

Supporting Information

Highly Regio- and Diastereoselective Synthesis of Novel Tri- and Tetracyclic Perhydroquinoline Architectures Through an Intramolecular [3 + 2] Cycloaddition Reaction

Manickam Bakthadoss,^{*a,b} Damodharan Kannan,^b Jayakumar Srinivasan^b and Varathan Vinayagam^b

^aDepartment of Chemistry, Pondicherry University, Pondicherry – 605 014, India

^bDepartment of Organic Chemistry, University of Madras, Guindy Campus, Chennai-600025, Tamil Nadu, India

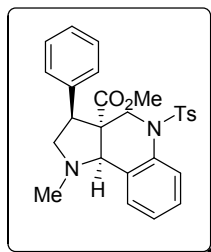
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Experimental Section

General Remarks: Melting points were recorded on a Superfit (India) capillary melting point apparatus and were uncorrected. IR spectra were recorded on a Bruker-FT-IR spectrometer using solid samples as KBr plates. For compounds ^1H NMR (300 MHz) and ^{13}C NMR (75 MHz) spectra **9a-l**, **12a-h**, **15a-d** and **17a-d** were recorded in deuteriochloroform (CDCl_3) on a Bruker 300 MHz spectrometer using tetramethylsilane (TMS, $\delta = 0$) as an internal standard at room temperature. Mass spectra were recorded on Agilent 1200 LC/MS-6110 mass spectrometer. The X-ray diffraction measurements were carried out on a Bruker AXS Kappa APEX 2 CCD diffractometer. All the compounds were synthesized as racemates.

Typical experimental procedure for the synthesis of Compound 9a: To a stirred solution of methyl (2*E*)-2- $\{[N-(2\text{-formylphenyl})(4\text{-methylbenzene})\text{ sulfonamido}]\text{methyl}\}$ -3-phenylprop-2-enoate (**6a**) (1 mmol, 0.45 g) in acetonitrile (10 mL), *N*-methyl glycine (**7**) (1.1 mmol, 0.10 g) was added and allowed to stir under reflux condition over a period of 6 h. After completion of the reaction as indicated by TLC, the reaction mixture was concentrated and the resulting crude mass was diluted with water (20 mL) and extracted with ethyl acetate (3 x 10 mL). The combined organic layer thus obtained was washed with brine (3 x 10 mL) and dried over anhydrous Na_2SO_4 . The organic layer was concentrated and the crude mass was recrystallized using ethyl acetate : hexane mixture (2:8) to provide **9a** as a colorless solid in 94% yield.

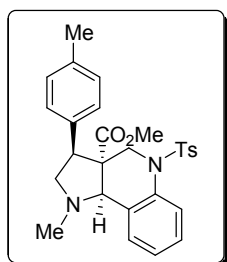
Methyl 1-methyl-5-[(4-methylbenzene)sulfonyl]-3-phenyl-1*H*,2*H*,3*H*,3*aH*,4*H*,5*H*,9*bH*-pyrrolo[3,2-*c*]quinoline-3*a*-carboxylate (9a**):**



Yield: 94%; mp: 226-228°C; IR (KBr): 1754, 1693 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3): δ 2.34 (s, 3H), 2.36 (s, 3H), 2.91 (t, 1H, $J = 9.9$ Hz), 3.35 (dd, 1H, $J = 4.2, 9.9$ Hz), 3.51 (d, 1H, $J = 12.3$ Hz), 3.64 (s, 1H), 3.69 (s, 3H), 3.89 (dd, 1H, $J = 4.2, 9.9$ Hz), 3.96 (d, 1H, $J = 12.6$ Hz), 6.96–7.58 (m, 13H); ^{13}C NMR (75 MHz, CDCl_3): δ 16.25, 34.64, 42.30, 43.80, 47.17, 48.79, 54.45,

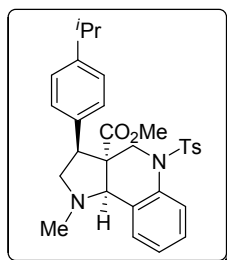
62.98, 114.48, 117.20, 119.19, 121.76, 122.17, 123.05, 123.23, 123.56, 124.29, 126.06, 131.52, 132.04, 132.50, 138.22, 168.30; MS (m/z): 478 ($M^{+}+1$); Anal. Calcd. for $C_{27}H_{28}N_2O_4S$: C, 68.04; H, 5.92; N, 5.88; Found: C, 68.13; H, 5.99; N, 6.01.

Methyl 1-methyl-5-[(4-methylbenzene)sulfonyl]-3-(4-methylphenyl)-1*H*,2*H*,3*H*,3*aH*,4*H*,5*H*,9*bH*-pyrrolo[3,2-*c*]quinoline-3*a*-carboxylate (9b)



Yield: 92%; mp: 229-231°C; IR (KBr): 1740, 1698 cm^{-1} ; 1H NMR: δ 2.20 (s, 3H), 2.30 (s, 3H), 2.35 (s, 3H), 2.89 (t, 1H, $J = 9.6$ Hz), 3.20 (d, 1H, $J = 9.3$ Hz), 3.44 (d, 1H, $J = 12.6$ Hz), 3.63 (s, 4H), 4.02 (t, 2H, $J = 12.6$ Hz), 6.89 – 7.54 (m, 12H); ^{13}C NMR ($CDCl_3$, 75 MHz): δ 19.72, 21.51, 40.30, 45.27, 47.65, 52.42, 62.10, 68.26, 119.43, 122.47, 125.94, 127.06, 127.19, 128.17, 128.45, 129.61, 130.65, 131.13, 136.76, 137.09, 137.52, 143.60, 149.61, 174.16; MS (m/z): 492 ($M^{+}+1$); Anal. Calcd. for $C_{28}H_{30}N_2O_4S$: C, 68.55; H, 6.16; N, 5.71; Found: C, 68.66; H, 6.24; N, 5.84.

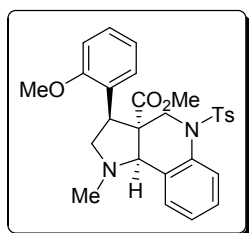
Methyl 1-methyl-5-[(4-methylbenzene)sulfonyl]-3-[4-(propan-2-yl)phenyl]-1*H*,2*H*,3*H*,3*aH*,4*H*,5*H*,9*bH*-pyrrolo[3,2-*c*]quinoline-3*a*-carboxylate (9c)



Yield: 91%; mp: 227-229°C; IR (KBr): 1732, 1698 cm^{-1} ; 1H NMR: δ 1.27 (d, 6H, $J = 6.9$ Hz), 2.31 (s, 3H), 2.36 (s, 3H), 2.81-2.99 (m, 2H), 3.34 (dd, 1H, $J = 4.8, 9.9$ Hz), 3.53 (d, 1H, $J = 12.3$

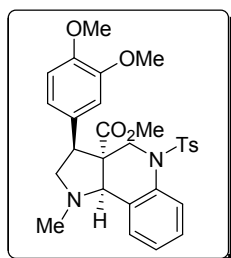
Hz), 3.64 (s, 1H), 3.68 (s, 3H), 3.87 (dd, 1H, $J = 4.5, 10.2$ Hz), 3.98 (d, 1H, $J = 12.6$ Hz), 6.96–7.59 (m, 12H); ^{13}C NMR (CDCl_3 , 75 MHz): δ 21.51, 23.96, 24.00, 33.73, 39.85, 47.40, 48.82, 52.40, 54.12, 59.62, 68.35, 119.81, 122.46, 124.44, 126.54, 127.05, 128.34, 128.72, 129.51, 131.30, 134.85, 136.74, 137.16, 143.47, 147.94, 173.56; MS (m/z): 520 ($M^{+}+1$); Anal. Calcd for $\text{C}_{30}\text{H}_{34}\text{N}_2\text{O}_4\text{S}$: C, 69.47; H, 6.61; N, 5.40; Found: C, 69.60; H, 6.73; N, 5.53.

Methyl 1-methyl-5-[(4-methylbenzene)sulfonyl]-3-(2-methoxyphenyl)-1*H*,2*H*,3*H*,3*aH*,4*H*,5*H*,9*bH*-pyrrolo[3,2-*c*]quinoline-3*a*-carboxylate (9d)



Yield: 94%; mp: 223–225°C; IR (KBr): 1761, 1656 cm^{-1} ; ^1H NMR: δ 2.29 (s, 3H), 2.36 (s, 3H), 2.89 (t, 1H, $J = 9.9$ Hz), 3.39 (dd, 1H, $J = 4.8, 9.9$ Hz), 3.51 (d, 1H, $J = 12.3$ Hz), 3.65 (s, 3H), 3.69 (s, 1H), 3.77 (s, 3H), 4.02 (d, 1H, $J = 12.3$ Hz), 4.37 (dd, 1H, $J = 4.5, 10.2$ Hz), 6.85–7.60 (m, 12H); ^{13}C NMR (CDCl_3 , 75 MHz): δ 21.51, 39.86, 42.58, 46.76, 52.13, 53.21, 55.32, 58.92, 69.29, 110.34, 119.68, 120.37, 122.24, 124.11, 125.56, 127.17, 128.32, 128.42, 128.54, 129.47, 131.37, 136.71, 137.14, 143.37, 157.65, 173.49; MS (m/z): 508 ($M^{+}+1$); Anal. Calcd. for $\text{C}_{28}\text{H}_{30}\text{N}_2\text{O}_5\text{S}$: C, 66.38; H, 5.97; N, 5.53; Found: C, 66.45; H, 6.09; N, 5.64.

Methyl 1-methyl-5-[(4-methylbenzene)sulfonyl]-3-(3,4-dimethoxyphenyl)-1*H*,2*H*,3*H*,3*aH*,4*H*,5*H*,9*bH*-pyrrolo[3,2-*c*]quinoline-3*a*-carboxylate (9e)



Yield: 95%; mp: 227–229°C; IR (KBr): 1777, 1687 cm^{-1} ; ^1H NMR: δ 2.37 (s, 3H), 2.38 (s, 3H), 2.92 (t, 1H, $J = 9.9$ Hz), 3.32 (dd, 1H, $J = 4.5, 10.2$ Hz), 3.48 (d, 1H, $J = 12.6$ Hz), 3.67 (s, 1H),

3.70 (s, 3H), 3.84 (s, 4H), 3.89 (s, 3H), 4.04 (d, 1H, $J = 12.9$ Hz), 6.83–7.61 (m, 11H); ^{13}C NMR (CDCl_3 , 75 MHz): δ 21.50, 40.20, 47.57, 49.10, 52.42, 54.90, 55.88, 55.95, 59.79, 67.97, 111.00, 112.11, 120.00, 121.02, 122.69, 125.33, 127.00, 128.20, 129.55, 130.20, 130.90, 136.83, 137.40, 143.49, 148.28, 148.81, 173.80; MS (m/z): 538 ($M^+ + 1$); Anal. Calcd. for $\text{C}_{29}\text{H}_{32}\text{N}_2\text{O}_6\text{S}$: C, 64.91; H, 6.01; N, 5.22; Found: C, 64.99; H, 6.12; N, 5.36.

Crystal data for Methyl 1-methyl-5-[(4-methylbenzene)sulfonyl]-3-(3,4-dimethoxyphenyl)-1*H*,2*H*,3*H*,3*aH*,4*H*,5*H*,9*bH*-pyrrolo[3,2-*c*]quinoline-3*a*-carboxylate (9e**)**

Empirical formula, $\text{C}_{29}\text{H}_{32}\text{N}_2\text{O}_6\text{S}$; Formula weight, 537; crystal color, colorless; Single crystal X-ray structure of the molecule shown in ORTEP diagram (Figure 1). Detailed X-ray crystallographic data is available from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK (for pyrroloquinoline (**9e**) CCDC # **764210**).

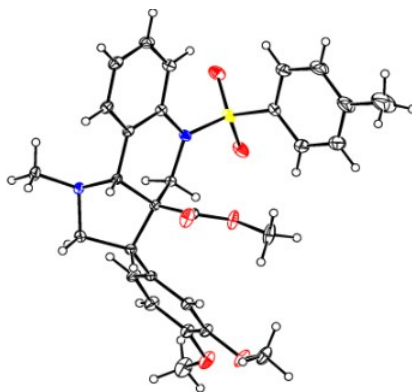
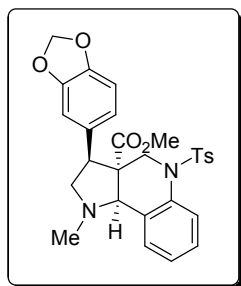


Figure 1. ORTEP diagram of compound 9e

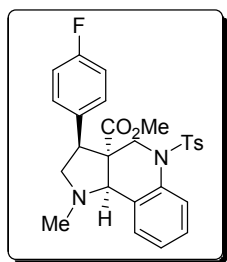
Methyl 3-(2*H*-1,3-benzodioxol-5-yl)-1-methyl-5-[(4-methylbenzene)sulfonyl]-1*H*,2*H*,3*H*,3*aH*,4*H*,5*H*,9*bH*-pyrrolo[3,2-*c*]quinoline-3*a*-carboxylate (9f**)**



Yield: 95%; mp: 226–228°C; IR (KBr): 1781, 1595 cm^{-1} ; ^1H NMR: δ 2.33 (s, 3H), 2.38 (s, 3H), 2.89 (t, 1H, $J = 10.2$ Hz), 3.25 (dd, 1H, $J = 3.9, 9.9$ Hz), 3.51 (d, 1H, $J = 12.3$ Hz), 3.61 (s, 1H),

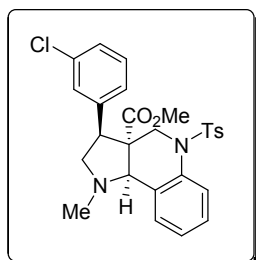
3.69 (s, 3H), 3.81 (dd, 1H, $J = 3.9, 9.9$ Hz), 4.05 (d, 1H, $J = 12.6$ Hz), 5.98 (s, 2H), 6.73–7.62 (m, 11H); ^{13}C NMR (CDCl_3 , 75 MHz): δ 21.52, 39.91, 47.48, 48.85, 52.46, 54.12, 60.01, 68.05, 101.11, 108.15, 109.19, 119.72, 122.01, 122.48, 124.46, 127.01, 128.28, 129.59, 131.27, 131.49, 136.74, 137.35, 143.53, 146.80, 147.74, 173.58; MS (m/z): 522 ($\text{M}^+ + 1$); Anal. Calcd. for $\text{C}_{28}\text{H}_{28}\text{N}_2\text{O}_6\text{S}$: C, 64.60; H, 5.42; N, 5.38; Found: C, 64.69; H, 5.52; N, 5.49.

Methyl 1-methyl-5-[(4-methylbenzene)sulfonyl]-3-(4-fluorophenyl)-1*H*,2*H*,3*H*,3*aH*,4*H*,5*H*,9*bH*-pyrrolo[3,2-*c*]quinoline-3*a*-carboxylate (9g)



Yield: 94%; mp: 230–232°C; IR (KBr): 1784, 1632 cm^{-1} ; ^1H NMR: δ 2.36 (s, 3H), 2.37 (s, 3H), 2.92 (t, 1H, $J = 9.9$ Hz), 3.29 (dd, 1H, $J = 3.9, 9.9$ Hz), 3.46 (d, 1H, $J = 12.3$ Hz), 3.62 (s, 1H), 3.69 (s, 3H), 3.87 (dd, 1H, $J = 3.6, 9.9$ Hz), 3.94 (d, 1H, $J = 12.6$ Hz), 6.97–7.59 (m, 12H); ^{13}C NMR (CDCl_3 , 75 MHz): δ 21.51, 39.91, 47.68, 48.15, 52.51, 53.82, 60.05, 67.94, 115.33 (d, $J = 21.1$ Hz), 119.61, 122.49, 124.36, 126.93, 128.30, 129.62, 130.36 (d, $J = 7.9$ Hz), 131.30, 133.62, 137.04 (d, $J = 48.3$ Hz), 143.59, 173.51. MS (m/z): 496 ($\text{M}^+ + 1$); Anal. Calcd. for $\text{C}_{27}\text{H}_{27}\text{FN}_2\text{O}_4\text{S}$: C, 65.57; H, 5.50; N, 5.66; Found: C, 65.68; H, 5.64; N, 5.79.

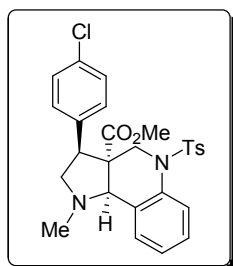
Methyl 1-methyl-5-[(4-methylbenzene)sulfonyl]-3-(3-chlorophenyl)-1*H*,2*H*,3*H*,3*aH*,4*H*,5*H*,9*bH*-pyrrolo[3,2-*c*]quinoline-3*a*-carboxylate (9h)



Yield: 90%; mp: 223–225°C; IR (KBr): 1729, 1686 cm^{-1} ; ^1H NMR: δ 2.36 (s, 6H), 2.91 (t, 1H, $J = 9.3$ Hz), 3.27 (t, 1H, $J = 9.9$ Hz), 3.46 (d, 1H, $J = 12.3$ Hz), 3.62 (s, 1H), 3.69 (s, 3H), 3.85 (d,

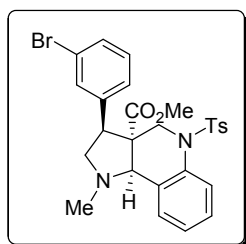
1H, $J = 6.6$ Hz), 3.94 (d, 1H, $J = 12.3$ Hz), 6.91–7.78 (m, 12H); ^{13}C NMR (CDCl_3 , 75 MHz): δ 21.51, 39.90, 47.67, 48.25, 52.53, 53.85, 59.87, 67.90, 119.64, 122.54, 124.35, 126.93, 127.28, 128.31, 128.61, 129.64, 129.78, 130.22, 131.27, 133.19, 136.51, 136.72, 137.36, 143.62, 173.42; MS (m/z): 512 ($\text{M}^+ + 1$); Anal. Calcd. for $\text{C}_{27}\text{H}_{27}\text{ClN}_2\text{O}_4\text{S}$: C, 63.46; H, 5.33; N, 5.48; Found: C, 63.52; H, 5.40; N, 5.61.

Methyl 1-methyl-5-[(4-methylbenzene)sulfonyl]-3-(4-chlorophenyl)-1*H*,2*H*,3*H*,3*aH*,4*H*,5*H*,9*bH*-pyrrolo[3,2-*c*]quinoline-3*a*-carboxylate (9i)



Yield: 92%; mp: 221–223°C; IR (KBr): 1780, 1673 cm^{-1} ; ^1H NMR: δ 2.37 (s, 3H), 2.38 (s, 3H), 2.91 (t, 1H, $J = 9.6$ Hz), 3.28 (d, 1H, $J = 7.5$ Hz), 3.45 (d, 1H, $J = 12.3$ Hz), 3.62 (s, 1H), 3.70 (s, 3H), 3.85 (d, 1H, $J = 6.9$ Hz), 3.94 (d, 1H, $J = 12.3$ Hz), 7.00–7.60 (m, 12H); ^{13}C NMR (CDCl_3 , 75 MHz): δ 21.51, 39.91, 47.67, 48.25, 52.53, 53.85, 59.90, 67.91, 119.65, 122.52, 124.37, 126.93, 128.30, 128.62, 129.62, 130.20, 131.25, 133.20, 136.51, 136.72, 137.40, 143.59, 173.43; MS (m/z): 512 ($\text{M}^+ + 1$); Anal. Calcd. for $\text{C}_{27}\text{H}_{27}\text{ClN}_2\text{O}_4\text{S}$: C, 63.46; H, 5.33; N, 5.48; Found: C, 63.53; H, 5.39; N, 5.61.

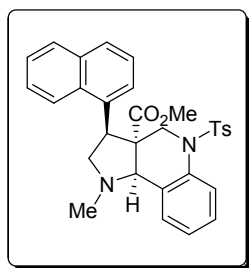
Methyl 1-methyl-5-[(4-methylbenzene)sulfonyl]-3-(3-bromophenyl)-1*H*,2*H*,3*H*,3*aH*,4*H*,5*H*,9*bH*-pyrrolo[3,2-*c*]quinoline-3*a*-carboxylate (9j)



Yield: 90%; mp: 232–234°C; IR (KBr): 1794, 1659 cm^{-1} ; ^1H NMR: δ 2.36 (s, 3H), 2.39 (s, 3H), 2.89 (t, 1H, $J = 9.9$ Hz), 3.26 (dd, 1H, $J = 3.6, 10.2$ Hz), 3.43 (d, 1H, $J = 12.3$ Hz), 3.60 (s, 1H),

3.72 (s, 3H), 3.83 (dd, 1H, $J = 3.6, 9.9$ Hz), 3.93 (d, 1H, $J = 12.3$ Hz), 6.99–7.60 (m, 12H); ^{13}C NMR (CDCl_3 , 75 MHz): δ 21.51, 39.89, 47.75, 48.53, 52.56, 53.95, 59.84, 67.86, 119.75, 122.56, 122.59, 124.43, 126.99, 127.78, 128.32, 129.64, 129.99, 130.55, 131.23, 131.74, 136.75, 137.12, 140.53, 143.60, 173.38; MS (m/z): 557 (M^{+2}); Anal. Calcd. for $\text{C}_{27}\text{H}_{27}\text{BrN}_2\text{O}_4\text{S}$: C, 58.38; H, 4.90; N, 5.04; Found: C, 58.45; H, 4.99; N, 5.17.

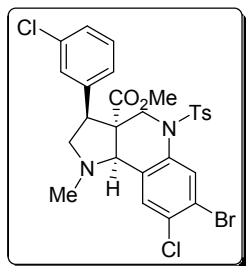
Methyl 1-methyl-5-[(4-methylbenzene)sulfonyl]-3-(naphthalen-1-yl)-1*H*,2*H*,3*H*,3*aH*,4*H*,5*H*,9*bH*-pyrrolo[3,2-*c*]quinoline-3*a*-carboxylate (9k)



Yield: 96%; mp: 226–228°C; IR (KBr): 1773, 1686 cm^{-1} ; ^1H NMR: δ 2.36 (s, 3H), 2.47 (s, 3H), 3.11 (t, 1H, $J = 9.9$ Hz), 3.53 (d, 2H, $J = 12.6$ Hz), 3.60 (s, 3H), 3.89 (s, 1H), 3.98 (d, 1H, $J = 12.6$ Hz), 4.70 (t, 1H, $J = 6.3$ Hz), 6.99–7.94 (m, 15H); ^{13}C NMR (CDCl_3 , 75 MHz): δ 21.50, 40.46, 44.74, 47.57, 52.44, 55.15, 61.40, 68.47, 119.87, 122.82, 123.01, 124.14, 125.63, 126.11, 126.16, 127.07, 128.20, 129.13, 129.54, 130.72, 132.64, 133.86, 133.97, 136.73, 137.23, 143.50, 174.15; MS (m/z): 528 (M^{+1}); Anal. Calcd. for $\text{C}_{31}\text{H}_{30}\text{N}_2\text{O}_4\text{S}$: C, 70.70; H, 5.74; N, 5.32; Found: C, 70.78; H, 5.83; N, 5.45.

Typical experimental procedure for the synthesis of Compound 9l: To a stirred solution of methyl (2*E*)-2- $\{[N-(5\text{-bromo-4-chloro-2-formylphenyl})(4\text{-methylbenzene})\text{sulfonamido}]\text{methyl}\}$ -3-(3-chlorophenyl)prop-2-enoate (**6l**) (1 mmol, 0.59 g) in acetonitrile (10 mL), *N*-methyl glycine (**7**) (1.1 mmol, 0.10 g) was added and allowed to stir under reflux condition over a period of 6 h. After completion of the reaction as indicated by TLC, the reaction mixture was concentrated and the resulting crude mass was diluted with water (20 mL) and extracted with ethyl acetate (3 x 10 mL). The combined organic layer thus obtained was washed with brine (3 x 10 mL) and dried over anhydrous Na_2SO_4 . The organic layer was concentrated and the crude mass was recrystallized using ethyl acetate : hexane mixture (2:8) to provide **9l** as a colorless solid in 86% yield.

Methyl 7-bromo-8-chloro-3-(3-chlorophenyl)-1-methyl-5-[(4-methylbenzene)sulfonyl]-1*H*,2*H*,3*H*,3*aH*,4*H*,5*H*,9*bH*-pyrrolo[3,2-*c*]quinoline-3*a*-carboxylate (9l)



Yield: 86%; mp: 239-241°C; IR (KBr): 1786, 1694 cm^{-1} ; ^1H NMR: δ 2.33 (s, 3H), 2.39 (s, 3H), 2.89 (t, 1H, $J = 9.6$ Hz), 3.25-3.36 (m, 2H), 3.52 (s, 1H), 3.72 (s, 3H), 3.81-3.91 (m, 2H), 7.14-7.89 (m, 10H); ^{13}C NMR (CDCl_3 , 75 MHz): δ 21.57, 39.77, 47.49, 48.53, 52.74, 53.96, 59.55, 67.26, 121.33, 124.64, 127.05, 127.22, 127.83, 128.32, 128.86, 129.71, 129.80, 130.59, 131.82, 134.46, 136.21, 139.65, 139.88, 143.91, 144.30, 172.92; MS (m/z): 626 ($\text{M}^+ + 2$); Anal. Calcd. for $\text{C}_{27}\text{H}_{25}\text{BrCl}_2\text{N}_2\text{O}_4\text{S}$: C, 51.94; H, 4.04; N, 4.49; Found: C, 51.99; H, 4.14; N, 4.60.

Typical experimental procedure for the synthesis of pyrroloquinoline (12a)

A mixture of (2*Z*)-2- $\{[N$ -(2-formylphenyl)(4-methylbenzene)sulfonamido]methyl}-3-phenylprop-2-enenitrile (**10a**) (1 mmol, 0.42 g) and sarcosine (**7a**) (1.1 mmol, 0.18 g) in acetonitrile (10 mL) was stirred under reflux temperature for 6 h. After the completion of the reaction as indicated by TLC, the reaction mixture was concentrated. Then the resulting crude mass was diluted with water (20 mL) and extracted with ethyl acetate (3 x 10 mL). The combined organic layer obtained was washed with brine (3 x 10 mL) and dried over anhydrous Na_2SO_4 . The organic layer was concentrated and the crude mass was recrystallized using ethylacetate:hexane mixture (3:7) to provide **12a** as a colorless solid in 94% yield.

Crystal data for 1-Methyl-5-[(4-methylbenzene)sulfonyl]-3-phenyl-1*H*,2*H*,3*H*,3*aH*,4*H*,5*H*,9*bH*-pyrrolo[3,2-*c*]quinoline-3*a*-carbonitrile (12a)

Empirical formula, $\text{C}_{26}\text{H}_{25}\text{N}_3\text{O}_2\text{S}$; Formula weight, 444; crystal color, colorless; Single crystal X-ray structure of the molecule shown in ORTEP diagram (Figure 2). Detailed X-ray

crystallographic data is available from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK (for pyrroloquinoline (**12a**) CCDC # **833470**).

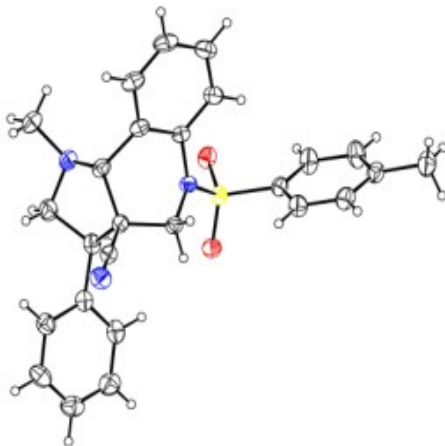
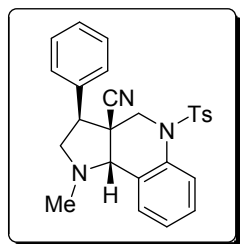


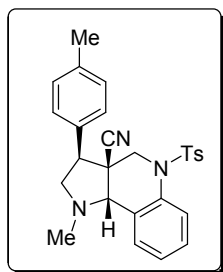
Figure 2. ORTEP diagram of compound **12a**

1-Methyl-5-[(4-methylbenzene)sulfonyl]-3-phenyl-1*H*,2*H*,3*H*,3*aH*,4*H*,5*H*, 9*bH*-pyrrolo[3,2-*c*]quinoline-3*a*-carbonitrile (12a**)**



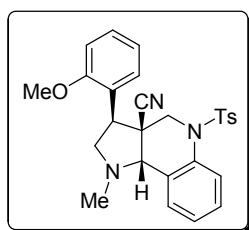
Yield: 94%; mp: 216-218°C; IR (KBr): 2242, 1514 cm^{-1} ; ^1H NMR: δ 2.28 (s, 3H), 2.41 (s, 3H), 2.93 (t, 1H, $J = 11.1$ Hz), 3.25 (dd, 1H, $J = 6.3, 9.3$ Hz), 3.58-3.61 (m, 2H), 3.85 (dd, 1H, $J = 6.3, 11.4$ Hz), 4.39 (d, 1H, $J = 13.2$ Hz), 7.11–7.83 (m, 13H); ^{13}C NMR (CDCl_3 , 75 MHz): δ 21.54, 39.53, 49.41, 52.10, 52.39, 59.97, 70.92, 120.32, 121.12, 124.53, 127.24, 127.93, 128.32, 128.78, 128.95, 129.16, 129.82, 130.47, 135.68, 137.32, 138.91, 144.10; MS (m/z): 445 ($\text{M}^+ + 1$); Anal. Calcd. for $\text{C}_{26}\text{H}_{25}\text{N}_3\text{O}_2\text{S}$: C, 70.40; H, 5.68; N, 9.47; Found: C, 70.52; H, 5.78; N, 9.59.

1-Methyl-5-[(4-methylbenzene)sulfonyl]-3-(4-methylphenyl-1*H*,2*H*,3*H*,3*aH*,4*H*,5*H*,9*bH*-pyrrolo[3,2-*c*]quinoline-3*a*-carbonitrile (12b)



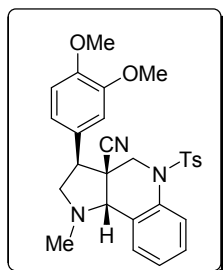
Yield: 92%; mp: 220-222 °C; IR (KBr): 2232, 1544 cm^{-1} ; ^1H NMR: δ 2.26 (s, 3H), 2.36 (s, 3H), 2.39 (s, 3H), 2.90 (t, 1H, $J = 10.5$ Hz), 3.21 (t, 1H, $J = 9.0$ Hz), 3.56 (s, 1H), 3.60 (d, 1H, $J = 13.2$ Hz), 3.79 (dd, 1H, $J = 6.0, 11.1$ Hz), 4.37 (d, 1H, $J = 12.9$ Hz), 7.12–7.82 (m, 12H); ^{13}C NMR (CDCl_3 , 75 MHz): δ 21.20, 21.56, 39.57, 49.15, 52.04, 52.33, 60.06, 70.83, 120.37, 121.14, 124.54, 127.27, 127.89, 128.96, 129.01, 129.50, 129.84, 130.51, 132.64, 137.28, 138.04, 138.86, 144.13; MS (m/z): 459 ($\text{M}^+ + 1$); Anal. Calcd. for $\text{C}_{27}\text{H}_{27}\text{N}_3\text{O}_2\text{S}$: C, 70.87; H, 5.95; N, 9.18; Found: C, 70.94; H, 6.09; N, 9.30.

1-Methyl-5-[(4-methylbenzene)sulfonyl]-3-(2-methoxyphenyl-1*H*,2*H*,3*H*,3*aH*,4*H*,5*H*,9*bH*-pyrrolo[3,2-*c*]quinoline-3*a*-carbonitrile (12c)



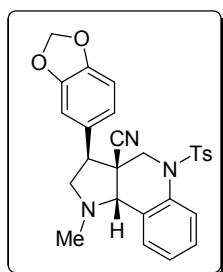
Yield: 96%; mp: 221-223°C; IR (KBr): 2251, 1526 cm^{-1} ; ^1H NMR: δ 2.38 (s, 3H), 2.40 (s, 3H), 3.01 (t, 1H, $J = 10.2$ Hz), 3.29 (dd, 1H, $J = 3.3, 9.7$ Hz), 3.57 (d, 1H, $J = 12.3$ Hz), 3.70 (s, 3H), 3.74 (d, 1H, $J = 7.5$ Hz), 4.15 (d, 1H, $J = 12.6$ Hz), 4.38-4.42 (m, 1H), 6.96–7.64 (m, 12H); ^{13}C NMR (CDCl_3 , 75 MHz): δ 21.51, 40.03, 45.75, 47.15, 52.52, 53.66, 60.86, 68.26, 119.31, 122.44, 124.35, 126.80, 127.14, 128.33, 128.69, 129.59, 129.76, 129.80, 131.21, 135.21, 135.80, 136.75, 137.31, 143.56; MS (m/z): 475 ($\text{M}^+ + 1$); Anal. Calcd. for $\text{C}_{27}\text{H}_{27}\text{N}_3\text{O}_3\text{S}$: C, 68.48; H, 5.75; N, 8.87; Found: C, 68.59; H, 5.84; N, 8.99.

1-Methyl-5-[(4-methylbenzene)sulfonyl]-3-(3,4-dimethoxyphenyl)-1*H*,2*H*,3*H*,3*aH*,4*H*,5*H*,9*bH*-pyrrolo[3,2-*c*]quinoline-3*a*-carbonitrile (12d)



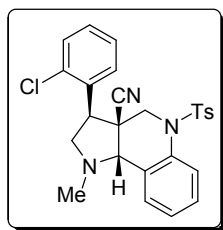
Yield: 95%; mp: 224-226°C; IR (KBr): 2245, 1511 cm^{-1} ; ^1H NMR: δ 2.32 (s, 3H), 2.41 (s, 3H), 2.94 (dd, 1H, $J = 9.6, 11.7$ Hz), 3.25 (dd, 1H, $J = 6.0, 9.3$ Hz), 3.51 (d, 1H, $J = 12.9$ Hz), 3.61 (s, 1H), 3.83-3.87 (m, 1H), 3.90 (s, 3H), 3.95 (s, 3H), 4.41 (d, 1H, $J = 12.9$ Hz), 6.91-7.83 (m, 11H); ^{13}C NMR (CDCl_3 , 75 MHz): δ 21.54, 39.64, 48.87, 52.20, 52.38, 55.89, 56.01, 59.98, 70.82, 111.29, 112.72, 120.54, 120.85, 121.31, 124.52, 127.17, 127.70, 128.19, 128.86, 129.91, 130.33, 137.32, 138.96, 144.17, 148.95, 149.00; MS (m/z): 505 ($\text{M}^+ + 1$); Anal. Calcd. for $\text{C}_{28}\text{H}_{29}\text{N}_3\text{O}_4\text{S}$: C, 66.78; H, 5.80; N, 8.34; Found: C, 66.89; H, 5.87; N, 8.46.

3-(2*H*-1,3-Benzodioxol-5-yl)-1-methyl-5-[(4-methylbenzene)sulfonyl]-1*H*,2*H*,3*H*,3*aH*,4*H*,5*H*,9*bH*-pyrrolo[3,2-*c*]quinoline-3*a*-carbonitrile (12e)



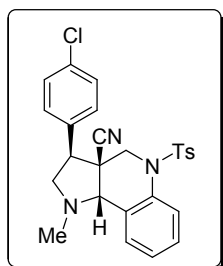
Yield: 92%; mp: 231-233°C; IR (KBr): 2276, 1503 cm^{-1} ; ^1H NMR: δ 2.26 (s, 3H), 2.41 (s, 3H), 2.84 (t, 1H, $J = 10.2$ Hz), 3.21 (t, 1H, $J = 7.8$ Hz), 3.55-3.59 (m, 2H), 3.76-3.81 (m, 1H), 4.37 (d, 1H, $J = 13.2$ Hz), 5.98 (s, 2H), 6.84-7.82 (m, 11H); ^{13}C NMR (CDCl_3 , 75 MHz): δ 21.54, 39.49, 49.10, 52.13, 52.35, 60.10, 70.83, 101.21, 108.51, 109.25, 120.30, 121.09, 122.69, 124.52, 127.23, 127.94, 128.93, 129.28, 129.83, 130.46, 137.34, 138.95, 144.11, 147.61, 147.92; MS (m/z): 489 ($\text{M}^+ + 1$); Anal. Calcd. for $\text{C}_{27}\text{H}_{25}\text{N}_3\text{O}_4\text{S}$: C, 66.51; H, 5.17; N, 8.62; Found: C, 66.66; H, 5.28; N, 8.77.

1-Methyl-5-[(4-methylbenzene)sulfonyl]-3-(2-chlorophenyl-1*H*,2*H*,3*H*,3*aH*,4*H*,5*H*,9*bH*-pyrrolo[3,2-*c*]quinoline-3*a*-carbonitrile (12f)



Yield: 91%; mp: 227-229°C; IR (KBr): 2258, 1529 cm⁻¹; ¹H NMR: δ 2.22 (s, 3H), 2.37 (s, 3H), 2.77 (t, 1H, *J* = 9.6 Hz), 3.23 (t, 1H, *J* = 9 Hz), 3.47 (s, 1H), 4.13 (t, 1H, *J* = 9 Hz), 4.36 (dd, 2H, *J* = 13.2, 26.4 Hz), 7.09–7.81(m, 12H); ¹³C NMR (CDCl₃, 75 MHz): δ 21.54, 39.30, 46.03, 49.32, 51.79, 60.40, 69.96, 119.48, 121.41, 123.95, 124.95, 127.14, 127.60, 128.12, 129.22, 129.54, 129.62, 130.11, 131.17, 135.01, 135.08, 137.03, 137.54, 143.94; MS (*m/z*): 479 (*M*⁺+1); Anal. Calcd. for C₂₆H₂₄ClN₃O₂S: C, 65.33; H, 5.06; N, 8.79; Found: C, 65.45; H, 5.19; N, 8.92.

1-Methyl-5-[(4-methylbenzene)sulfonyl]-3-(4-chlorophenyl-1*H*,2*H*,3*H*,3*aH*,4*H*,5*H*,9*bH*-pyrrolo[3,2-*c*]quinoline-3*a*-carbonitrile (12g)

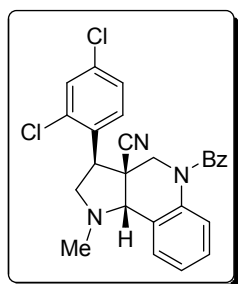


Yield: 93%; mp: 219-221°C; IR (KBr): 2248, 1526 cm⁻¹; ¹H NMR: δ 2.29 (s, 3H), 2.42 (s, 3H), 2.90 (t, 1H, *J* = 10.2 Hz), 3.24 (t, 1H, *J* = 8.1 Hz), 3.53 (d, 1H, *J* = 13.2 Hz), 3.59 (s, 1H), 3.89 (dd, 1H, *J* = 5.7, 10.8 Hz), 4.37 (d, 1H, *J* = 12.9 Hz), 7.13–7.82 (m, 12H); ¹³C NMR (CDCl₃, 75 MHz): δ 21.55, 39.46, 48.54, 52.16, 52.28, 59.86, 70.86, 120.11, 120.96, 124.58, 127.15, 127.85, 128.98, 129.91, 130.44, 130.55, 134.12, 13.31, 137.33, 138.99, 142.07, 144.22; MS (*m/z*): 479 (*M*⁺+1); Anal. Calcd. for C₂₆H₂₄ClN₃O₂S: C, 65.33; H, 5.06; N, 8.79; Found: C, 65.47; H, 5.14; N, 8.92.

Typical experimental procedure for the synthesis of pyrroloquinoline (12h)

A mixture of *N*-[(2*Z*)-2-cyano-2-[(2,4-dichlorophenyl)methylidene]ethyl]-*N*-(2-formylphenyl) benzamide (**10h**) (1 mmol, 0.43 g) and sarcosine (**7a**) (1.1 mmol, 0.10 g) in acetonitrile (10 mL) was stirred under reflux temperature for 6 h. After the completion of the reaction as indicated by TLC, the reaction mixture was concentrated. Then the resulting crude mass was diluted with water (20 mL) and extracted with ethyl acetate (3 x 10 mL). The combined organic layer obtained was washed with brine (3 x 10 mL) and dried over anhydrous Na₂SO₄. The organic layer was concentrated and the crude mass was recrystallized using ethylacetate:hexane mixture (3:7) to provide **12h** as a colorless solid in 84% yield.

5-benzoyl-3-(2,4-dichlorophenyl)-1-methyl-1*H*,2*H*,3*H*,3*aH*,4*H*,5*H*,9*bH*-pyrrolo[3,2-*c*]quino- -line-3*a*-carbonitrile (**12h**)



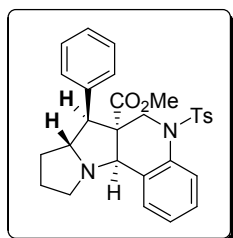
Yield: 84%; mp: 209-211°C; IR (KBr): 2258, 1542 cm⁻¹; ¹H NMR: δ 2.40 (s, 3H), 2.84 (t, 1H, *J* = 10.2 Hz), 3.33-3.41 (m, 4H), 3.72 (s, 1H), 4.34-4.40 (m, 1H), 5.29 (d, 1H, *J* = 13.2 Hz), 6.59-7.58 (m, 12H); ¹³C NMR (CDCl₃, 75 MHz): δ 39.38, 45.90, 51.30, 52.48, 61.01, 72.67, 122.39, 125.18, 125.64, 127.23, 128.00, 128.11, 128.67, 129.15, 129.98, 130.18, 130.83, 131.22, 132.57, 134.51, 134.80, 135.92, 141.99, 169.63; MS (*m/z*): 463 (*M*⁺+1); Anal. Calcd. for C₂₆H₂₁Cl₂N₃O: C, 67.54; H, 4.58; N, 9.09; Found: C, 67.64; H, 4.70; N, 9.20.

Typical experimental procedure for the synthesis of pyrrolizinoquinoline (15a)

A mixture of methyl (2*E*)-2-[[*N*-(2-formylphenyl)(4-methylbenzene)sulfonamido]methyl]-3-phenylprop-2-enoate (**6a**) (1 mmol, 0.45g) and *L*-proline (**7b**) (1.1 mmol, 0.23 g) in acetonitrile (10 mL) was refluxed for 10 h. After the completion of the reaction as indicated by TLC, the reaction mixture was concentrated. Then the resulting crude mass was diluted with water (20 mL) and extracted with ethyl acetate (3 x 10 mL). The combined organic layer

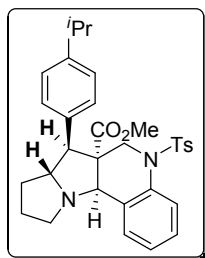
obtained was washed with brine (3 x 10 mL) and dried over anhydrous Na₂SO₄. The organic layer was concentrated and the crude mass was recrystallized using ethylacetate:hexane mixture (1:1) to provide **15a** as a colorless solid in 88% yield.

Methyl 8-[(4-methylbenzene)sulfonyl]-11-phenyl-8,16-diazatetracyclo[8.6.0.0^{2,7}.0^{12,16}]hexadeca-2,4,6-triene-10-carboxylate (15a)



Yield : 88%; mp: 186-188°C; IR (KBr): 1784, 1685 cm⁻¹; ¹H NMR: δ 1.56-2.13 (m, 4H), 2.39 (s, 3H), 3.05-3.14 (m, 2H), 3.52 (d, 1H, *J* = 10.5 Hz), 3.62 (s, 3H), 3.78 (d, 1H, *J* = 12.3 Hz), 4.04-4.10 (m, 1H), 4.33 (s, 1H), 4.53 (d, 1H, *J* = 12.6 Hz), 6.97–7.68 (m, 13H); ¹³C NMR (CDCl₃, 75 MHz): δ 21.52, 27.18, 31.62, 45.69, 52.26, 54.99, 58.76, 58.94, 66.85, 68.89, 119.36, 123.14, 127.05, 127.55, 127.88, 128.02, 128.52, 128.73, 129.61, 129.76, 135.15, 135.78, 137.68, 143.53, 172.53; MS (*m/z*): 504 (*M*⁺+1); Anal. Calcd. for C₂₉H₃₀N₂O₄S: C, 69.30; H, 6.02; N, 5.57; Found: C, 69.41; H, 6.17; N, 5.73.

Methyl 8-[(4-methylbenzene)sulfonyl]-11-[4-(propan-2-yl)phenyl]-8,16-diazatetracyclo[8.6.0.0^{2,7}.0^{12,16}]hexa deca-2,4,6-triene-10-carboxylate (15b)



Yield: 86%; mp: 189-191°C; IR (KBr): 1787, 1639 cm⁻¹; ¹H NMR: δ 1.26 (s, 3H), 1.29 (s, 3H), 1.57-2.11 (m, 5H), 2.38 (s, 3H), 2.85-3.10 (m, 2H), 3.51 (d, 1H, *J* = 10.2 Hz), 3.63 (s, 3H), 3.77 (d, 1H, *J* = 5.7 Hz), 4.04-4.06 (m, 1H), 4.30 (s, 1H), 4.54 (d, 1H, *J* = 12.6 Hz), 6.96–7.71 (m,

12H); ^{13}C NMR (CDCl_3 , 75 MHz): δ 21.50, 23.88, 27.10, 31.66, 33.68, 45.70, 52.25, 54.88, 58.58, 58.72, 66.89, 68.96, 119.50, 123.11, 126.78, 127.09, 128.02, 128.39, 129.57, 129.73, 132.29, 135.82, 137.71, 143.47, 148.25, 172.62; MS (m/z): 546 (M^++1); Anal. Calcd. for $\text{C}_{32}\text{H}_{36}\text{N}_2\text{O}_4\text{S}$: C, 70.56; H, 6.66; N, 5.14; Found: C, 70.66; H, 6.75; N, 5.26.

Crystal data for Methyl 8-[(4-methylbenzene)sulfonyl]-11-[4-(propan-2-yl)phenyl]-8,16-diazatetracyclo [8.6.0.0^{2,7}.0^{12,16}]hexa deca-2,4,6-triene-10-carboxylate (15b**)**

Empirical formula, $\text{C}_{32}\text{H}_{36}\text{N}_2\text{O}_4\text{S}$; Formula weight, 545; crystal color, colorless; Single crystal X-ray structure of the molecule shown in ORTEP diagram (Figure 3). Detailed X-ray crystallographic data is available from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK (for pyrrolizinoquinoline (**15b**) CCDC # **976506**).

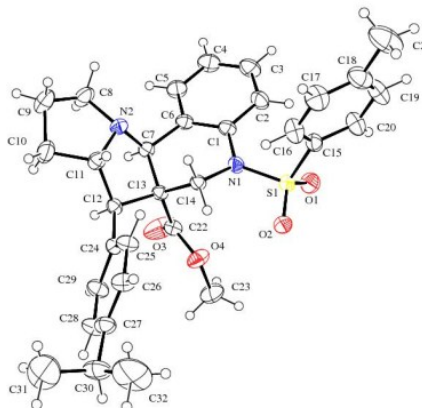
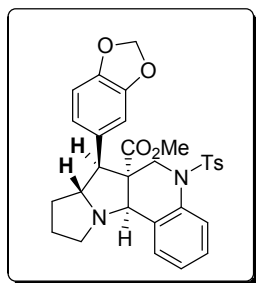


Figure 3. ORTEP diagram of compound 15b

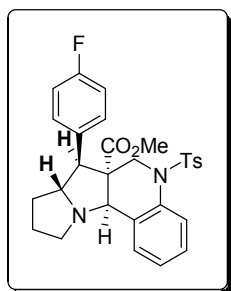
Methyl 11-(2H-1,3-benzodioxol-5-yl)-8-[(4-methylbenzene) sulfonyl]-8,16-diazatetracyclo [8.6.0.0^{2,7}.0^{12,16}]hexadeca-2,4,6-triene-10-carboxylate (15c**)**



Yield: 84%; mp: 190-192°C; IR (KBr): 1779, 1648 cm^{-1} ; ^1H NMR: δ 1.62-2.11 (m, 4H), 2.41 (s, 3H), 3.03-3.13 (m, 2H), 3.36-3.44 (m, 1H), 3.47 (s, 3H), 3.60-3.87 (m, 4H), 6.01-7.71 (m, 13H); ^{13}C NMR (CDCl_3 , 75 MHz): δ 21.62, 26.12, 30.32, 47.75, 52.29, 53.75, 57.47, 58.69, 66.98,

68.78, 74.67, 101.32, 108.56, 109.12, 122.23, 123.86, 124.70, 126.82, 127.04, 129.62, 132.07, 135.18, 135.35, 143.87, 147.02, 147.97, 148.13, 174.22; MS (m/z): 548 (M⁺+1); Anal. Calcd. for C₃₀H₃₀N₂O₆S: C, 65.92; H, 5.53; N, 5.12; Found: C, 66.08; H, 5.62; N, 5.28.

Methyl 11-(4-fluorophenyl)-8-[(4-methylbenzene)sulfonyl]-8,16-diazatetracyclo[8.6.0.0^{2,7}.0^{12,16}]hexa deca-2,4,6-triene-10-carboxylate (15d)

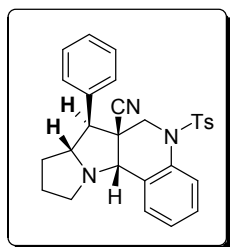


Yield: 87%; mp: 196-198°C; IR (KBr): 1787, 1678 cm⁻¹; ¹H NMR: δ 1.59-2.08 (m, 4H), 2.41 (s, 3H), 2.91-3.06 (m, 2H), 3.37-3.42 (m, 1H), 3.49 (s, 3H), 3.56-3.87 (m, 4H), 7.05-7.69 (m, 12H); ¹³C NMR (CDCl₃, 75 MHz) : δ 21.59, 26.23, 30.41, 47.91, 52.32, 53.76, 56.69, 59.55, 66.85, 74.59, 115.81 (d, *J* = 21.0 Hz), 123.99, 124.15, 124.58, 126.80, 129.57, 130.37 (d, *J* = 7.5 Hz), 134.82 (d, *J* = 84.5 Hz), 143.82, 174.07; MS (m/z): 522 (M⁺+1); Anal. Calcd. for C₂₉H₂₉FN₂O₄S: C, 66.90; H, 5.61; N, 5.38; Found: C, 66.99; H, 5.74; N, 5.53.

Typical experimental procedure for the synthesis of pyrrolizinoquinoline (17a)

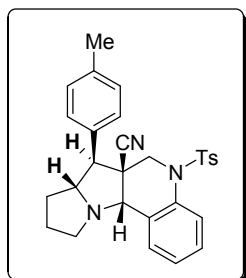
To a stirred solution of (2*Z*)-2-{[*N*-(2-formylphenyl)(4-methylbenzene)sulfonamido]methyl}-3-phenylprop-2-enenitrile (**10a**) (1 mmol, 0.42 g) and *L*-proline (**7b**) (1.1 mmol, 0.17 g) in acetonitrile (10 mL) was refluxed for 10 h. After the completion of the reaction as indicated by TLC, the reaction mixture was concentrated. Then the resulting crude mass was diluted with water (20 mL) and extracted with ethyl acetate (3 x 10 mL). The combined organic layer obtained was washed with brine (3 x 10 mL) and dried over anhydrous Na₂SO₄. The organic layer was concentrated and the crude mass was recrystallized using ethylacetate:hexane mixture (4:6) to provide **17a** as a colorless solid in 83% yield.

8-[(4-Methylbenzene)sulfonyl]-11-phenyl-8,16-diazatetracyclo[8.6.0.0^{2,7}.0^{12,16}]hexadeca-2,4,6-triene-10-carbonitrile (17a)



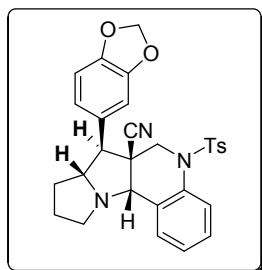
Yield: 83%; mp: 196-198°C; IR (KBr): 2254, 1571 cm⁻¹; ¹H NMR: δ 1.60-2.07 (m, 4H), 2.40 (s, 3H), 2.88-2.96 (m, 1H), 3.27-3.32 (m, 1H), 3.47 (d, 1H, J = 7.8 Hz), 3.51 (s, 1H), 3.67 (d, 1H, J = 14.1 Hz), 3.84-3.92 (m, 1H), 4.61 (d, 1H, J = 14.1 Hz), 7.21–7.70 (m, 13H); ¹³C NMR (CDCl₃, 75 MHz): δ 21.55, 26.78, 28.60, 47.22, 51.71, 54.40, 56.10, 68.86, 69.21, 122.85, 123.83, 126.16, 127.59, 127.68, 128.22, 128.34, 128.75, 128.90, 129.28, 129.84, 132.11, 135.18, 135.53, 136.62, 144.20; MS (m/z): 471 (M⁺+1); Anal. Calcd. for C₂₈H₂₇N₃O₂S: C, 71.61; H, 5.80; N, 8.95; Found: C, 71.69; H, 5.89; N, 9.09.

8-[(4-Methylbenzene)sulfonyl]-11-(4-methylphenyl)-8,16-diazatetracyclo[8.6.0.0^{2,7}.0^{12,16}]hexadeca-2,4,6-triene-10-carbonitrile (17b)



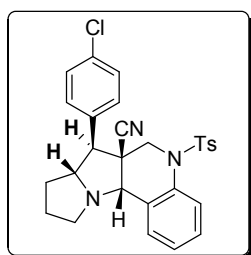
Yield: 84%; mp: 200-202°C; IR (KBr): 2259, 1528 cm⁻¹; ¹H NMR: δ 1.58-2.05 (m, 4H), 2.34 (s, 3H), 2.40 (s, 3H), 2.87-2.95 (m, 1H), 3.27-3.32 (m, 1H), 3.43 (d, 1H, J = 7.8 Hz), 3.51 (s, 1H), 3.66 (d, J = 14.1 Hz, 1H), 3.78-3.88 (m, 1H), 4.59 (d, 1H, J = 14.1 Hz), 7.16-7.70 (m, 12H); ¹³C NMR (CDCl₃, 75 MHz): δ 21.03, 21.54, 26.81, 28.58, 47.36, 51.68, 54.08, 56.09, 68.89, 69.17, 122.84, 123.74, 126.09, 127.60, 128.24, 128.29, 128.83, 129.44, 129.82, 132.04, 132.10, 135.54, 136.64, 137.42, 144.17; MS (m/z): 485 (M⁺+1); Anal. Calcd. for C₂₉H₂₉N₃O₂S: C, 72.02; H, 6.04; N, 8.69; Found: C, 72.13; H, 6.15; N, 8.84.

11-(2*H*-1,3-Benzodioxol-5-yl)-8-[(4-methylbenzene)sulfonyl]-8,16-diazatetracyclo[8.6.0.0^{2,7}.0^{12,16}] hexa deca-2,4,6-triene-10-carbonitrile (17c)

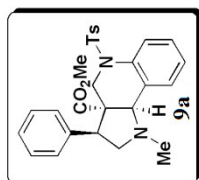
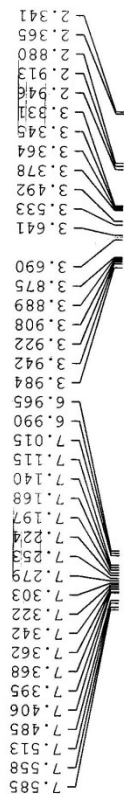


Yield: 82%; mp: 209-211°C; IR (KBr): 2268, 1532 cm⁻¹; ¹H NMR: δ 1.63-2.05 (m, 4H), 2.40 (s, 3H), 2.87-2.95 (m, 1H), 3.28-3.80 (m, 5H), 4.53 (d, 1H, *J* = 14.1 Hz), 5.97 (d, 2H, *J* = 5.7 Hz), 6.80-7.71 (m, 11H); ¹³C NMR (CDCl₃, 75 MHz): δ 21.56, 26.84, 28.45, 47.53, 51.52, 53.91, 55.86, 67.54, 68.90, 69.04, 101.23, 108.39, 109.27, 122.55, 123.43, 126.01, 126.90, 127.00, 127.55, 128.35, 128.70, 129.86, 131.71, 135.57, 136.65, 144.23, 147.16, 148.00; MS (*m/z*): 515 (*M*⁺+1); Anal. Calcd. for C₂₉H₂₇N₃O₄S: C, 67.82; H, 5.30; N, 8.18; Found: C, 67.93; H, 5.39; N, 8.32.

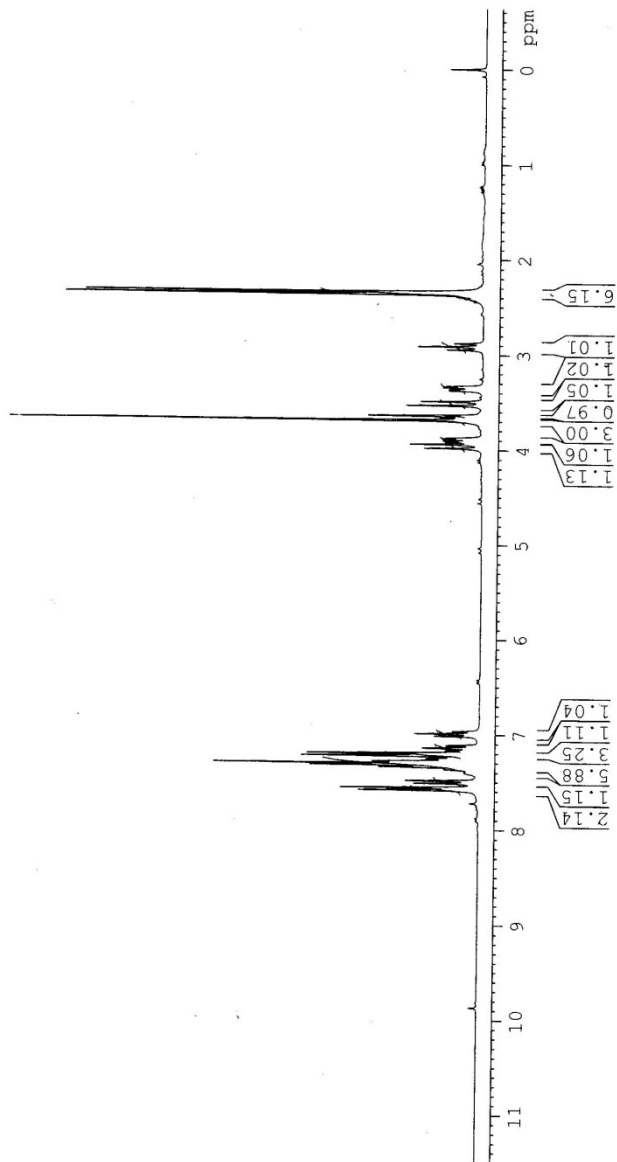
11-(4-Chlorophenyl)-8-[(4-methylbenzene)sulfonyl]-8,16-diazatetracyclo[8.6.0.0^{2,7}.0^{12,16}] hexadeca-2,4,6-triene-10-carbonitrile (17d)



Yield: 86%; mp: 201-203°C; IR (KBr): 2259, 1548 cm⁻¹; ¹H NMR: δ 1.73-2.06 (m, 4H), 2.40 (s, 3H), 2.89-2.97 (m, 1H), 3.22-3.31 (m, 1H), 3.51 (d, 1H, *J* = 7.5 Hz), 3.59 (s, 1H), 3.71 (d, 1H, *J* = 14.1 Hz), 3.80-3.85 (m, 1H), 4.50 (d, 1H, *J* = 14.1 Hz), 7.22-7.70 (m, 12H); ¹³C NMR (CDCl₃, 75 MHz): δ 21.56, 26.71, 28.53, 47.19, 51.51, 53.33, 55.92, 68.79, 69.16, 122.50, 123.39, 126.09, 127.48, 128.41, 128.94, 129.06, 129.61, 129.92, 130.37, 131.61, 133.74, 135.59, 136.65, 144.32; MS (*m/z*): 505 (*M*⁺+1); Anal. Calcd. for C₂₈H₂₆ClN₃O₂S: C, 66.72; H, 5.20; N, 8.34; Found: C, 66.86; H, 5.29; N, 8.47.



Current Data Parameters
 Name: 0X-VH-EST
 EXPNO: 1
 PROCNO: 1
 F2 - Acquisition Parameters
 Date_: 20101218
 Time: 18.32
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 PULPROG: zgpg30
 PRG: 5 mm DUL 13C-1
 PULPROG: zgpg30
 TD: 65536
 SOLVENT: CDCl3
 NS: 7
 DS: 2
 SWH: 6172.839 Hz
 FIDRES: 0.094190 Hz
 AQ: 5.308460 sec
 RG: 400
 DW: 81.000 usec
 DE: 6.00 usec
 TE: 300.0 K
 D1: 1.00000000 sec
 TDO: 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





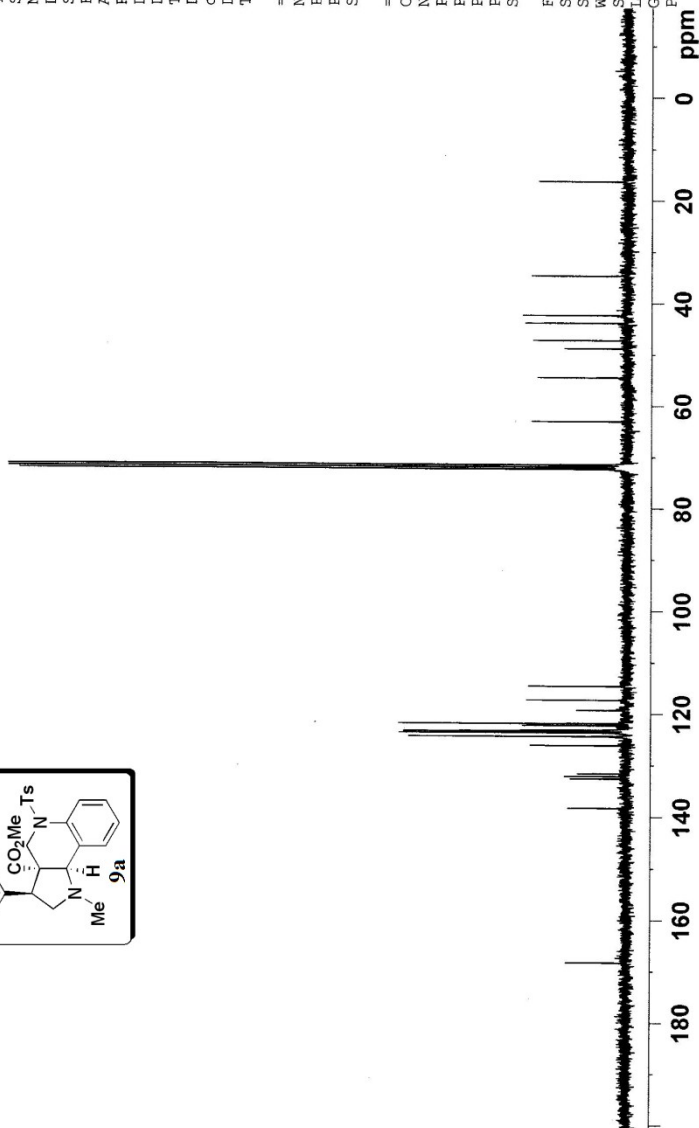
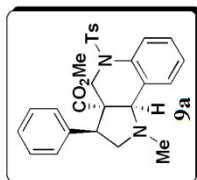
Current Data Parameters
 NAME DK-V-HEST-SA
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20101218
 Time_ 17:53
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 433
 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
 TDO 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

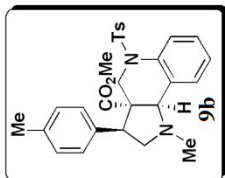
F2 - Processing parameters
 SI 32768
 SF 75.4677867 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40





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3.213
3.422
3.464
3.628
3.991
4.025
4.067

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6.943
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7.044
7.077
7.084
7.142
7.172
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7.361
7.389
7.514
7.541

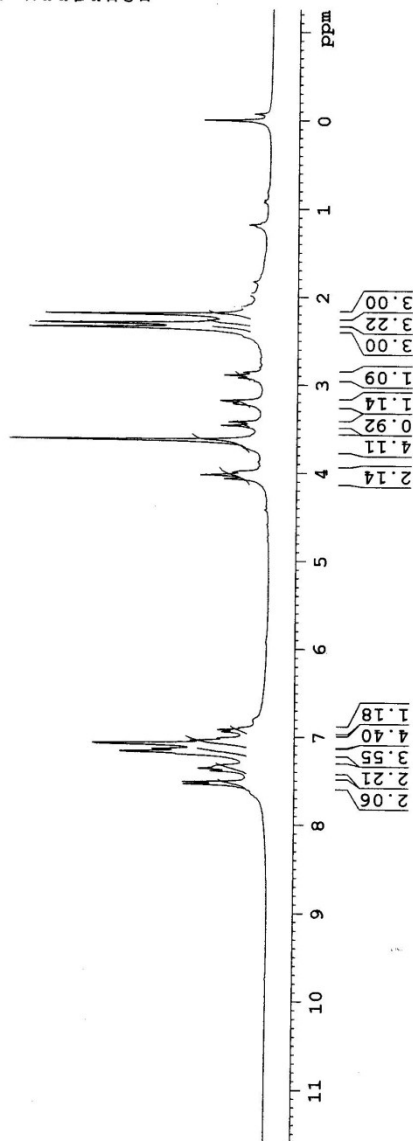


Current Data Parameters
NAME DR-V-H-Est-COUM
EXPNO 3
PROCNO 1

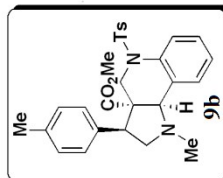
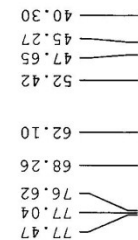
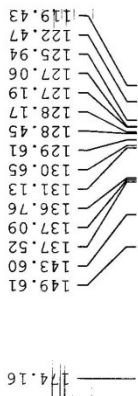
F2 - Acquisition Parameters
Date_ 20110102
Time 2.06
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 101.6
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

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

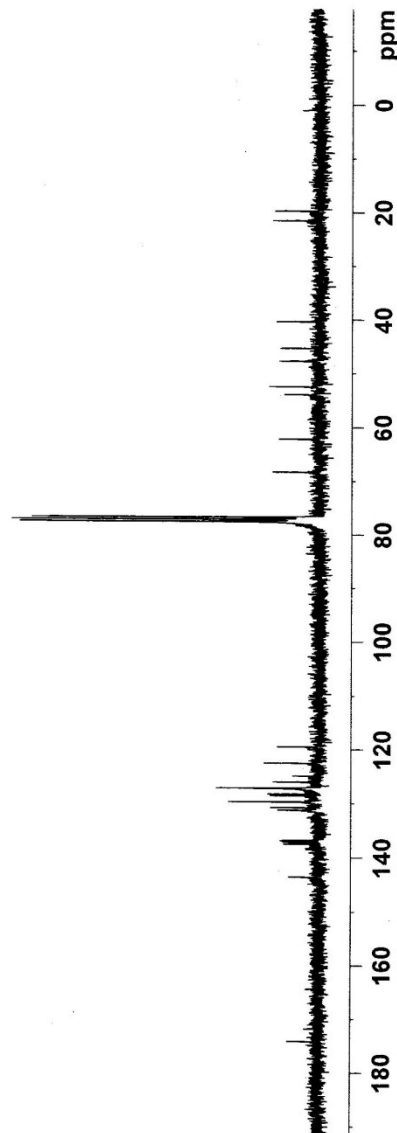
F2 - Processing parameters
SI 32768
SF 300.1300290 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



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Current Data Parameters
NAME DK-V-4-est-6000
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110102
Time 1.45
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 319
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 362
DW 27.800 usec
DE 6.000 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
PL -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
FC 1.40



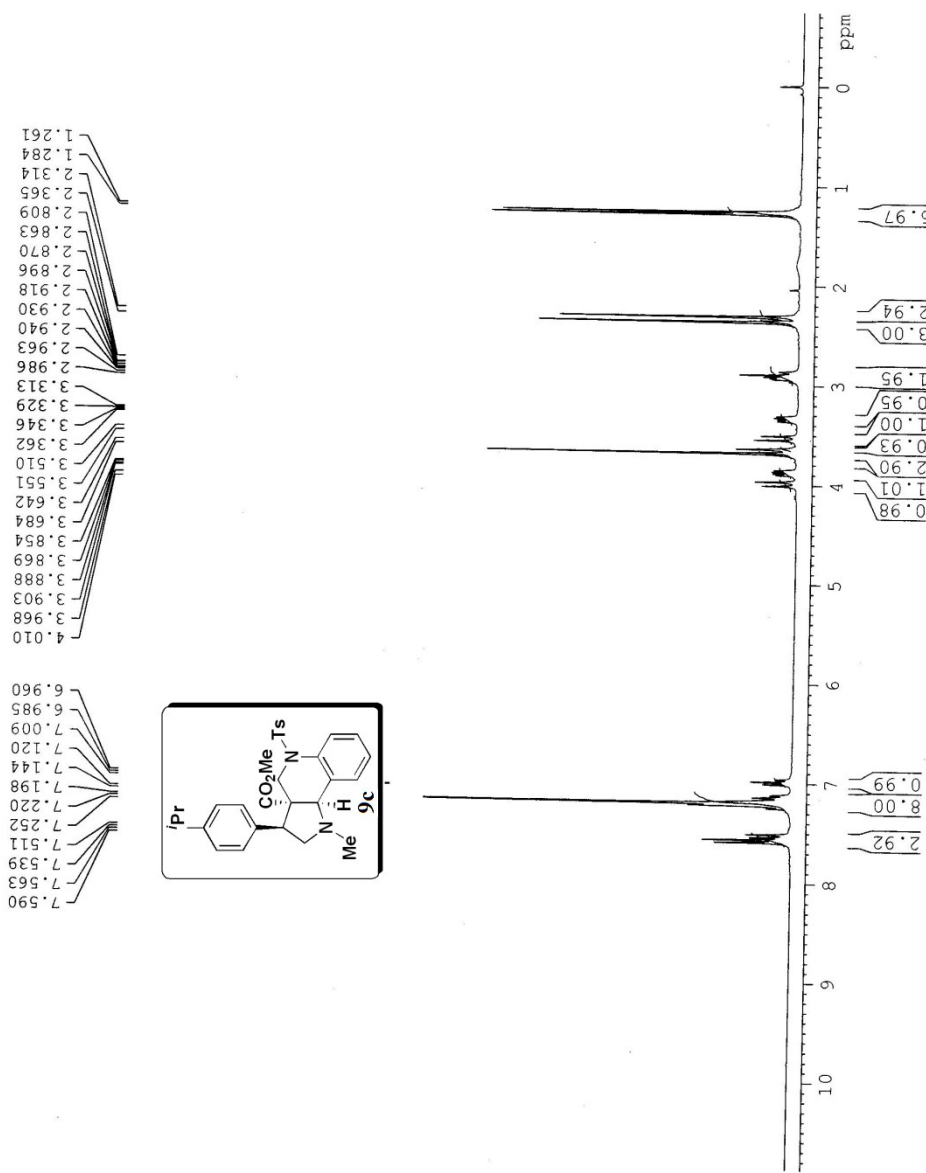


Current Data Parameters
 NAME DR-V-41FF-E5C-SA
 EXNO
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20101218
 Time_ 19.04
 INSTRUM spect
 PROBHD 5 mm DUL
 PULPROG zgpg30
 TD 65536
 SOLVENT cdc13
 NS 16
 DS 2
 SH 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 5.309466 sec
 RG 71.8
 DW 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.0000000 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 300.1300090 MHz
 WDW EM
 SSB 0
 GB 0
 PC 1.00





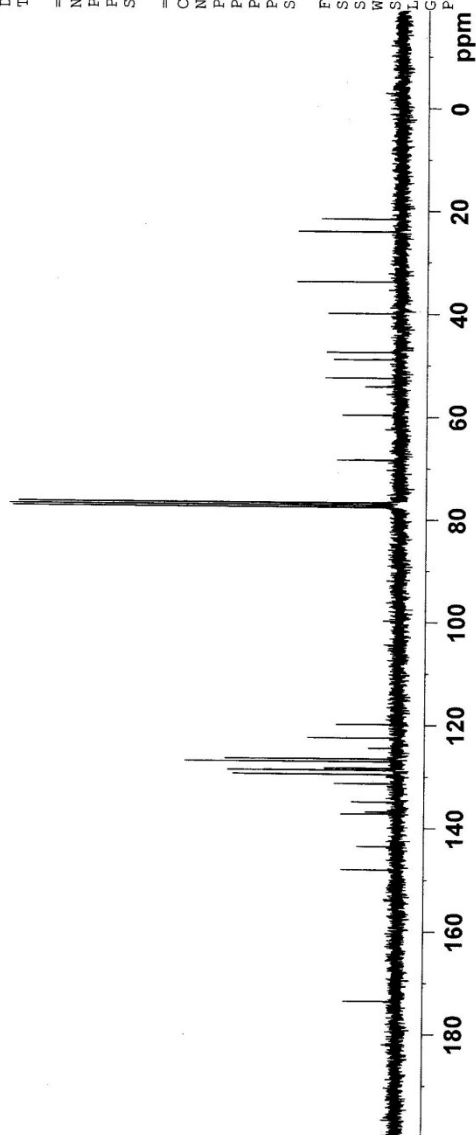
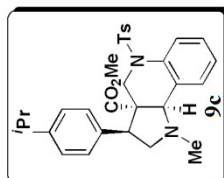
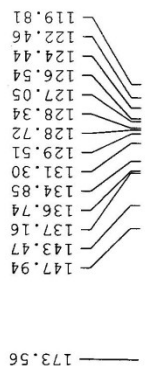
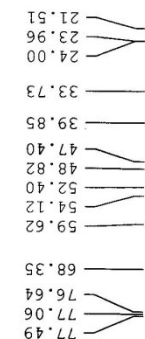
Current Data Parameters
 NAME DK-V-4IPr-EST SA
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20101218
 Time_ 19.10
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 83
 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 7.40 usec
 PL1 -2.00 dB
 SFO1 75.4752953 MHz

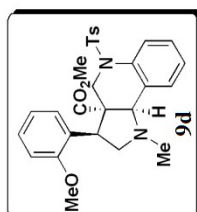
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PL12 15.68 dB
 PL13 16.00 dB
 SFO2 300.1312005 MHz

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

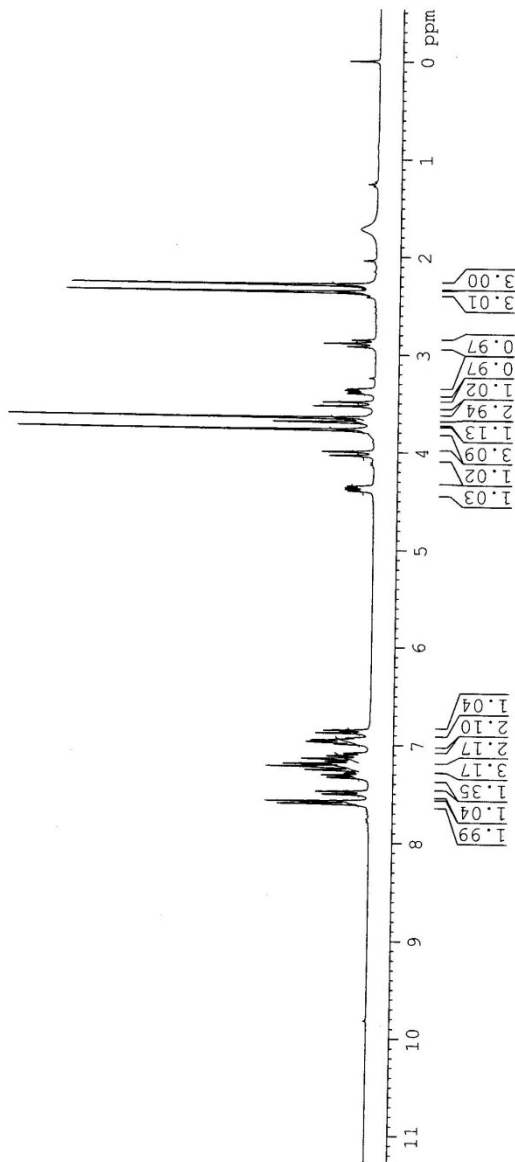


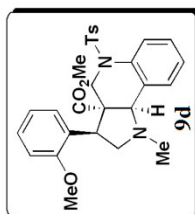
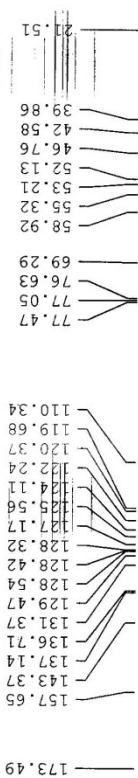


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2.365
2.291



Current Data Parameters
NAME DR-V-100-ESI-SA
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110102
Time 4.02
INSTRUM spect
PROBHD 5 mm BBL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 327.4
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 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





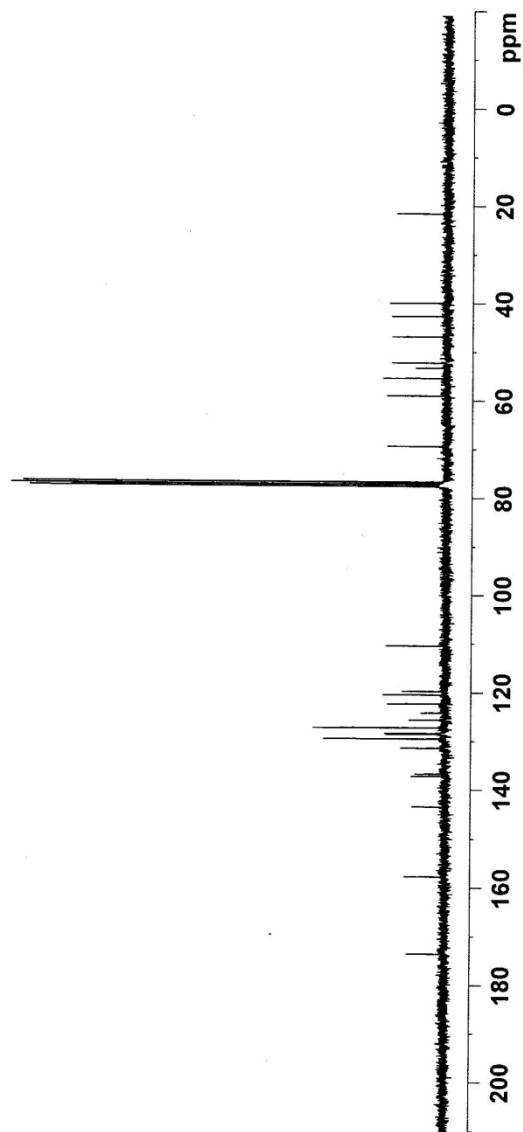
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 NAME DK-V-1008-EST-SA
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110102
 Time_ 3.58
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 175
 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
 TDO 1

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

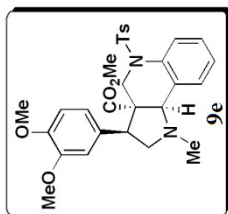
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 P2 80.00 usec
 PL2 0.00 dB
 PL12 15.68 dB
 PL13 16.00 dB
 SFO2 300.1312005 MHz

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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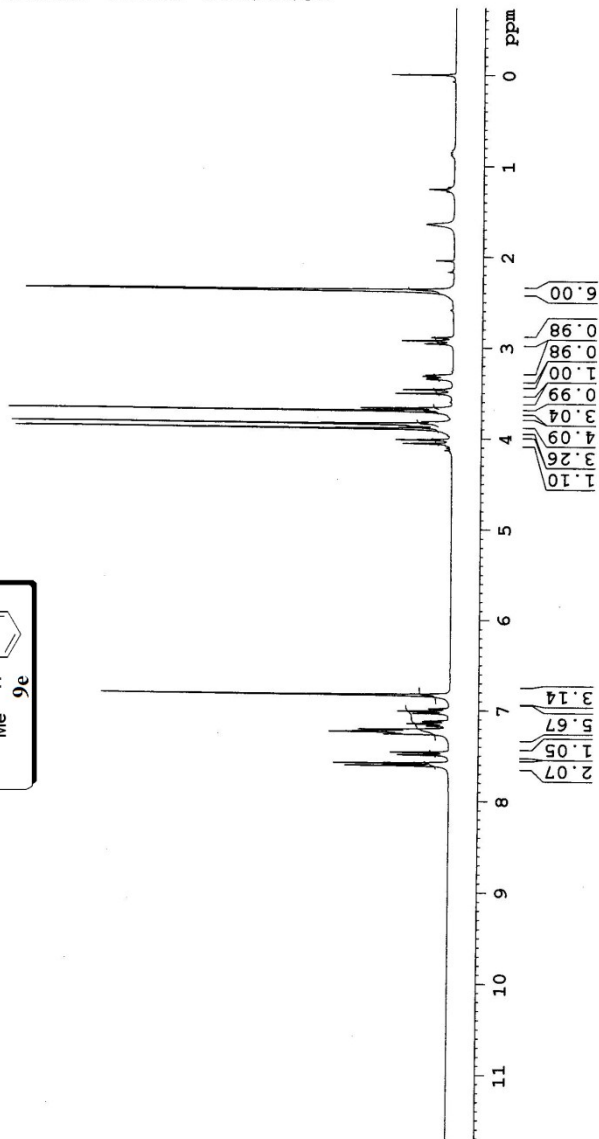


Current Data Parameters
NAME DK-V-2-Me Est SA
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20101225
Time 23.33
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 13.15 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





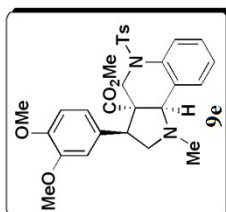
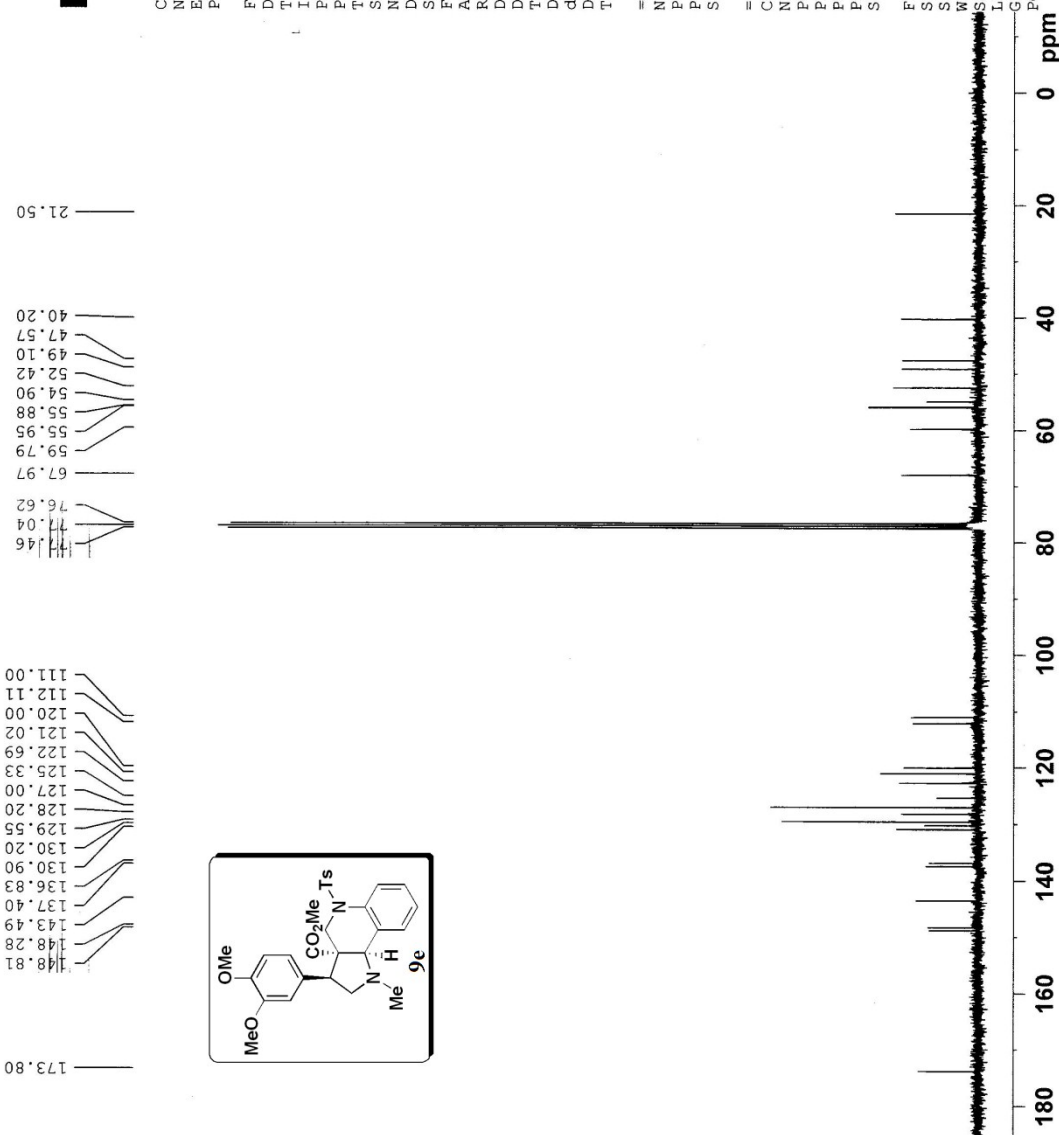
Current Data Parameters
 NAME DK-V-(4Me)₂ SA
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20101225
 Time_ 23.56
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl₃
 NS 350
 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
 TDO 1

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

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCDP2 80.00 usec
 PL2 0.00 dB
 PL12 15.68 dB
 PL13 16.00 dB
 SFO2 300.1312005 MHz

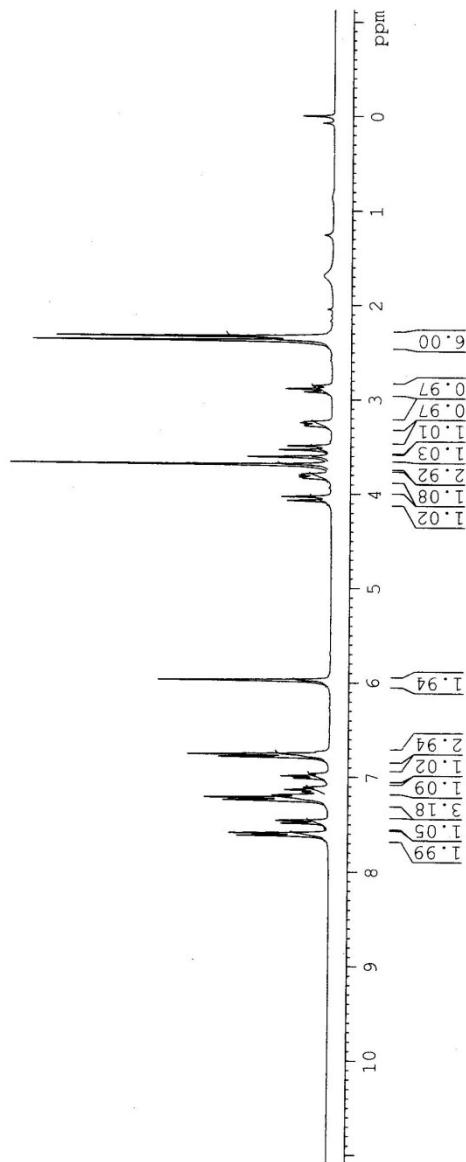
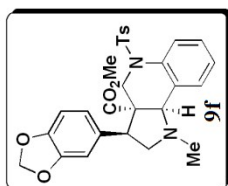
F2 - Processing parameters
 SI 32768
 SF 75.4677490 MHz
 EM 0
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40





Current Data Parameters
 NAME DK-V-Est PIP
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20100818
 Time_ 20.05
 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 300.2 K
 DI 1.00000000 sec
 TD0 1
 CHANNEL f1
 NUC1 1H
 P1 13.15 usec
 PL1 0.00 dB
 SFO1 300.1318594 MHz
 F2 - Processing parameters
 SI 32768
 SF 300.1300067 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

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6.732
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4.029
3.836
3.823
3.803
3.790
3.691
3.609
3.535
3.494
3.282
3.249
3.236
2.920
2.886
2.853
2.377
2.334





Current Data Parameters
 NAME DK-V-Est PIP
 EXPNO 2
 PROCNO 1

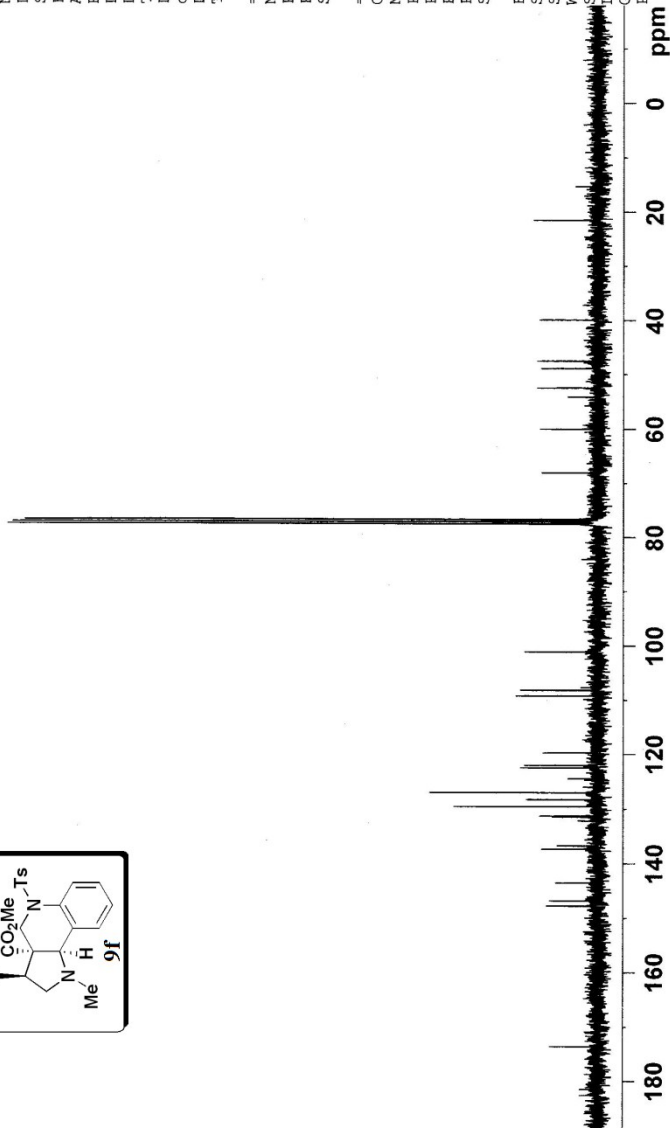
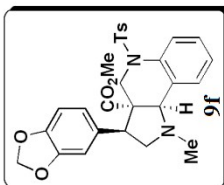
F2 - Acquisition Parameters
 Date_ 20101218
 Time 20.09
 INSTRUM spect
 PROBD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 66
 DS 4
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 645.1
 DE 27.800 usec
 TE 300.0 K
 D1 2.0000000 sec
 d11 0.0300000 sec
 DELTA 1.8999998 sec
 TDO 1

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

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 P2 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

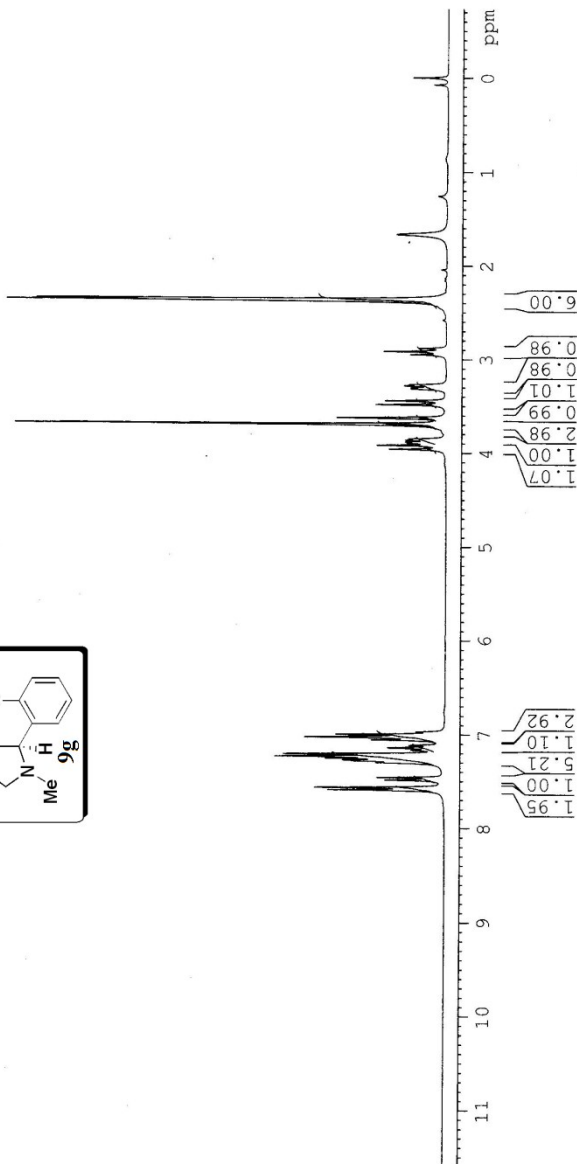
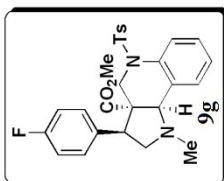
173.58
 147.74
 146.80
 143.53
 137.35
 136.74
 131.49
 131.27
 129.59
 128.28
 127.01
 124.46
 122.48
 122.01
 119.72
 109.19
 108.15
 101.11
 77.48
 77.05
 76.63
 68.05
 60.01
 54.12
 52.46
 48.85
 47.48
 39.91
 21.52





Current Data Parameters
 NAME DR-V-F-ES-
 EXPNO 2
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20101218
 Time 18.55
 INSTRUM spect
 PULPROG 5 mm DUL 13C-1
 FIDRES 0.094190 Hz
 RG 5.300461 sec
 DW 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.0000000 sec
 TDO 1
 ===== CHANNEL f1 =====
 NUC1 1H
 P1 13.15 usec
 PL1 0.00 dB
 SFO1 300.1318534 MHz
 F2 - Processing parameters
 SF 300.1318534 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

7.595
7.568
7.489
7.461
7.303
7.284
7.275
7.257
7.237
7.210
7.166
7.142
7.117
7.058
7.029
7.000
6.973
3.961
3.919
3.896
3.884
3.863
3.851
3.693
3.625
3.483
3.442
3.316
3.303
3.283
3.270
3.270
3.949
2.916
2.883
2.372
2.358





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

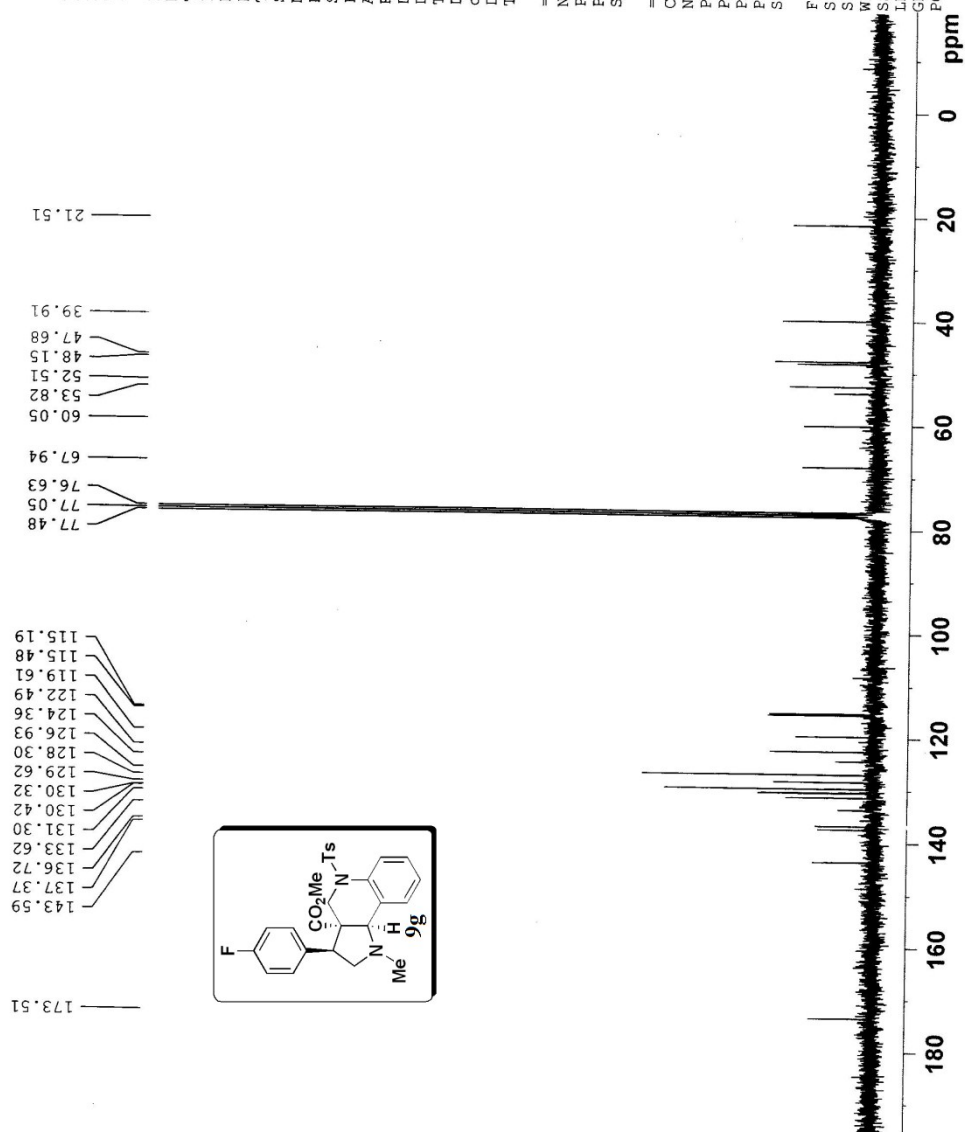
F2 - Acquisition Parameters

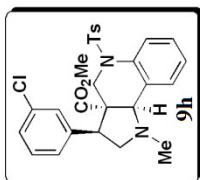
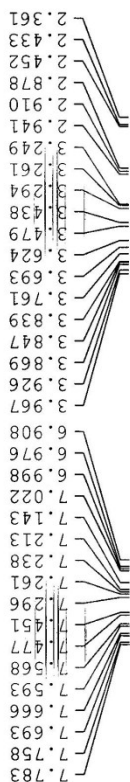
Date_ 20101218
 Time 16.46
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 103
 DS 4
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 645.1
 DW 27.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

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

===== CHANNEL f2 =====
 CPDPRG2 waitz16
 NUC2 1H
 FCPD2 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
 EM 0
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



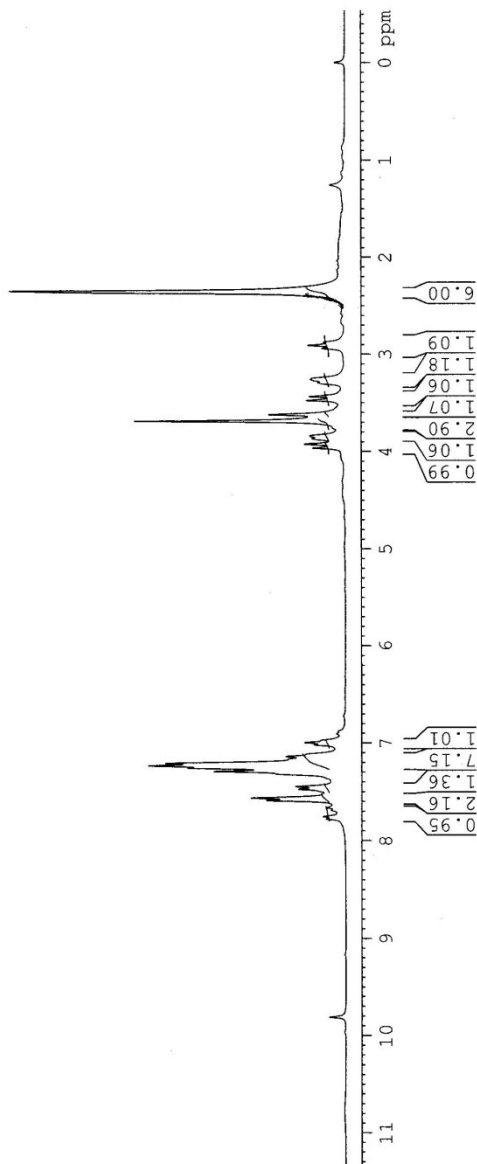


Current Data Parameters
 NAME DK-V-3-Cl-Est SA
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110101
 Time_ 23.35
 INSTRUM spect
 PROBD 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
 DI 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 300.1300070 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





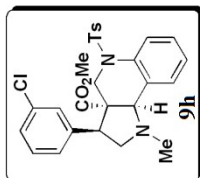
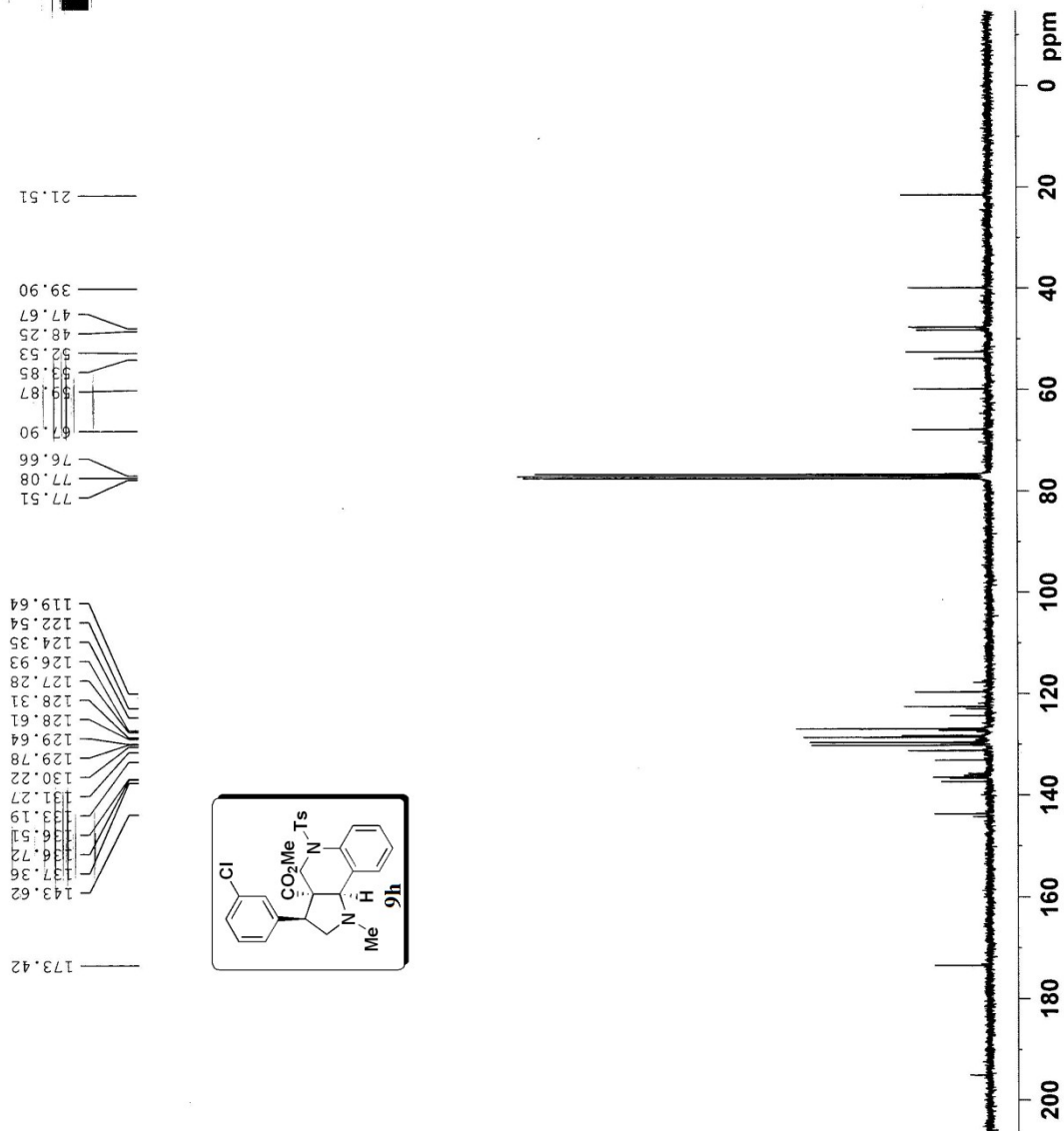
Current Data Parameters
 NAME DK-V-3-Cl-Est-SA
 EXPNO 2
 PROCNO 1

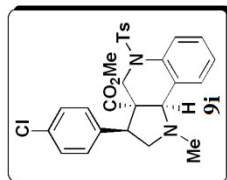
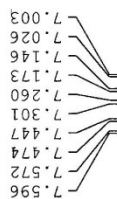
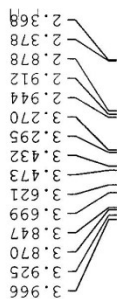
F2 - Acquisition Parameters
 Date_ 20110101
 Time 23.49
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 279
 DS 4
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 645.1
 DW 27.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.0000000 sec
 d11 0.0300000 sec
 DELTA 1.8999998 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



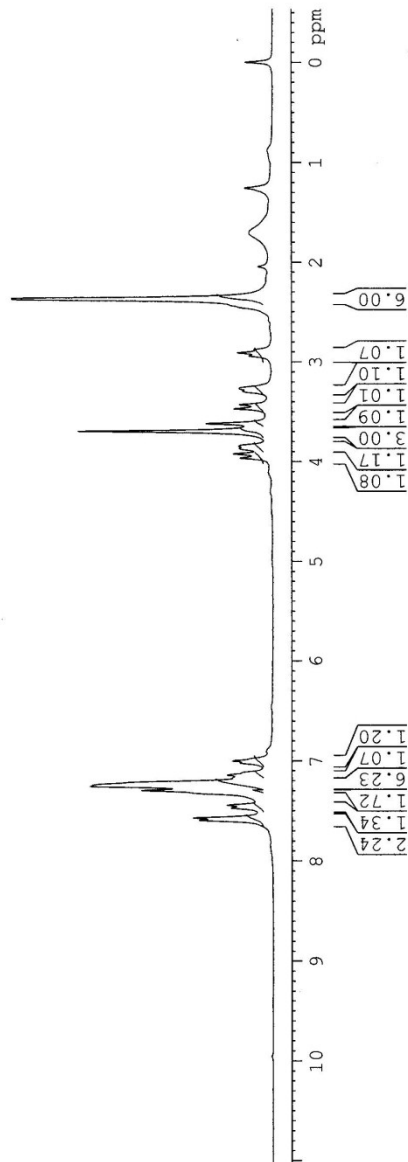


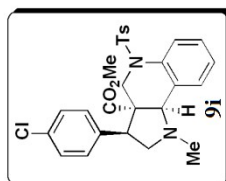
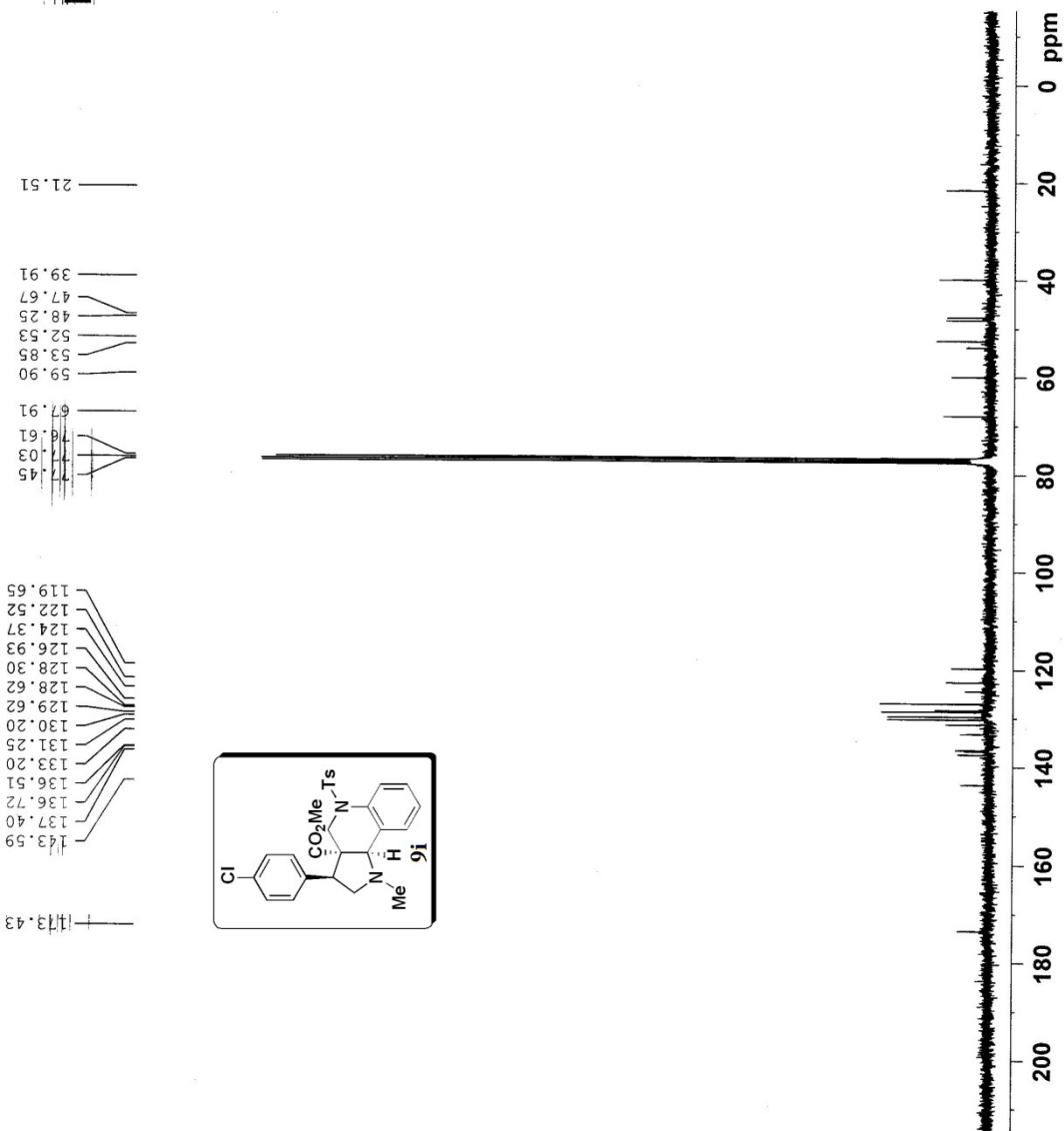
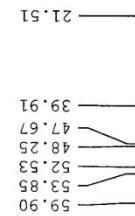
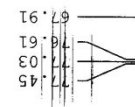
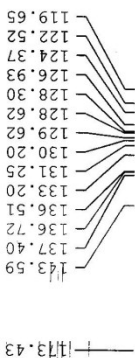
Current Data Parameters
NAME DK-V-4-Me-Est-SA
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110102
Time 0.28
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 14377
DE 816.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 13.15 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300061 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





Current Data Parameters
 NAME DK-V-4-Me-Est-SA
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110102
 Time_ 0.32
 INSTRUM spect
 PROBD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 414
 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
 TDO 1

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

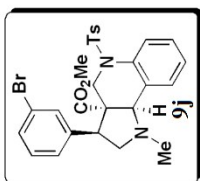
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 P2 80.00 usec
 PL2 0.00 dB
 PL12 15.68 dB
 PL13 16.00 dB
 SFO2 300.1312005 MHz

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

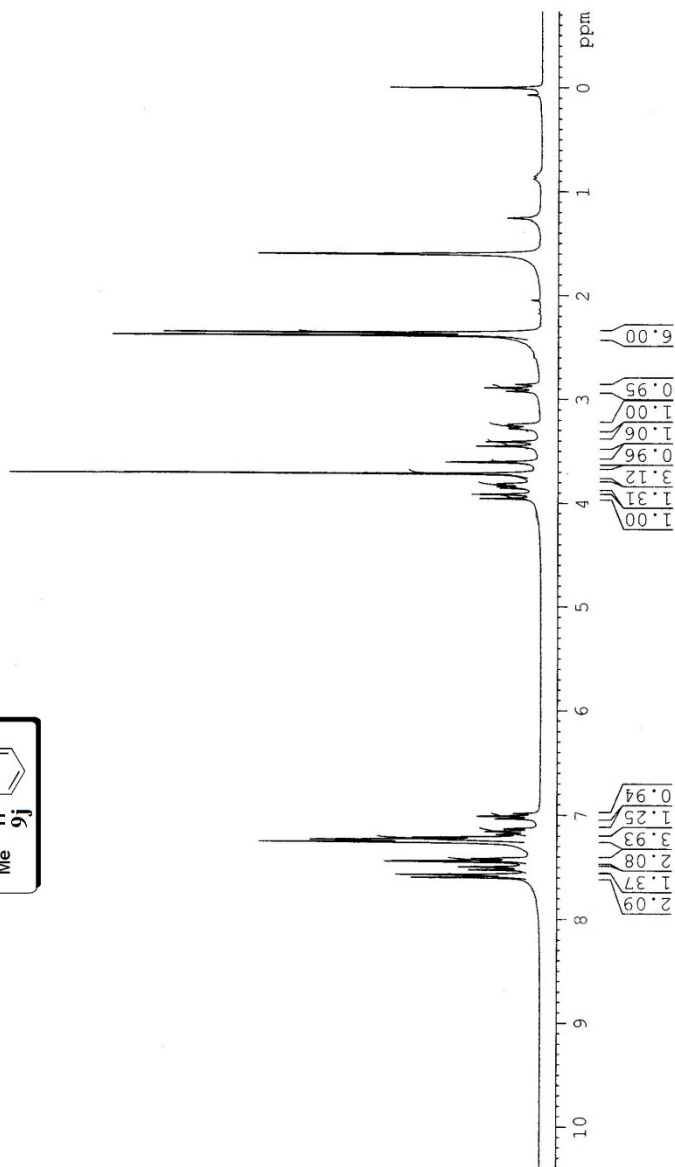


2.359
2.387
2.559
2.592
2.925
3.240
3.252
3.274
3.286
3.410
3.451
3.605
3.716
3.811
3.823
3.844
3.915
3.956

6.989
7.014
7.039
7.135
7.162
7.189
7.217
7.241
7.262
7.418
7.423
7.446
7.497
7.525
7.570
7.598



Current Data Parameters
NAME: DRV-3-BR-5A
EXPNO: 1
PROCNO: 1
F2 - Acquisition Parameters
Date_: 20101226
Time: 21.48
INSTRUM: spect
PROBHD: 5 mm DUL 125-1
PULPROG: zg30
TD: 65536
SOLVENT: CDCl3
NS: 16
DS: 2
SWH: 6172.839 Hz
FIDRES: 0.04150 Hz
AQ: 5.308160 sec
RG: 287.4
DM: 81.000 usec
DE: 6.00 usec
TE: 300.0 K
D1: 1.0000000 sec
D11: 1
===== CHANNEL f1 =====
NUC1: 1H
P1: 13.15 usec
PL1: 0.00 dB
SFO1: 300.1318534 MHz
F2 - Processing parameters
SI: 32768
SF: 300.130057 MHz
WDW: EM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00





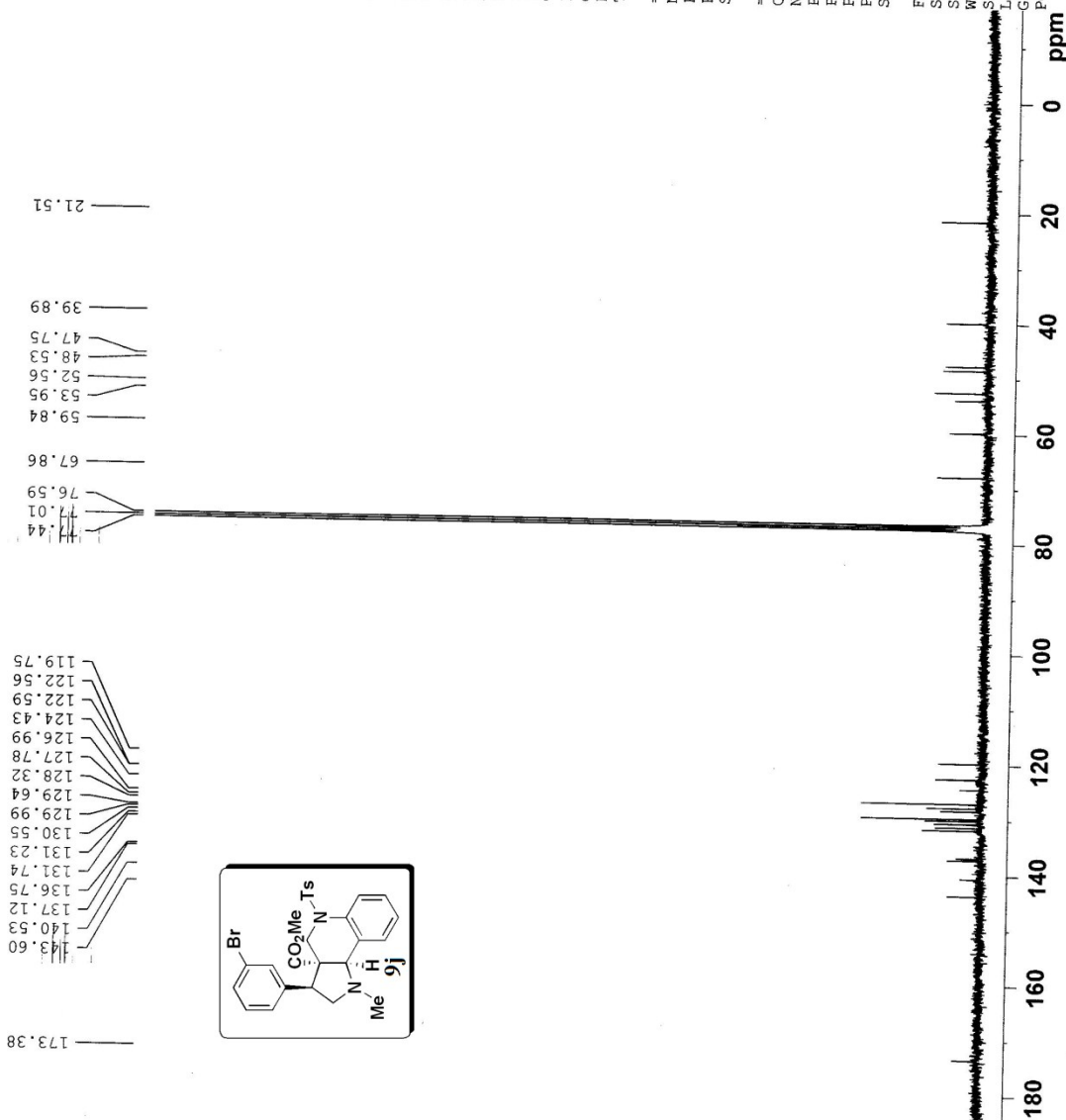
Current Data Parameters
 NAME DKV-3-BF-4-NSA
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20101226
 Time_ 21.53
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1787
 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 7.40 usec
 PL1 -2.00 dB
 SFO1 75.4752953 MHz

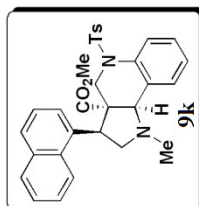
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 P2 80.00 usec
 PL2 0.00 dB
 PL12 15.68 dB
 PL13 16.00 dB
 SFO2 300.1312005 MHz

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

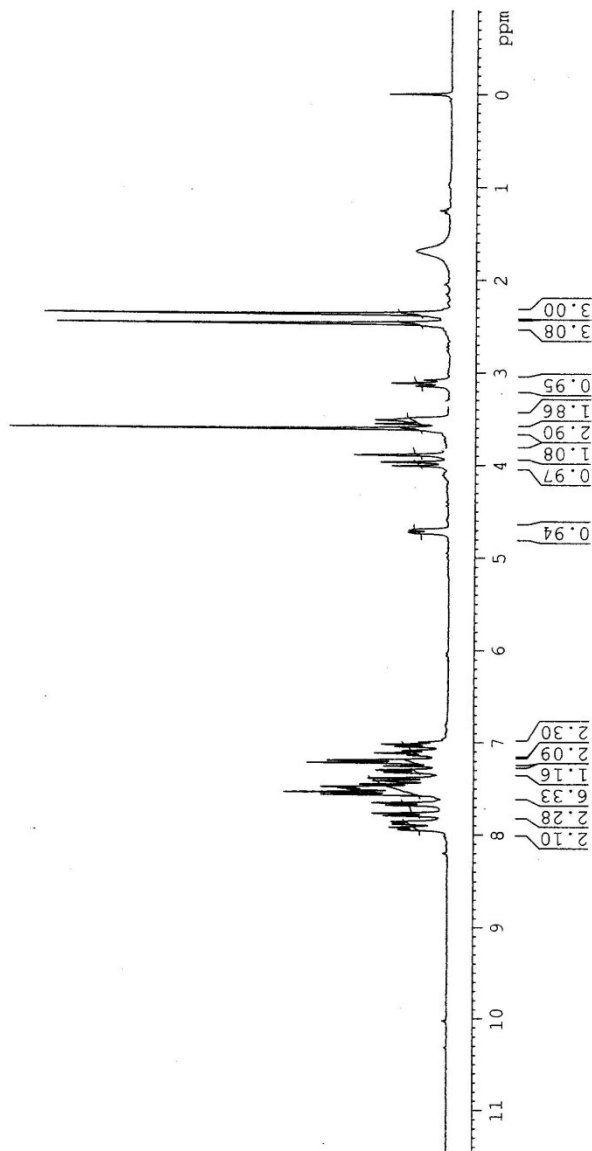




2.365
2.468
2.080
3.113
3.146
3.514
3.554
3.605
3.829
3.890
3.967
4.009
4.692
4.704
4.725
6.994
7.019
7.043
7.087
7.113
7.139
7.191
7.217
7.256
7.298
7.323
7.388
7.416
7.452
7.479
7.495
7.508
7.537
7.564
7.656
7.680
7.767
7.794
7.856
7.885
7.919
7.944



Current Data Parameters
NAME DK-V-Nap-**5ST**
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 2010116
Time 0041
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 2
DS 2
SWH 6172.826 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 300.1300077 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





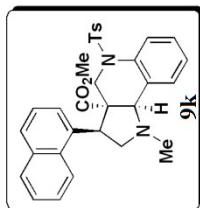
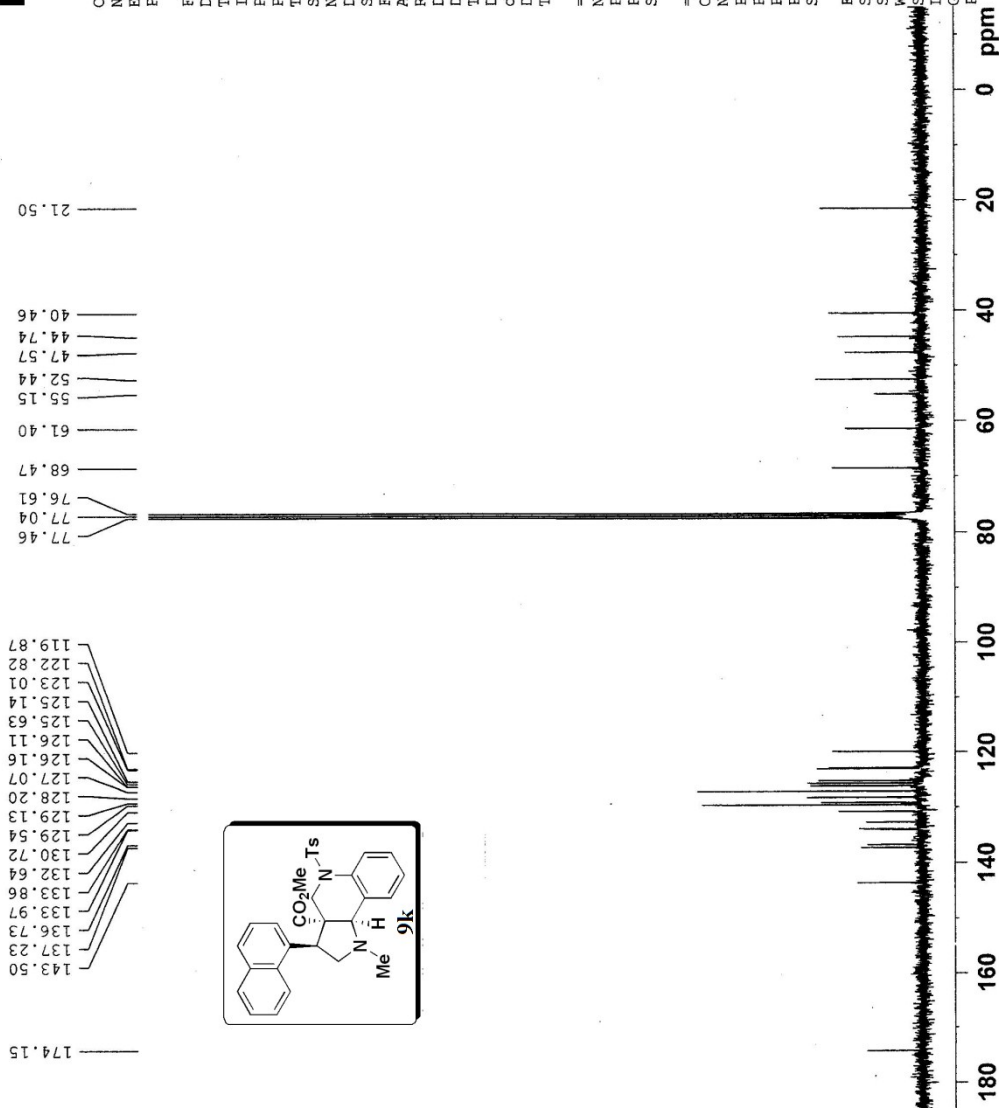
Current Data Parameters
 NAME DK-V-Nap-**5f**
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20101116
 Time_ 20.50
 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 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
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 7.40 usec
 PL1 -2.00 dB
 SF01 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
 SF02 300.1312005 MHz

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





Current Data Parameters
 NAME VV-FINAL
 EXPNO 1
 PROCNO 1

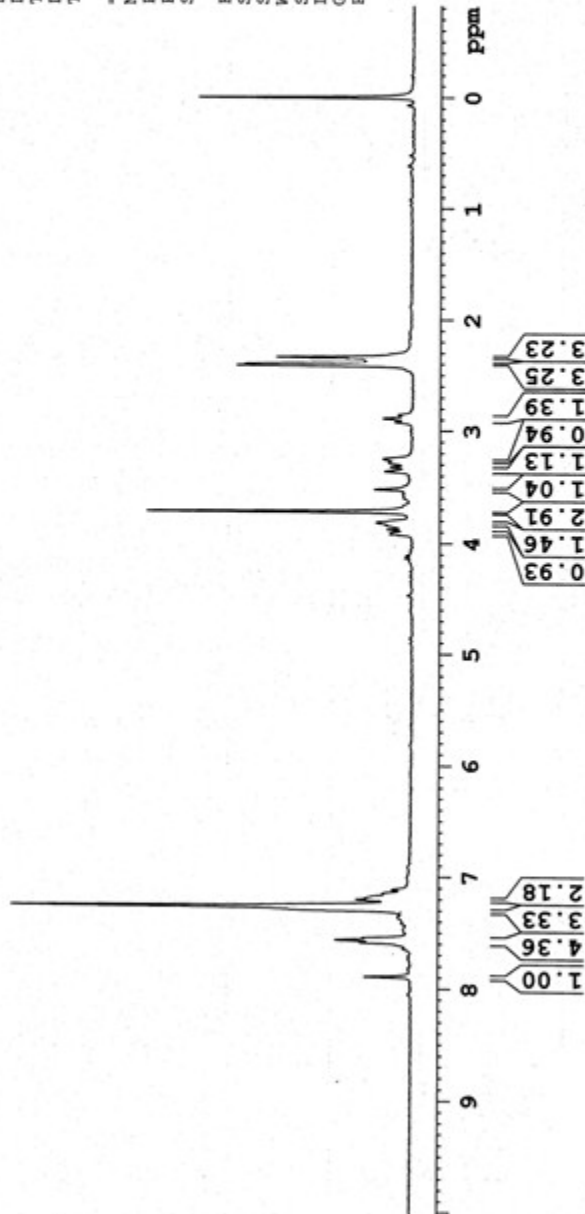
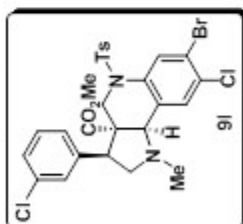
F2 - Acquisition Parameters
 Date_ 20141121
 Time_ 15.17
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 5.3084660 sec
 RG 362
 DW 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 13.15 usec
 PL1 0.00 dB
 SF01 300.1318534 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300065 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

3.919
3.906
3.841
3.817
3.720
3.523
3.363
3.323
3.288
3.254
2.922
2.890
2.857
2.399
2.338

7.894
7.589
7.566
7.549
7.265
7.204
7.187
7.148





Current Data Parameters
NAME VV-14
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

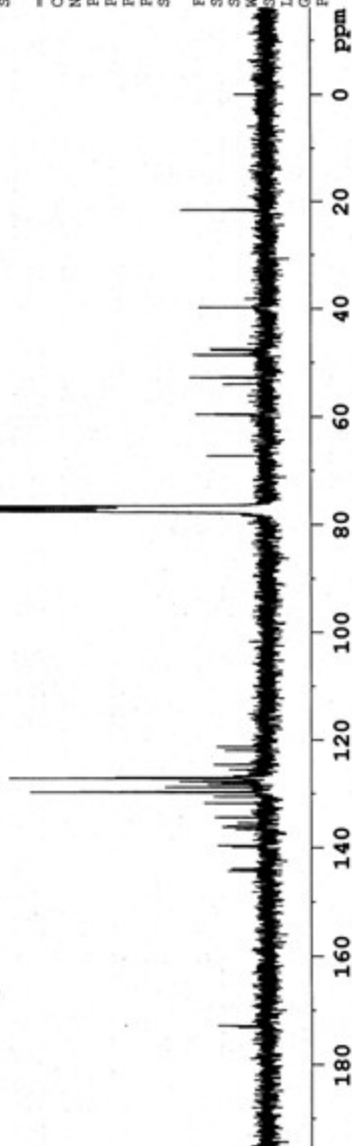
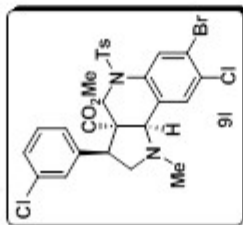
Date_ 20141126
Time 6.05
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 8000
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 3649.1
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

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

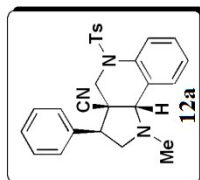
F2 - Processing parameters
SI 32768
SF 75.4677479 MHz
EX 0
GB 1.00 Hz
PC 1.40

172.92
144.30
143.91
139.88
139.65
136.21
134.46
131.82
130.59
129.80
129.71
128.86
128.32
127.83
127.22
127.05
124.64
121.33
77.44
77.02
76.60
67.26
59.55
53.96
52.74
48.53
47.49
39.77
21.57





7.828
7.801
7.566
7.542
7.525
7.458
7.435
7.410
7.391
7.368
7.344
7.305
7.277
7.262
7.241
7.209
7.189
7.160
7.136
7.112
4.417
4.373
3.880
3.859
3.842
3.822
3.615
3.577
3.275
3.254
3.244
3.224
2.971
2.934
2.902
2.407
2.283

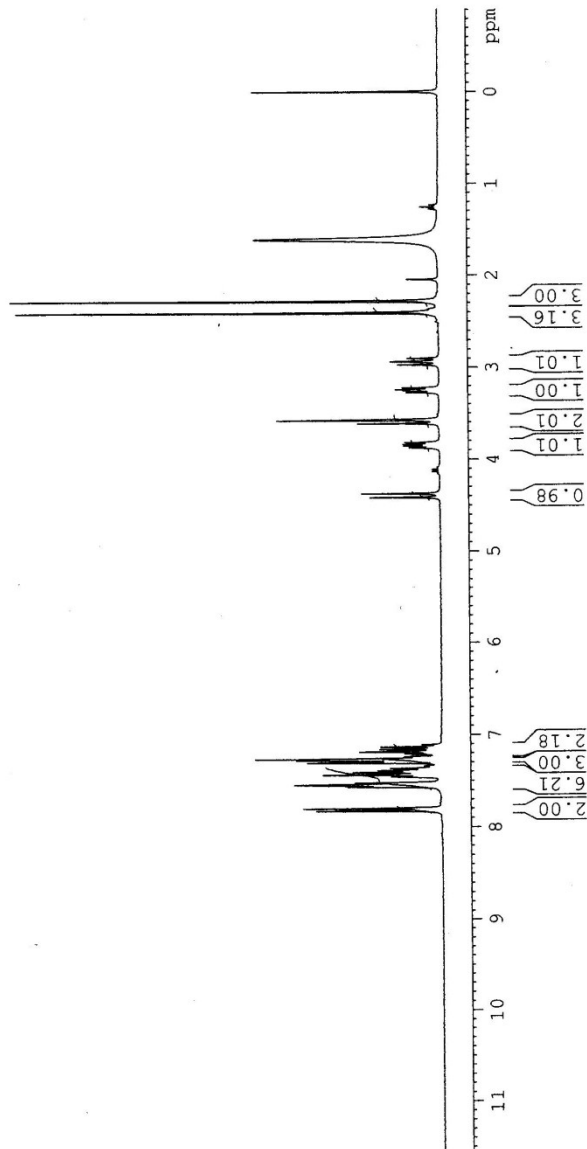


Current Data Parameters
NAME DK-V-H-CN
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20101116
Time_ 21:24
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 456.1
DM 81.000 usec
DE 6.00 usec
TE 300.2 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





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

F2 - Acquisition Parameters
 Date_ 20101116
 Time 22.22
 INSTRUM spect
 PROBD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1095
 DS 4
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQC 1.8219508 sec
 RG 362
 DE 27.800 usec
 TE 300.0 K
 DI 2.0000000 sec
 d11 0.0300000 sec
 DELTA 1.8999998 sec
 TDO 1

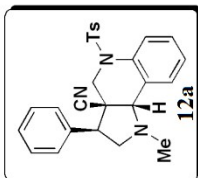
===== CHANNEL f1 =====
 NUC1 13C
 P1 7.40 usec
 PL1 -2.00 dB
 SFO1 75.4752953 MHz

===== 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
 EM 0
 WDW 0
 SSB 1.00 Hz
 GB 0
 PC 1.40

77.44
 77.01
 76.59
 70.92
 59.97
 52.39
 52.10
 49.41
 39.53
 21.54

144.10
 138.91
 137.32
 135.68
 130.47
 129.82
 129.16
 128.95
 128.78
 128.32
 127.93
 127.24
 124.53
 121.12
 120.32

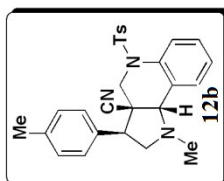


180 160 140 120 100 80 60 40 20 0 ppm

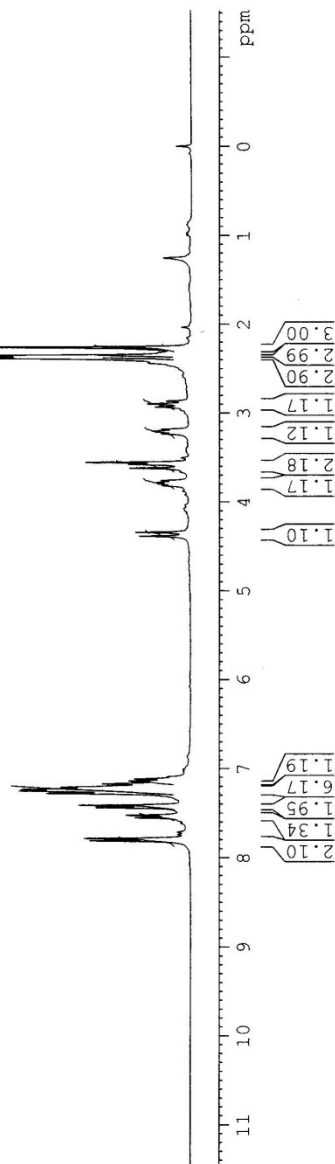


2.265
2.361
2.387
2.867
2.901
2.936
3.187
3.207
3.237
3.559
3.580
3.624
3.763
3.783
3.800
3.820
4.345
4.386

7.120
7.145
7.177
7.215
7.241
7.259
7.285
7.418
7.443
7.530
7.557
7.789
7.816



Current Data Parameters
NAME DR-V-4-95-CN-1A
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101226
Time 0.50
INSTRUM spect
PROBHD 5 mm DUL 125
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 7
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3068469 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 300.1300113 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





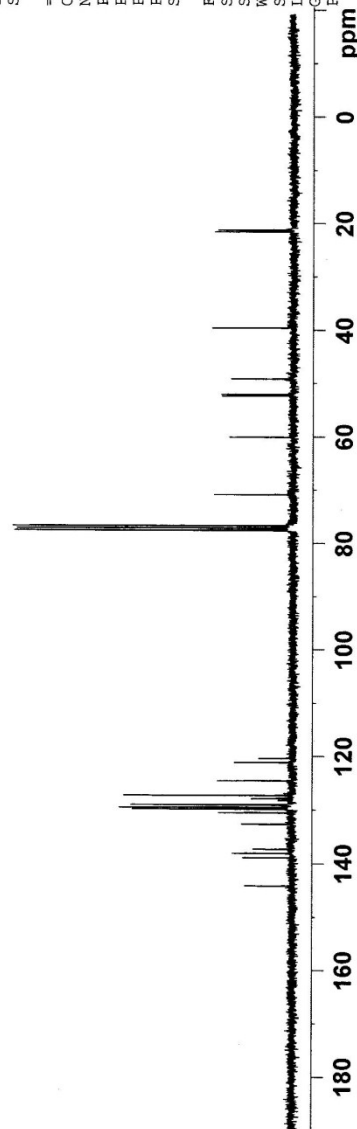
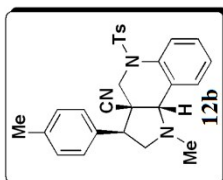
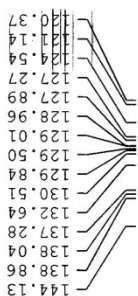
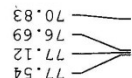
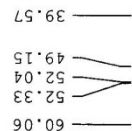
Current Data Parameters
 NAME DK-V-4-Me-CN SA
 EXNO 2
 PROCNO 1

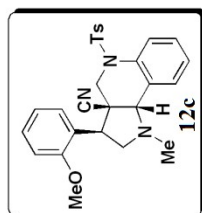
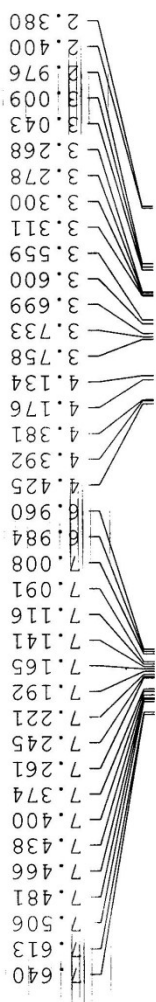
F2 - Acquisition Parameters
 Date_ 20101226
 Time_ 0.56
 INSTRUM spect
 PROBD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 101
 DS 4
 SMH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQC 1.8219508 sec
 RG 362
 DW 27.800 usec
 DE 6.00 usec
 TE 300.0 K
 DI 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TDO 1

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

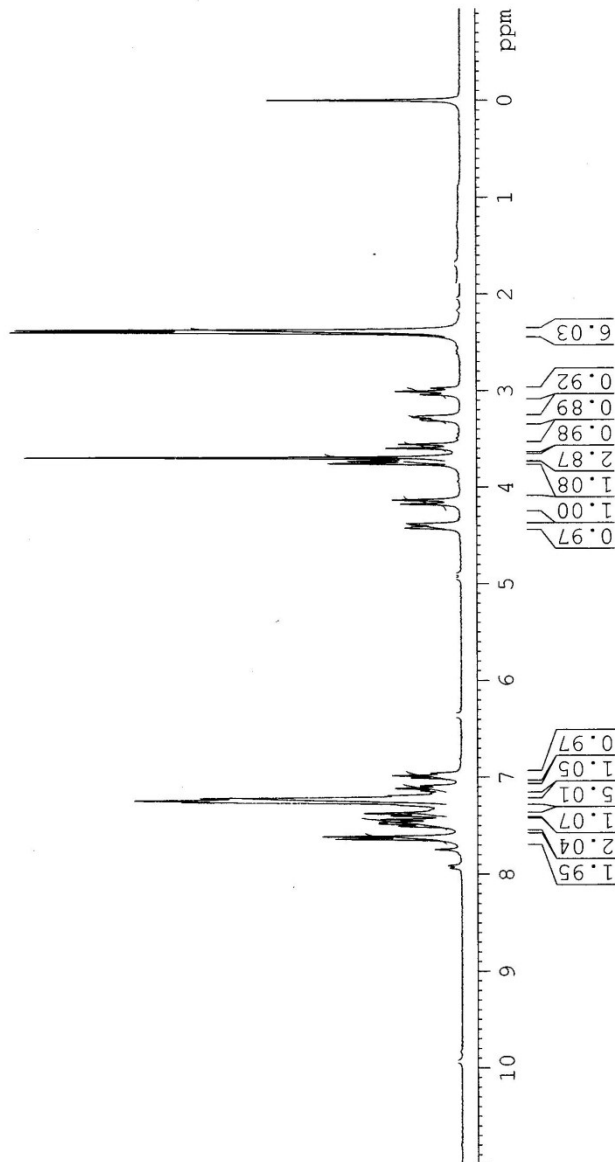
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PL12 15.68 dB
 PL13 16.00 dB
 SFO2 300.1312005 MHz

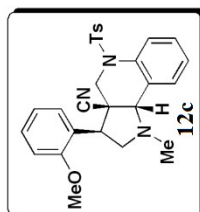
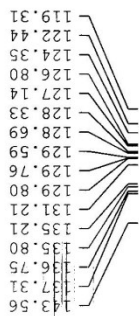
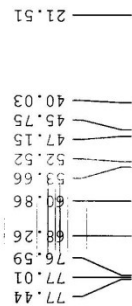
F2 - Processing parameters
 SI 32768
 SF 75.4677490 MHz
 EM 0
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40





Current Data Parameters
NAME DK-V-20Me-EST-SA
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190227
Time 0.15
INSTRUM spect
PROBHD 5 mm DUL 13c-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 12
DS 2
SWH 6172.439 Hz
FIDRES 0.04190 Hz
AQ 5.3084660 sec
RG 322.5
DM 81.000 usec
DE 6.00 usec
TE 300.2 K
D1 1.0000000 sec
TD0 1
===== CHANNEL f1 =====
NUC1 1H
P1 13.15 usec
PL1 0.00 dB
SFO1 300.1318934 MHz
F2 - Processing parameters
SI 32768
SF 300.130061 MHz
WDW EM
SSB 0
CB 0.30 Hz
GB 0
PC 1.00





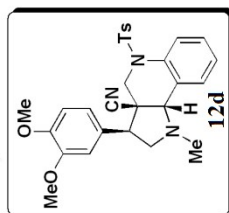
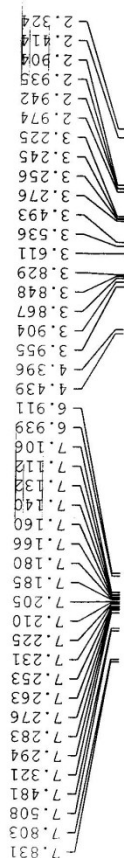
Current Data Parameters
NAME DK-V-2-OMe-1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20101224
Time 8.16
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 6709
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 362
DM 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TDO 1

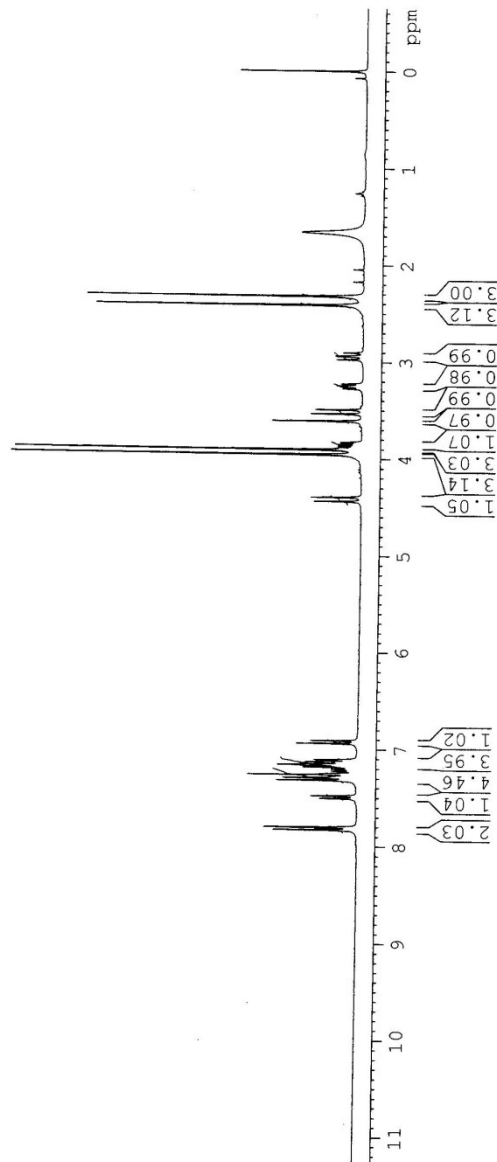
===== CHANNEL f1 =====
NUC1 13C
P1 7.40 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz

===== 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



Current Data Parameters
 NAME DK-V-OMe2 CN SA
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20101225
 Time_ 12:02
 INSTRUM spect
 PROHD 5 mm DUL 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 9
 DS 2
 SWH 6172.830 Hz
 FIDRES 0.094190 Hz
 AQ 5.3084660 sec
 RG 256
 DW 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 TDO 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
 GB 0
 PC 1.00





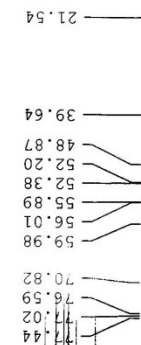
Current Data Parameters
 NAME DK-V-OMe2 CN SA
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20101225
 Time_ 22.19
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 848
 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
 TDO 1

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

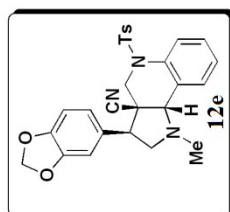
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 FCPD2 80.00 usec
 PL2 0.00 dB
 PL12 15.68 dB
 PL13 16.00 dB
 SFO2 300.1312005 MHz

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





2.261
2.406
2.811
2.845
2.879
3.185
3.206
3.232
3.550
3.593
3.757
3.776
3.792
3.812
4.350
4.394
4.984
5.984
6.839
6.864
7.014
7.040
7.126
7.151
7.171
7.261
7.279
7.303
7.509
7.534
7.795
7.821

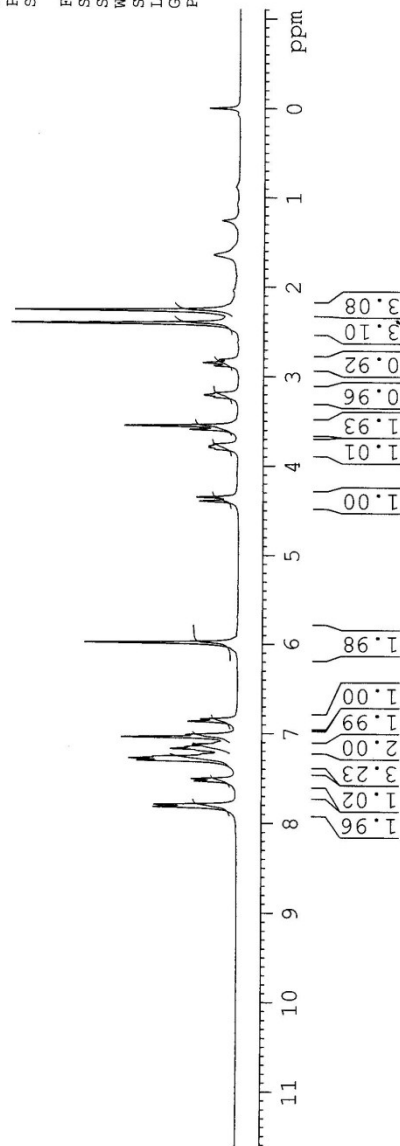


Current Data Parameters
NAME DK-V-FIP-CN-SAR
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130223
Time_ 16.49
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 300.1300076 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





Current Data Parameters
 NAME DK-V-PIP-CN-SAR
 EXPNO 2
 PROCNO 1

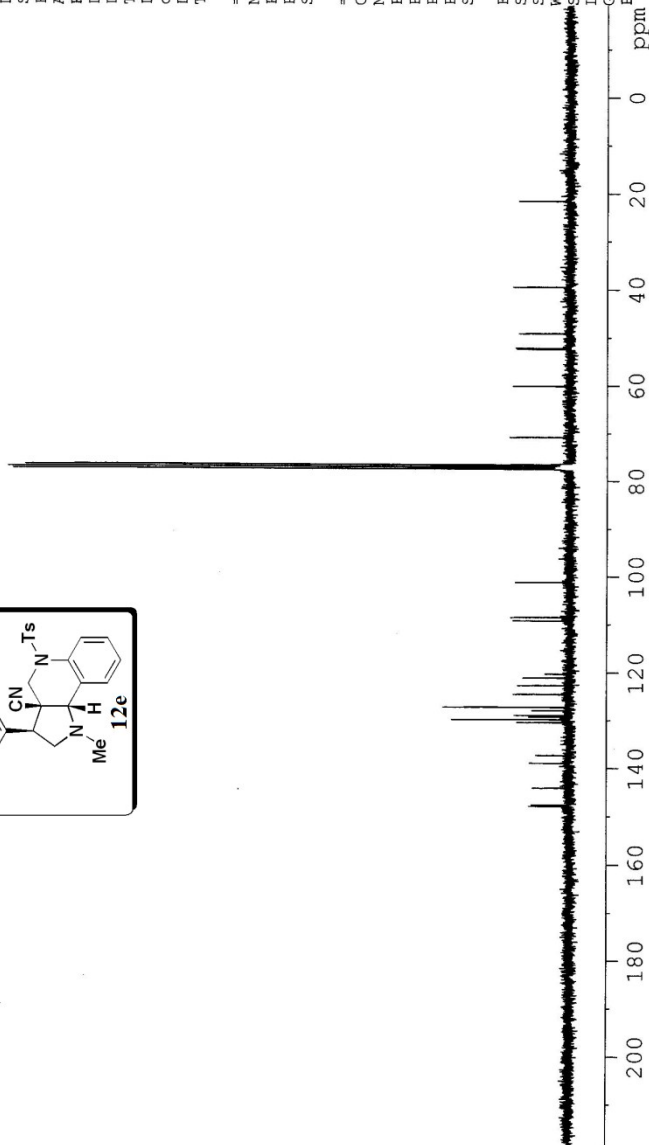
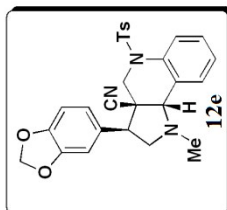
F2 - Acquisition Parameters
 Date_ 20130223
 Time 16.54
 INSTRUM spect
 PROBD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 353
 DS 4
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 456.1
 DW 27.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.30 usec
 PL1 0.00 dB
 SF01 75.4752953 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 FCPD2 80.00 usec
 PL2 0.00 dB
 PL12 15.68 dB
 PL13 16.00 dB
 SF02 300.1312005 MHz

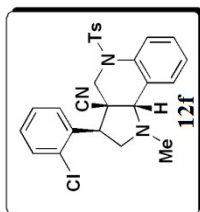
F2 - Processing parameters
 SI 32768
 SF 75.4677490 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

147.92
 147.61
 144.11
 138.95
 137.34
 130.46
 129.83
 129.28
 128.93
 127.94
 127.23
 124.52
 122.69
 121.09
 120.30
 109.25
 108.51
 101.21
 77.45
 77.03
 76.61
 70.83
 60.10
 52.35
 52.13
 49.10
 39.49
 21.54

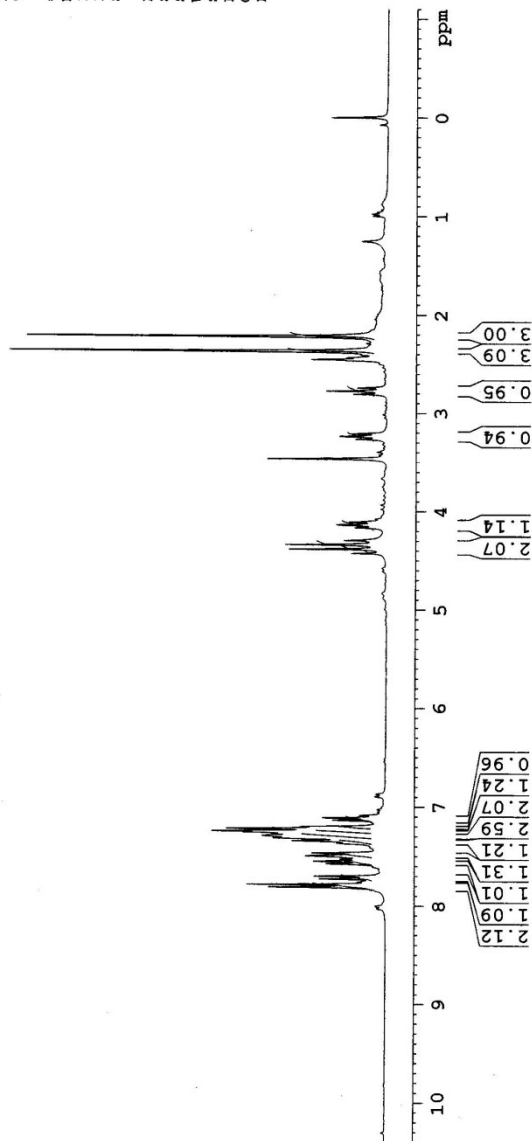




7.812
7.785
7.759
7.728
7.700
7.606
7.575
7.549
7.527
7.497
7.466
7.412
7.368
7.344
7.317
7.293
7.271
7.259
7.246
7.220
7.203
7.135
7.110
7.086
4.427
4.383
4.339
4.294
4.164
4.134
4.108
3.466
3.265
3.235
3.209
2.807
2.775
2.743
2.367
2.218



Current Data Parameters
NAME DK-V-2Cl-CN-SA
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101228
Time 0.23
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 128
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.0000000 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 300.1300068 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





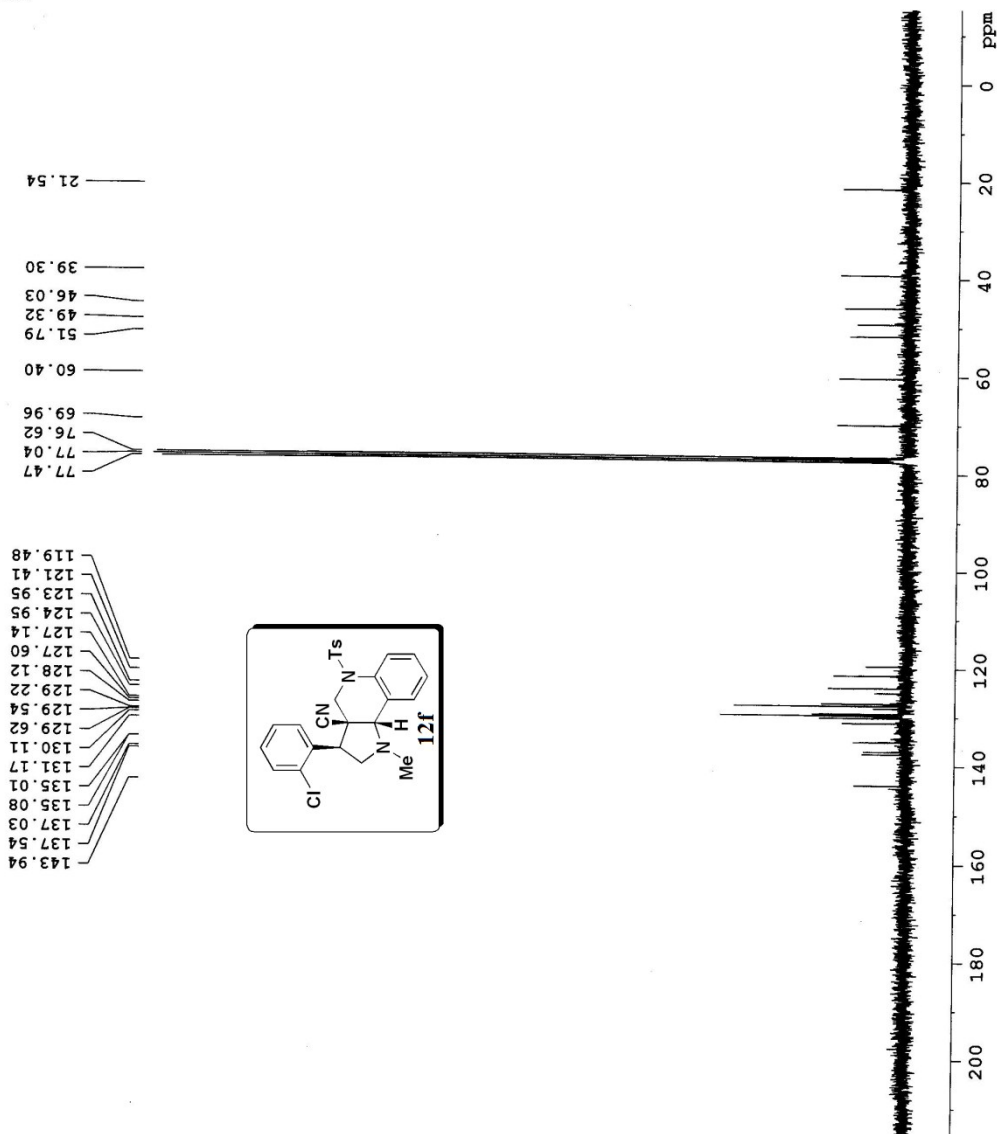
Current Data Parameters
NAME DK-V-2C1-CN-SA
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20101228
Time 0.31
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 215
DS 4
SWH 17985.61 Hz
FIDRES 0.27432 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
PL 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

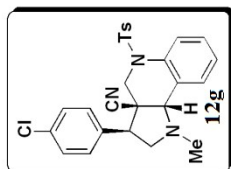
F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



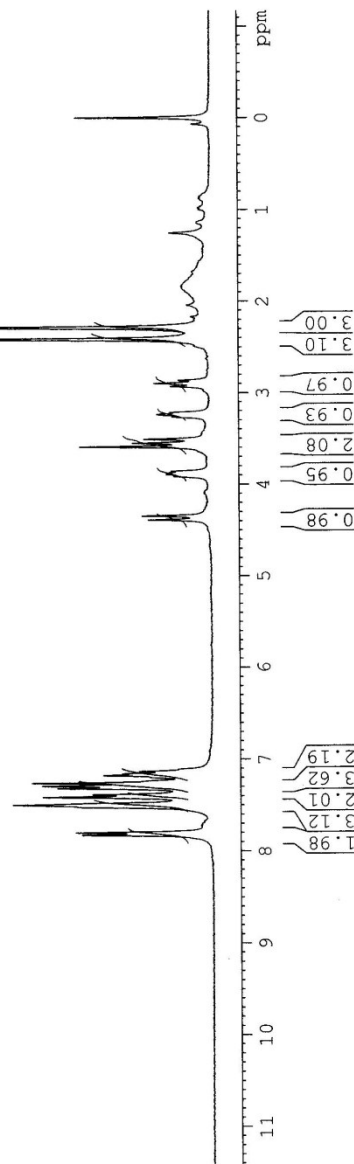


4.390
4.347
3.917
3.898
3.881
3.861
3.594
3.555
3.511
3.267
3.240
3.219
3.933
2.899
2.864
2.416
2.289

7.825
7.799
7.497
7.415
7.389
7.319
7.293
7.262
7.179
7.160
7.135



Current Data Parameters
NAME: 12g
EXPNO: 1
PROCNO: 1
F2 - Acquisition Parameters
Date_: 20101226
Time: 0.04
INSTRUM: spect
PROBHD: 5 mm DUL 125-1
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl3
NS: 16
DS: 2
SWH: 6172.939 Hz
FIDRES: 0.021430 Hz
AQ: 5.3084660 sec
RG: 287.4
DE: 81.000 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: 300.1300061 MHz
WDW: EM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00





Current Data Parameters
 NAME DK-V-4-Cl CN SA
 EXNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20101226
 Time_ 0.38
 INSTRUM spect
 PROBD 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 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
 FCPD2 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

121.55

39.46

48.54

52.28

52.16

59.86

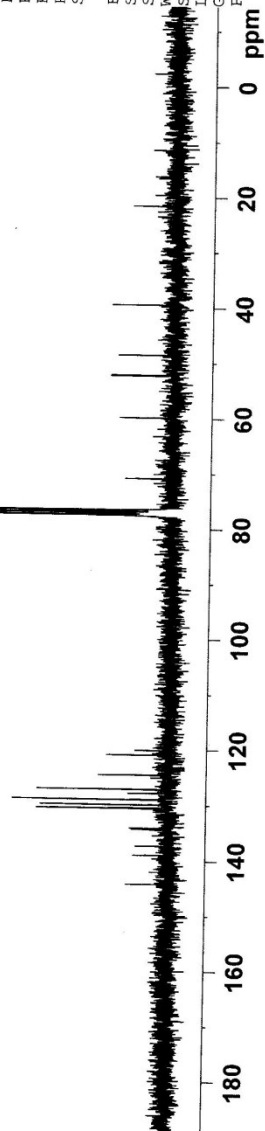
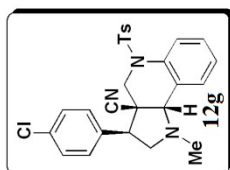
70.86

76.59

77.02

77.44

144.22
 142.07
 138.99
 137.33
 134.31
 134.12
 130.55
 130.44
 129.91
 128.98
 127.85
 127.15
 124.58
 120.96
 120.11





Current Data Parameters
 NAME VV-28
 EXPNO 1
 PROCNO 1

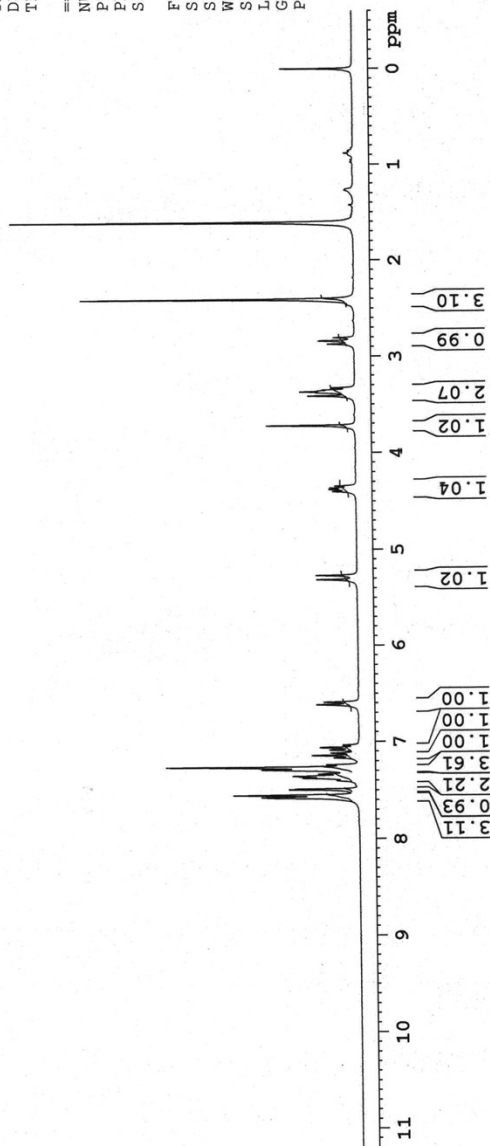
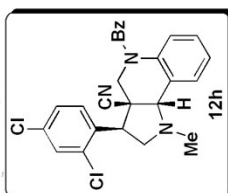
F2 - Acquisition Parameters

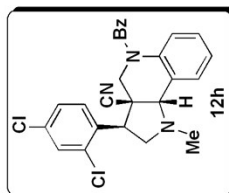
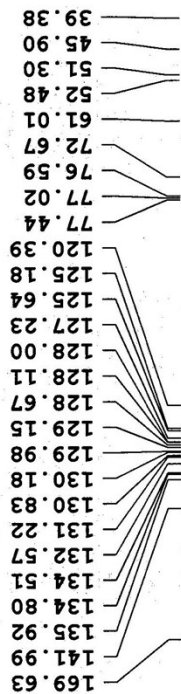
Date_ 20141209
 Time_ 22.27
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 5.3084660 sec
 RG 256
 DW 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 D11
 D10 1

===== 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

7.583
 7.577
 7.555
 7.496
 7.490
 7.402
 7.379
 7.366
 7.358
 7.338
 7.331
 7.292
 7.265
 7.242
 7.169
 7.145
 7.120
 7.089
 7.064
 7.038
 6.619
 6.593
 5.314
 5.270
 4.402
 4.381
 4.366
 4.344
 3.722
 3.416
 3.383
 3.372
 3.363
 3.353
 3.331
 2.875
 2.841
 2.806
 2.407





Current Data Parameters
NAME VV-28
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141210
Time_ 7.40
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 8500
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

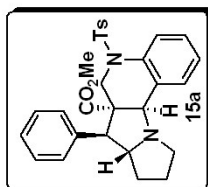
===== CHANNEL f1 =====
NUC1 13C
P1 9.30 usec
PL1 0.00 dB
SFO1 75.4752953 MHz

===== 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
EM 0
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



1.563
1.582
1.599
1.618
1.642
1.903
1.941
1.955
1.976
1.994
2.048
2.071
2.088
2.109
2.126
2.386
3.054
3.075
3.100
3.121
3.139
3.504
3.539
3.623
3.760
3.801
4.064
4.078
4.098
4.334
4.511
4.553
6.968
6.993
7.017
7.074
7.100
7.124
7.167
7.187
7.211
7.237
7.262
7.319
7.347
7.371
7.391
7.428
7.456
7.684

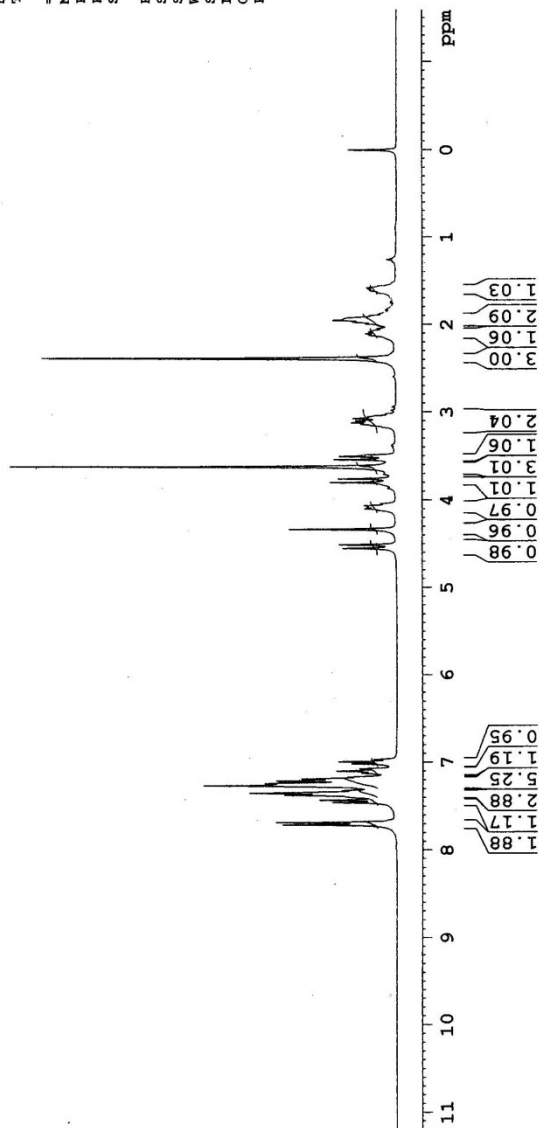


Current Data Parameters
NAME DK-V-ts-PYZ
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110923
Time_ 19.43
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 1.0000000 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 300.1300061 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





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

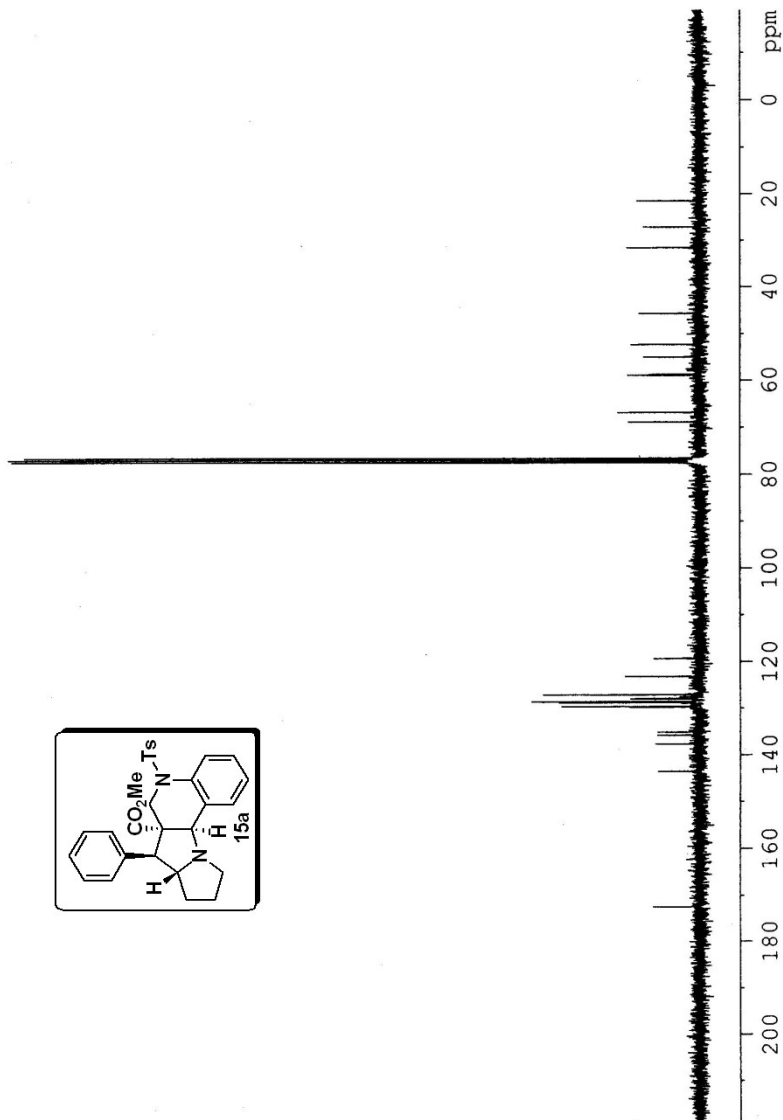
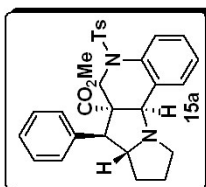
F2 - Acquisition Parameters
 Date_ 20110923
 Time_ 19.48
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 261
 DS 4
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 724.1
 DW 27.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TDO 1

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

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCD2 80.00 usec
 PL2 0.00 dB
 PL12 15.68 dB
 PL13 16.00 dB
 SFO2 300.1312005 MHz

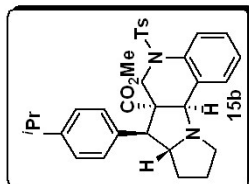
F2 - Processing parameters
 SI 32768
 SF 75.4677490 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

172.53
 143.53
 137.68
 135.78
 135.15
 129.76
 129.61
 128.73
 128.52
 128.02
 127.88
 127.55
 127.05
 123.14
 119.36
 77.46
 77.04
 76.62
 68.89
 66.85
 58.94
 58.76
 54.99
 52.26
 45.69
 31.62
 27.18
 21.52





7.714
7.687
7.460
7.433
7.259
7.231
7.196
7.165
7.117
7.094
7.010
6.986
6.962
4.559
4.517
4.305
4.061
4.042
3.798
3.757
3.629
3.524
3.490
3.104
3.086
3.054
2.984
2.961
2.939
2.916
2.893
2.870
2.848
2.382
2.110
2.093
2.073
1.944
1.924
1.883
1.861
1.636
1.612
1.590
1.575
1.564

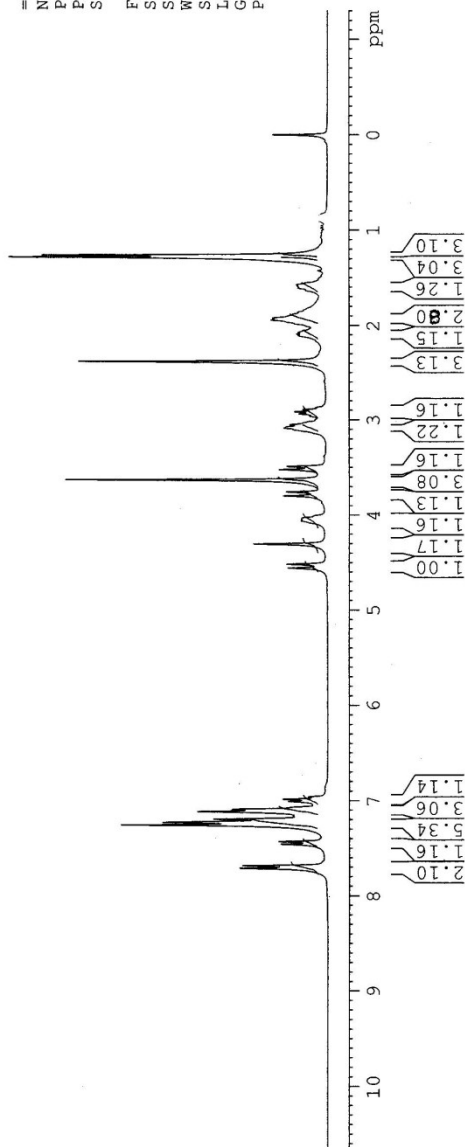


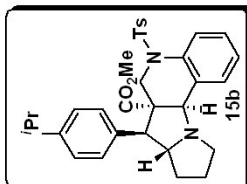
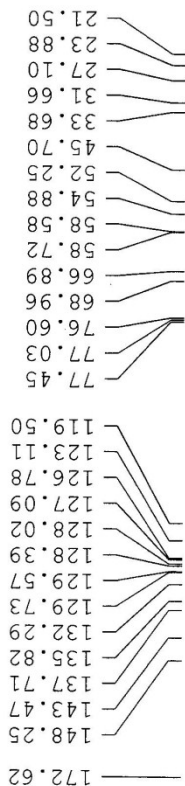
Current Data Parameters
NAME DK-4-1PRO PROL
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130221
Time_ 17.33
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 13.15 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300070 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





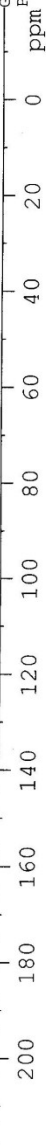
Current Data Parameters
NAME DK-4-1PRO PROL
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130221
Time_ 17.43
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 385
DS 4
SWH 17985.611 Hz
FIDRES 0.27439 Hz
AQ 1.8219508 sec
RG 1024
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.8999998 sec
TD0 1

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

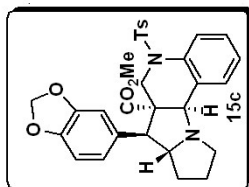
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.68 dB
PL13 16.00 dB
SFO2 300.1312005 MHz

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





1.617
1.636
1.655
1.876
1.898
1.915
1.935
1.955
1.977
1.996
2.012
2.031
2.052
2.074
2.109
2.409
3.027
3.051
3.089
3.130
3.365
3.391
3.443
3.474
3.604
3.622
3.659
3.703
3.722
3.763
3.829
3.869
6.013
6.049
6.080
6.556
6.595
6.680
6.706
6.798
6.824
7.150
7.176
7.219
7.255
7.282
7.391
7.416
7.457
7.687
7.715

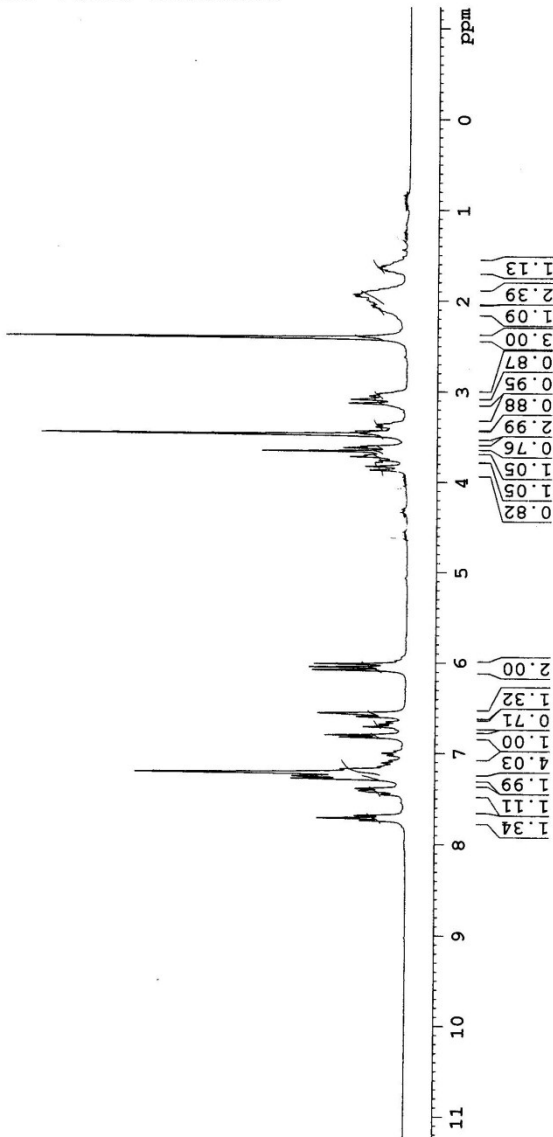


Current Data Parameters
NAME DK-V-pip-TS-FYZ
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 2011024
Time_ 22.47
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 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 13.15 usec
PL1 0.00 dB
SF01 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





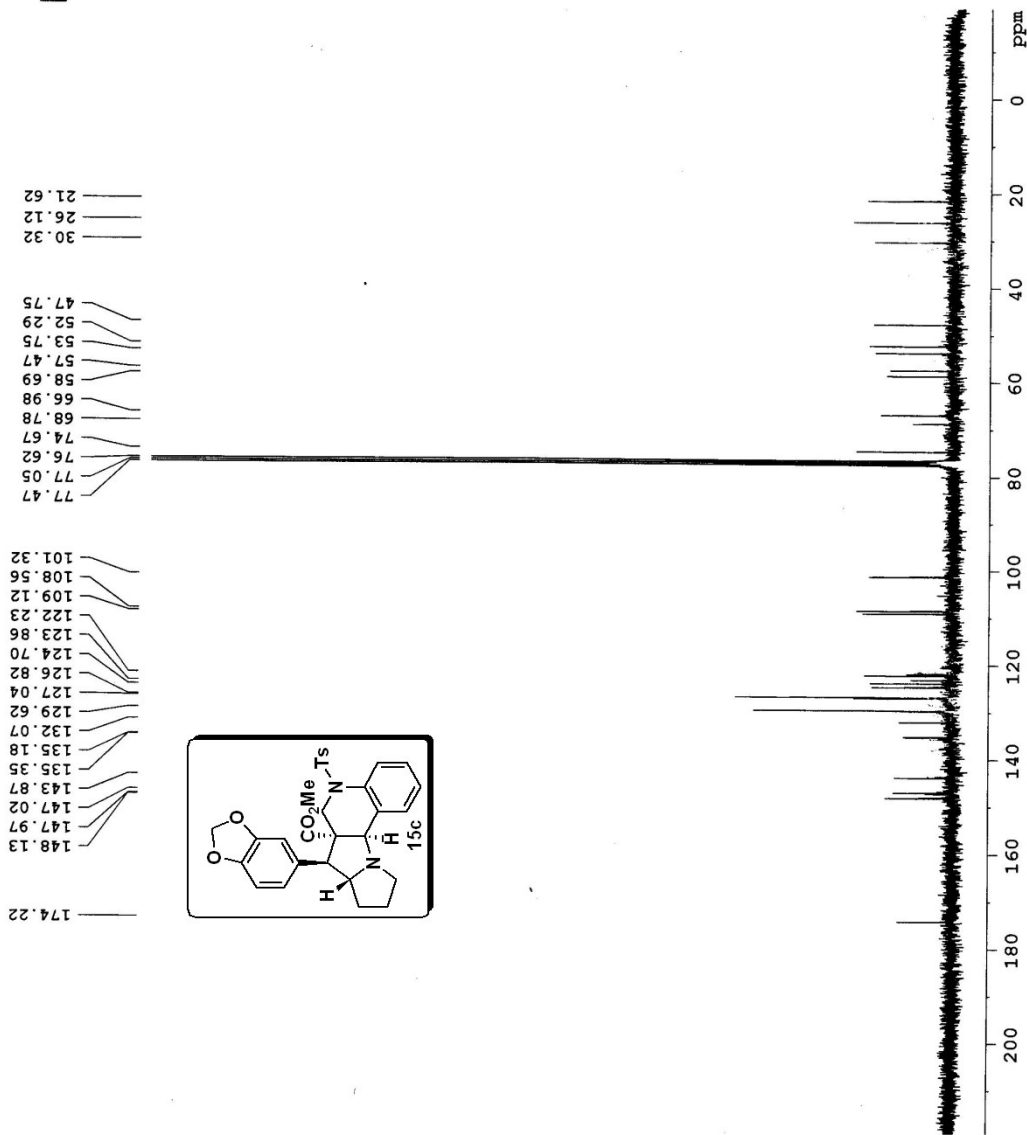
Current Data Parameters
 NAME DR-V-PIP-TS-Pyz
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110614
 Time 22.51
 INSTRUM 5 mm DUL 13C-1
 PROBD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 379
 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 2.0000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.30 usec
 PL1 0.00 dB
 SF01 75.4752953 MHz

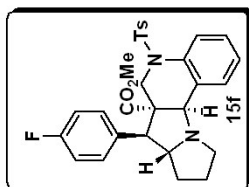
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 FCPD2 80.00 usec
 PL2 0.00 dB
 PL12 15.68 dB
 PL13 16.00 dB
 SF02 300.1312005 MHz

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





1.589
1.611
1.632
1.651
1.673
1.809
1.839
1.863
1.881
1.904
1.928
1.947
1.966
1.989
2.017
2.036
2.055
2.078
2.409
2.913
2.953
3.044
3.065
3.372
3.394
3.418
3.486
3.561
3.687
3.705
3.712
3.733
3.752
3.827
3.867
7.053
7.076
7.139
7.168
7.197
7.274
7.413
7.435
7.667
7.692

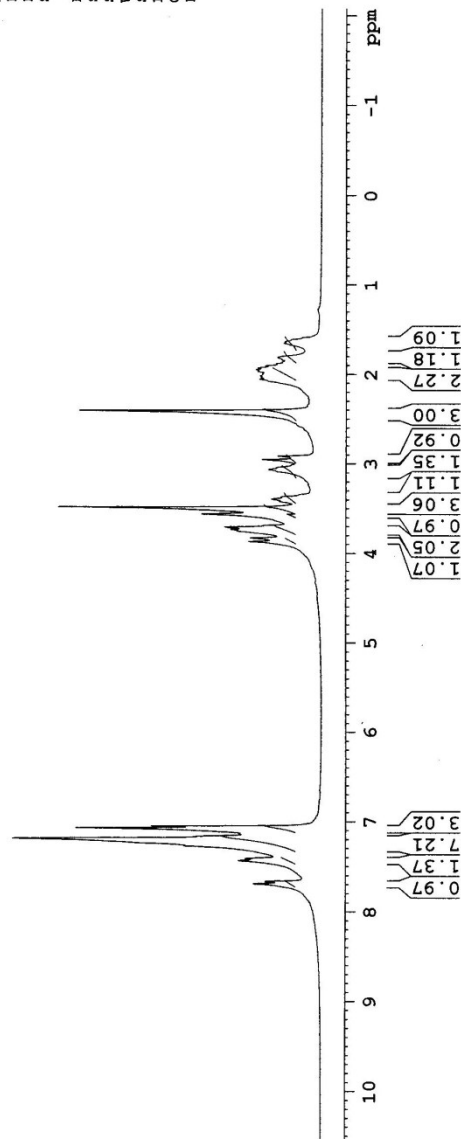


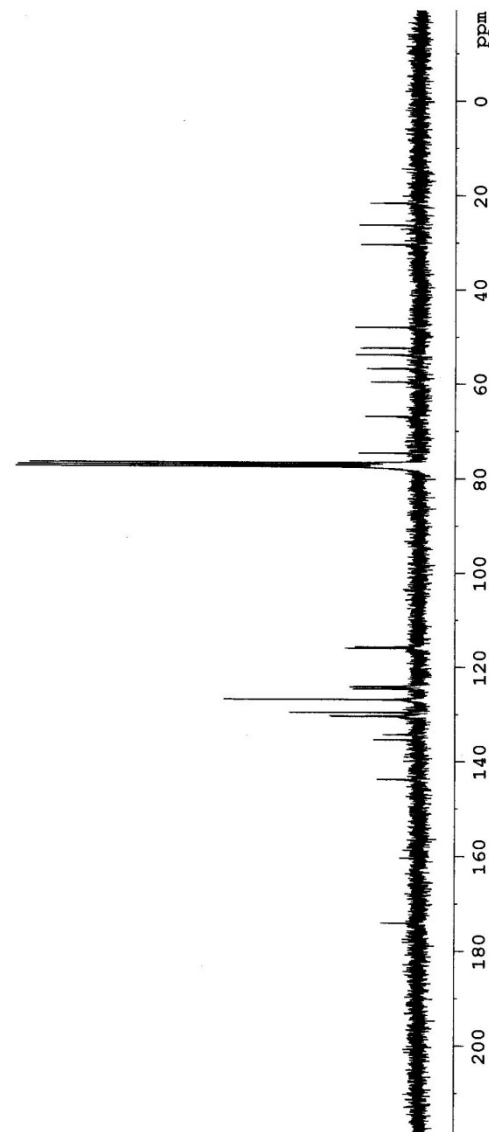
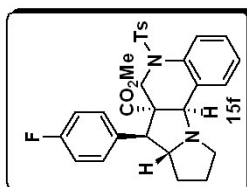
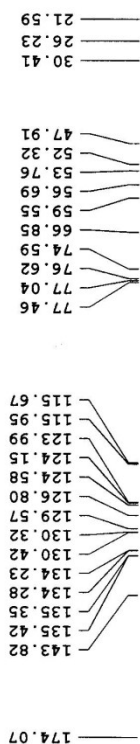
Current Data Parameters
NAME DK-V-4-F-EST-DC-PYZ
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 2011017
Time 18.36
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 114
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-F-EST-DC-PYZ
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 201107
Time_ 18.46
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 400
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

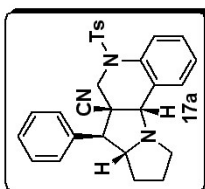
===== CHANNEL f1 =====
NUC1 13C
PL 9.30 usec
PL1 0.00 dB
SFO1 75.4752953 MHz

===== 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
GB 1.00 Hz
PC 1.40



1.600
1.617
1.639
1.749
1.787
1.812
1.821
1.837
1.857
2.024
2.046
2.068
2.403
2.880
2.911
2.932
2.964
3.275
3.298
3.322
3.453
3.479
3.509
3.646
3.693
3.837
3.862
3.869
3.892
3.917
4.593
4.640
7.209
7.233
7.253
7.260
7.279
7.302
7.314
7.324
7.330
7.339
7.365
7.387
7.441
7.552
7.574
7.578
7.675
7.702

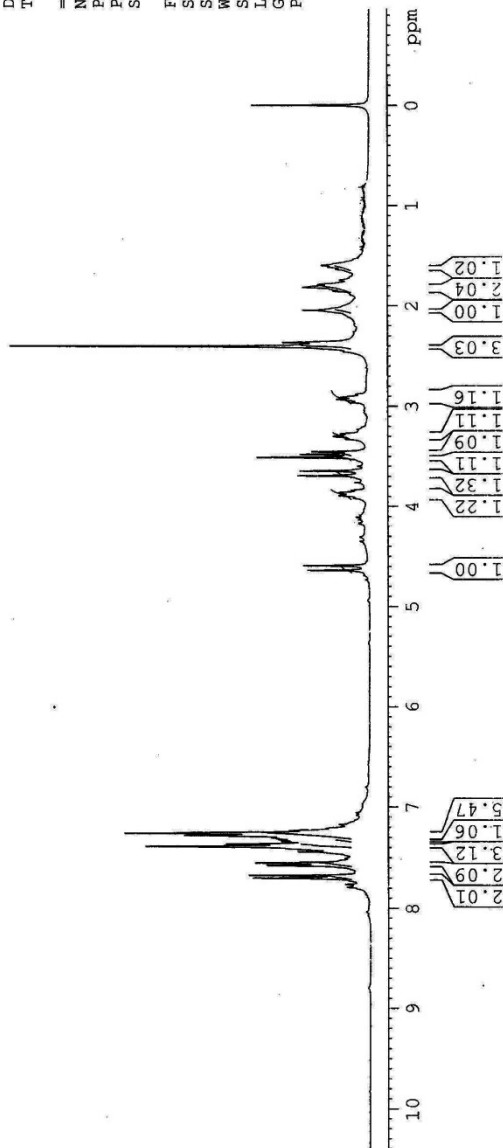


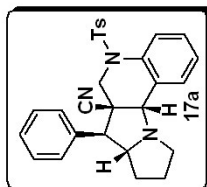
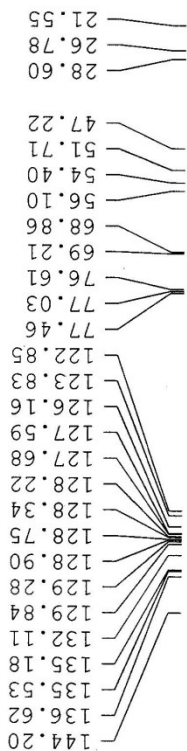
Current Data Parameters
NAME DK-HCN-PYZ
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121218
Time_ 23.03
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 13.15 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





Current Data Parameters
NAME DK-HCN-PYZ
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121218
Time_ 23.21
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 504
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
EM 0
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
 NAME 4-Me-CN-Ts-Pyrz
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters

Date 20121226
 Time 18.50
 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 128
 DW 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 TD0 1

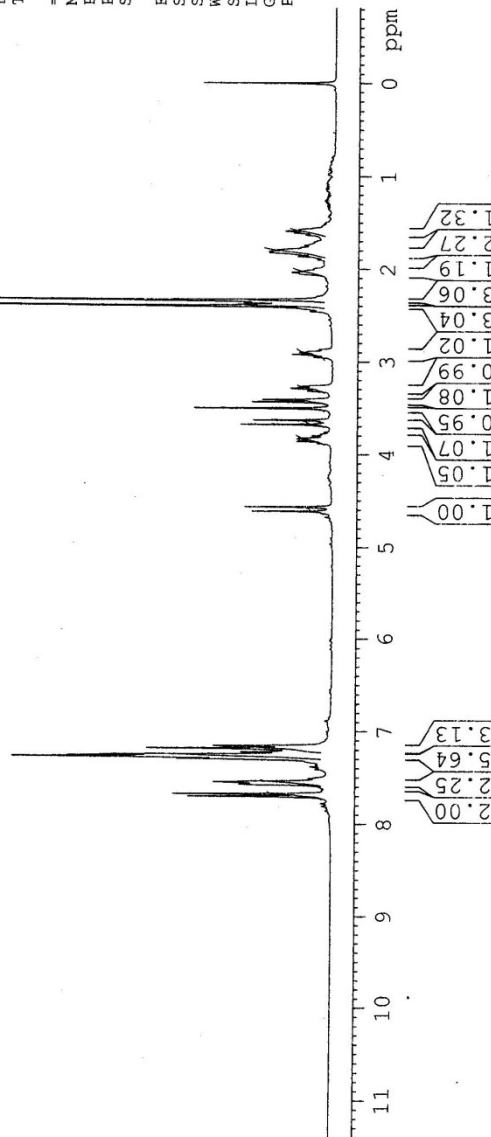
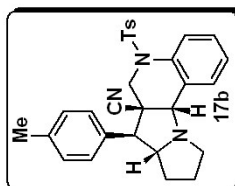
===== CHANNEL f1 =====

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

F2 - Processing parameters

SI 32768
 SF 300.1300070 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1.579
1.595
1.614
1.636
1.746
1.771
1.794
1.816
1.828
1.866
2.022
2.040
2.052
2.341
2.365
2.384
2.400
2.901
2.922
3.267
3.291
3.413
3.439
3.506
3.634
3.681
3.829
3.837
3.861
4.568
4.615
7.156
7.182
7.220
7.224
7.249
7.259
7.274
7.296
7.546
7.561
7.572
7.674
7.701





Current Data Parameters
 NAME 4-Me-CN-Ts-Pyrz
 EXPNO 2
 PROCNO 1

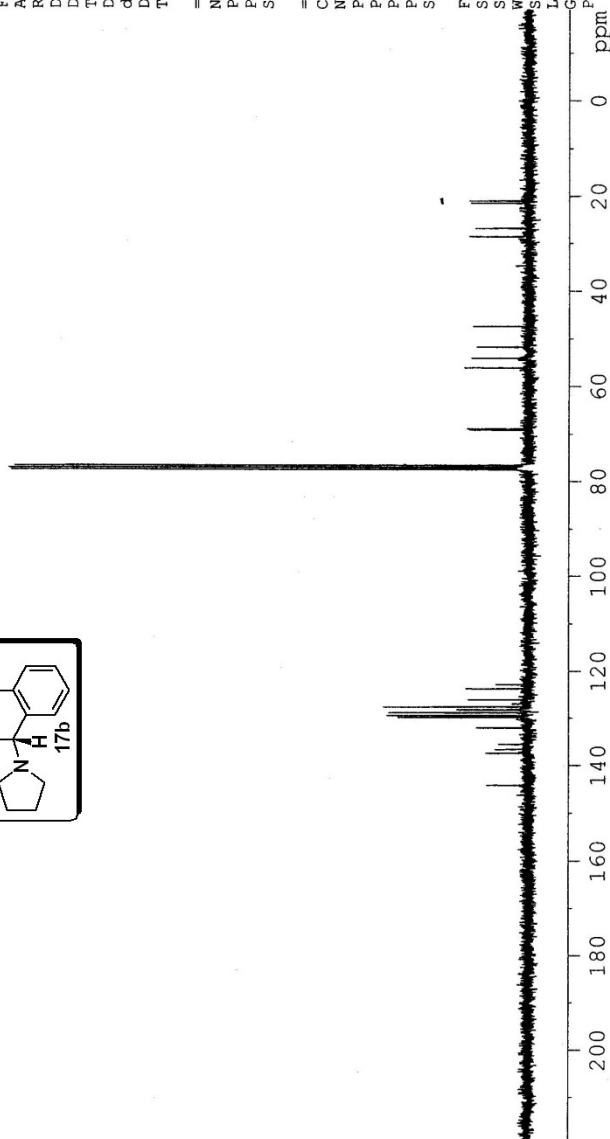
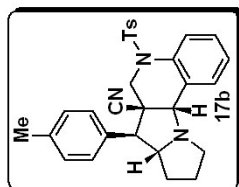
F2 - Acquisition Parameters
 Date_ 20121226
 Time_ 19.00
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 320
 DS 4
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 456.1
 DE 27.800 usec
 TE 300.0 K
 D1 2.0000000 sec
 d11 0.0300000 sec
 DELTA 1.8999998 sec
 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

144.17
 137.42
 136.64
 135.54
 132.10
 132.04
 129.82
 129.44
 128.83
 128.29
 128.24
 127.60
 126.09
 123.74
 122.87
 77.45
 77.03
 76.61
 69.17
 68.89
 56.09
 54.08
 51.68
 47.36
 28.58
 26.81
 21.54
 21.03



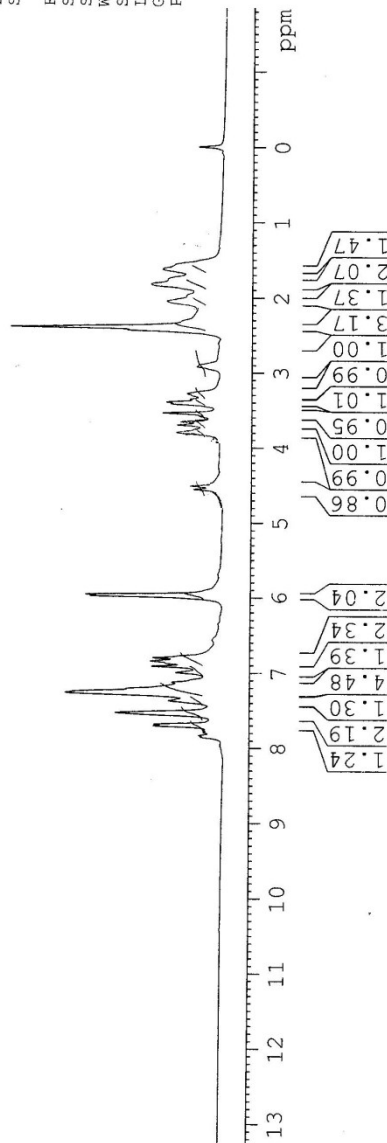
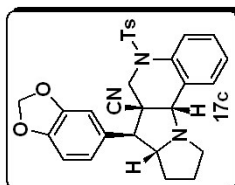
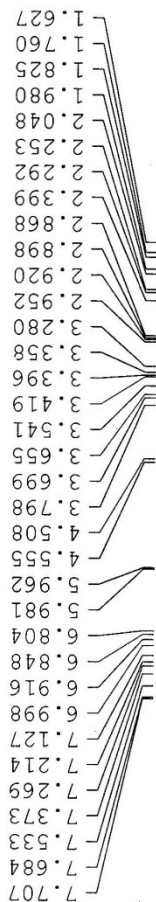


Current Data Parameters
 NAME DK-PIP-CN-PYZ
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20121211
 Time 20.12
 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 50.8
 DW 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 TD0 1

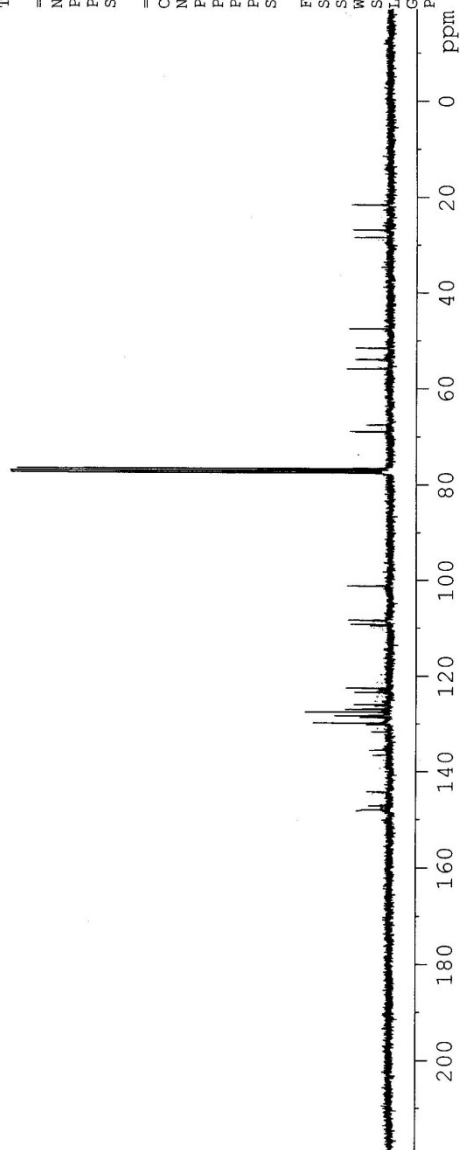
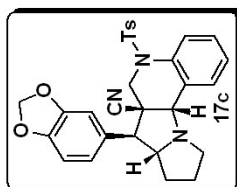
===== CHANNEL f1 =====
 NUC1 1H
 P1 13.15 usec
 PL1 0.00 dB
 SFO1 300.1318534 MHz

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





148.00
 147.16
 144.23
 136.65
 135.57
 131.71
 129.86
 128.70
 128.35
 127.55
 127.00
 126.90
 126.01
 123.43
 122.55
 109.27
 108.39
 101.23
 77.51
 77.09
 76.66
 69.04
 68.90
 67.54
 55.86
 53.91
 51.52
 47.53
 28.45
 26.84
 21.56



Current Data Parameters
 NAME DK-FIP-CN-FY2
 EXPNO 2
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20121211
 Time_ 20.17
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 198
 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
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.30 usec
 PL1 0.00 dB
 SFO1 75.4752953 MHz
 ===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 P2 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
 EM 0
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



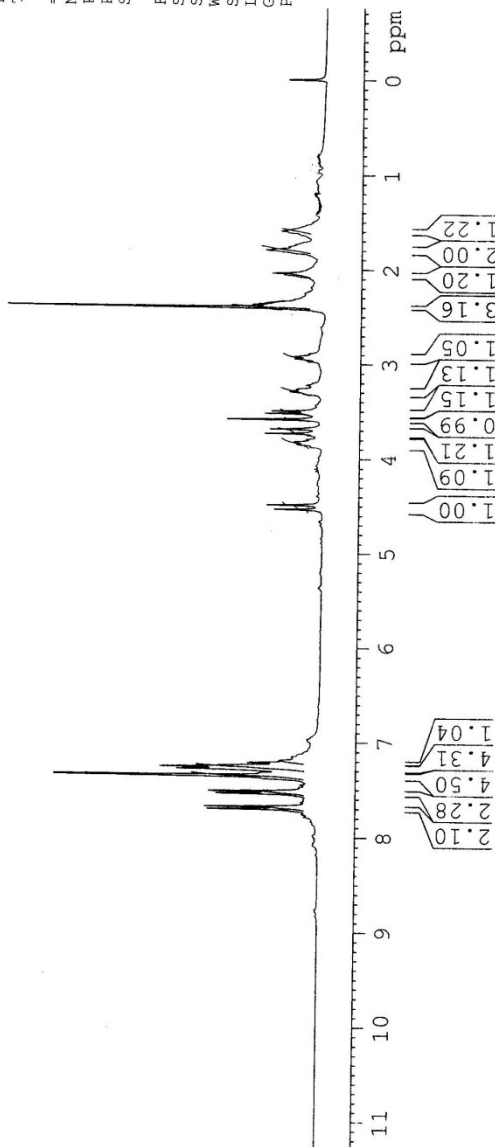
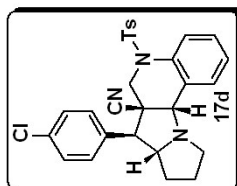
Current Data Parameters
 NAME DK-4-CL-CN-TS-PYZ
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20121226
 Time_ 19.24
 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
 TDO 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

7.705
7.678
7.540
7.515
7.355
7.350
7.328
7.320
7.285
7.260
7.245
7.217
4.534
4.487
3.850
3.821
3.796
3.734
3.687
3.587
3.523
3.498
3.315
3.292
3.269
3.223
2.973
2.942
2.920
2.889
2.402
2.057
2.042
1.798
1.760
1.737
1.726





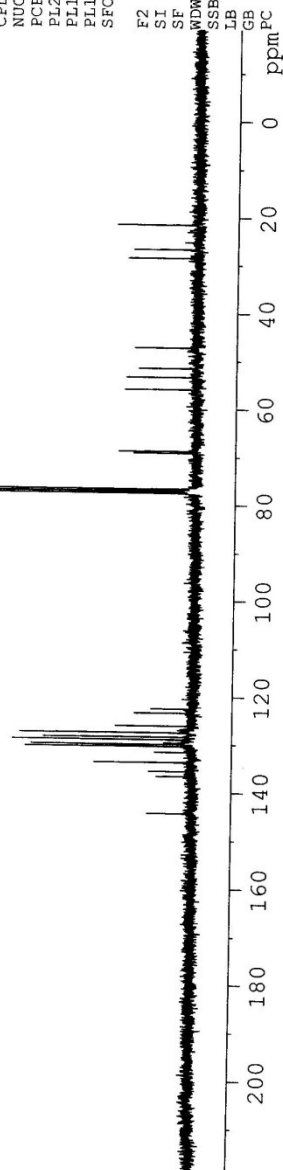
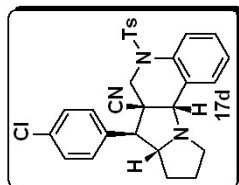
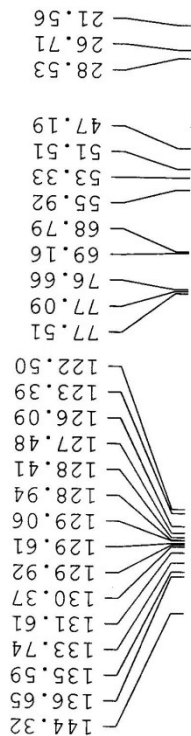
Current Data Parameters
 NAME DR-4-CL-CN-TS-FYZ
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20121226
 Time_ 19.29
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 143
 DS 4
 SWH 17985.611 Hz
 FIDRES 0.27439 Hz
 AQ 1.8219508 sec
 RG 512
 DW 27.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.0000000 sec
 d11 0.0300000 sec
 DELTA 1.8999998 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



gsk proline
iitm-Proton(-5to15)

7.700
7.679
7.541
7.538
7.521
7.519
7.381
7.376
7.360
7.346
7.340
7.330
7.324
7.278
7.273
7.267
7.258
7.248
7.236
7.233
7.217
7.214
4.518
4.482
3.843
3.818
3.724
3.689
3.590
3.516
3.497
3.298
3.292
2.945
2.929
2.402
2.383
2.366
1.835
1.808
1.793
1.782
1.609
1.595

Current Data Parameters
NAME gskrs41114
EXPNO 4
PROCNO 1

F2 - Acquisition Parameter
Date_ 20141120
Time 13.15

INSTRUM spect
PROBHD 5 mm PABBO
PULPROG zg30

TD 65536
SOLVENT CDCl3

NS 16
DS 2

SWH 8012.820 Hz
FIDRES 0.122266 Hz

AQ 4.0894966 sec
RG 95.73

DW 62.400 usec
DE 6.50 usec

TE 301.1 K
D1 0.50000000 sec

TD0 1
===== CHANNEL f1 =====

NUC1 1H
P1 15.70 usec

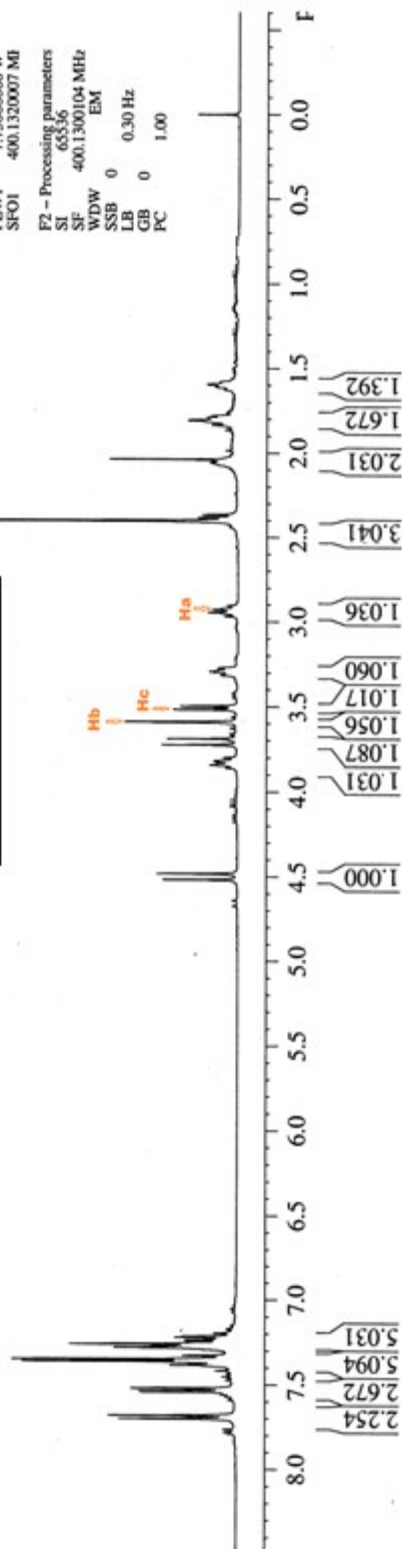
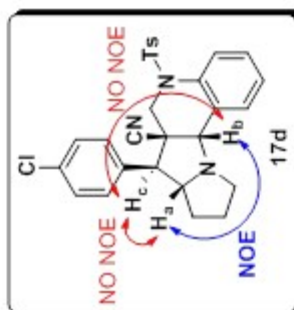
PLW1 7.7500000 W
SFO1 400.1320007 MHz

F2 - Processing parameters
SI 65536

SF 400.1300104 MHz
WDW EM

SSB 0 0.30 Hz
LB 0

GB 0 1.00
PC



Current Data Parameters
 NAME gskrs41114
 EXPNO 7
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20141120
 Time 13.32
 INSTRUM spect
 PROBDH 5 mm PABBO BB-
 PULPROG selnogr
 TD 65536
 SOLVENT CDCl3
 NS 32
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894966 Sec
 RG 31.3
 DE 62.400 usec
 DW 6.50 usec
 TE 301.1 K
 CNU21 2.9359000
 D1 2.00000000 sec
 D8 0.30000001 sec
 D16 0.00020000 sec
 D20 0.14880000 sec
 TD0 1
 ZGPTNS -DCALC_SPOFFS

===== CHANNEL f1 =====
 NUC1 ¹H
 P1 15.70 usec
 P2 31.40 usec
 PL12 80000.00 usec
 PLW0 0 W
 PLW1 7.75000000 W
 SFO1 400.131775 MHz
 SPNAM2 Gaus1_180r.1000
 SFOAL2 0.500
 SPOFFS2 -602.73 Hz
 SPW2 0.00000705 W

===== GRADIENT CHANNEL =====
 GPNAM1 SMSQ10.100
 GPNAM2 SMSQ10.100
 GF21 15.00 %
 GF22 40.00 %
 P16 1000.00 usec

F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

