      1.40
```

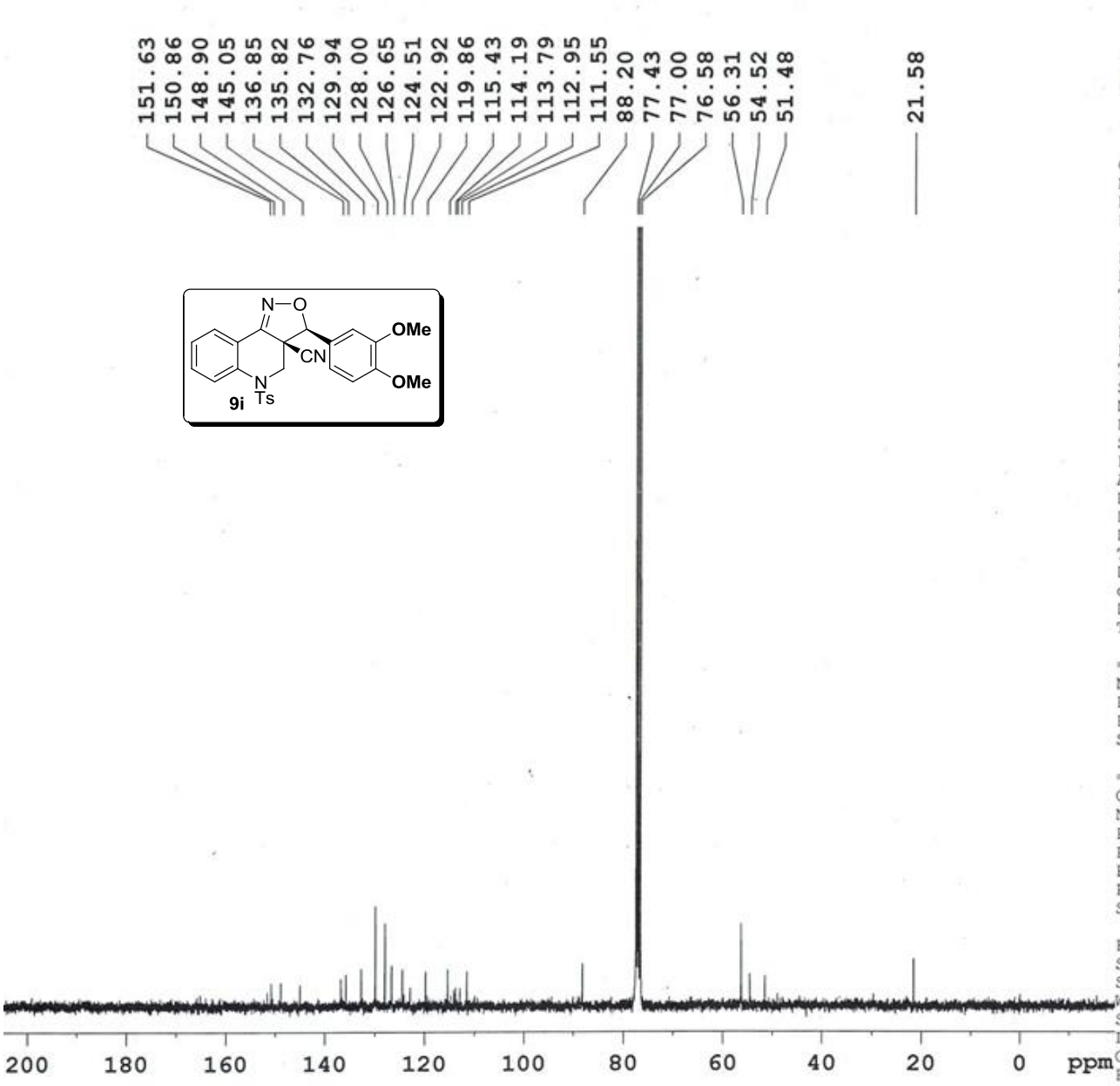






BRUKER

```
Current Data Parameters
NAME                  VV-78
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20140827
Time                  0.27
INSTRUM              spect
PROBHD    5 mm DUL 13C-1
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH               6172.839 Hz
FIDRES            0.094190 Hz
AQ                5.3084660 sec
RG                   228.1
DW                  81.000 usec
DE                   6.00 usec
TE                  300.0 K
D1               1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                  13.15 usec
PL1                  0.00 dB
SFO1          300.1318534 MHz

F2 - Processing parameters
SI                   32768
SF            300.1300066 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```



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Current Data Parameters
NAME VV-78
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140827
Time 3.17
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2651
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 456.1
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.30 usec
PL1 0.00 dB
SFO1 75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.68 dB
PL13 16.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Sample Name	MM-78CN	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	MM-78CNn.d	**ACQ Method**	Pondicherry Universi	**Comment**	MSK-MB-489.1358	**Acquired Time**	05-06-2015 12:37:16