Convenient Syntheses of *Benzo*-Fluorinated Dibenz[*b,f*]azepines: Rearrangements of Isatins, Acridines and Indoles

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Supporting Information

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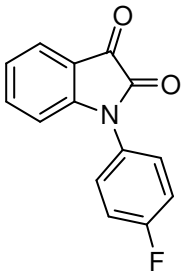
1. General Experimental

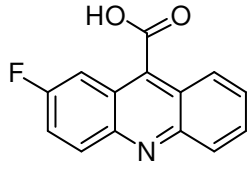
All reactions were carried out under an inert nitrogen or argon atmosphere unless otherwise stated. Reactions were monitored using thin layer chromatography (TLC) performed on Merck Silica gel 60 F_{254} plates. Fluorinated reagents were purchased from Fluorochem: all other reagents were purchased from SigmaAldrich and used as received. All reaction solvents were purchased from Fisher Scientific and used as received. ^{1}H, ^{13}C and ^{19}F NMR Spectra were obtained using a Bruker Avance instrument operating at 400, 100 and 376 MHz respectively. ^{1}H and ^{13}C NMR spectral data are reported in ppm (δ) relative to their residual solvent peaks. For ^{1}H NMR the chemical shifts are relative to 7.26 ($CDCl_3$) and 2.50 (DMSO-d_6); for ^{13}C NMR the chemical shifts are relative to 77.00 ($CDCl_3$) and 39.50 (DMSO-d_6).[1] Coupling constants (*J*) are reported in Hz. High resolution mass spectrometry for the N-aryl indoles and Iminostilbenes were performed by the National Mass Spectrometry Service based in Swansea; all other samples were obtained in electrospray mode (ES) with a micromass LCT mass spectrometer operating in the positive or negative ion mode as indicated. Elemental analyses for the N-aryl indoles and iminostilbenes were performed by Mr. Stephen Boyer of London Metropolitan University, all other analyses were performed by Mr. Steven Apter of the University of Liverpool. Infra red spectra were recorded on a Jasco FTIR ATR spectrometer. Melting points were recorded

using Bibby-Sterlin Stuart SMP3 melting point apparatus. Flash chromatography was performed on VWR silica gel (40-63 μm).

2. Experimental Procedures

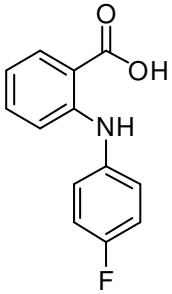


1-(4-Fluorophenyl)indoline-2,3-dione 10: Isatin (4 g, 27.19 mmol) and CuO (4.33 g, 54.37 mmol) were suspended in dimethylacetamide (DMA) (70 mL). 1-Bromo-4-fluorobenzene (4.19 mL, 38.06 mmol) was added dropwise over 1 h, then the reaction mixture was heated to 150 °C (±5 °C) for 24 h. The reaction was then filtered through Celite® 521 and the filtrate poured into an ice-water slurry (700 mL).ii then stirred for 30 min. The resulting red/brown precipitate was isolated by filtration, dried, redissolved in acetone and filtered for a second time through Celite® 521 to remove any insoluble material. The filtrate was concentrated and purified by column chromatography (dichloromethane) to afford the product as an orange crystalline solid (3.93 g, 60 %). ^{1}H NMR (400.13 MHz, DMSO-d_6) δ 7.65 (d, J = 7.4 Hz, 1 H), 7.61 (dt, J = 7.8, 1.3 Hz, 1 H), 7.57 - 7.51 (m, 2 H), 7.47 - 7.40 (m, 2 H), 7.19 (t, J = 7.5 Hz, 1 H) and 6.79 (d, J = 8.0 Hz, 1 H); ^{13}C NMR [100.62 MHz, DMSO d_6] δ 182.6, 161.4 (d, $^{1}J_{CF}$ = 245.4 Hz), 157.5, 151.2, 138.0, 129.6 (d, $^{4}J_{CF}$ = 3.0 Hz), 128.9 (d, $^{3}J_{CF}$= 9.0 Hz), 124.6, 123.6, 117.6, 116.6 (d, $^{2}J_{CF}$ = 22.8 Hz) and 110.6; ^{19}F NMR (376.46 MHz, DMSO-d_6) δ -112.82; *m/z* [CI, NH_3] 259; Found: m/z, 259.0878. $C_{14}H_{12}FN_2O_2$ (MNH_4^+) req. m/z, 259.0883; Found: C 69.66, H 3.31, N 5.78; $C_{14}H_8FNO_2$ req. C 69.71, H 3.34, N 5.81%; ν_{max} (cm^{-1}) [ground solid] 1736 (s), 1604 (s),1506 (m), 1460 (m), 1180 (m, C-F stretch), 835 (m) and 756 (m); m.p. = 236 °C.

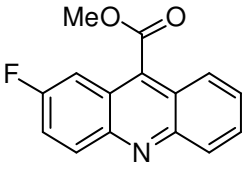


2-Fluoroacridine-9-carboxylic acid 11: 1-(4-Fluorophenyl)indoline-2,3-dione (3.044 g, 12.63 mmol) was dissolved in ethanol (100 mL) and 60 % $KOH_{(aq)}$ (25 mL) added cautiously to the mixture forming a clear, yellow solution. The reaction was then heated to gentle reflux overnight, during which time the mixture became dark yellow-brown. After 45 h the reaction was cooled to room temperature, concentrated and re-dissolved in water (400 mL). The alkaline solution (~ pH 14) was washed with ether (3 × 100 mL). The aqueous phase was then acidified with 2 M HCl to pH 1-2 and the resulting precipitate isolated by filtration, washed with ether and dried. Product that remained in the acidified aqueous phase was extracted with a 1:1 mixture of EtOAc/THF (3 × 100 mL). The combined organic extracts were dried (sodium sulphate), filtered and evaporated. The desired acridine-9-carboxylic acid was obtained as a yellow solid (2.50 g, 82 %); ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.37 (dd, J = 5.6, 9.6 Hz, 1 H), 8.29 - 8.25 (m, 1 H), 8.16 (d, J = 8.4 Hz, 1 H), 8.00 - 7.91 (m, 2 H) and 7.83 - 7.77 (m, 2 H); ^{13}C NMR (100.13 MHz, DMSO-d_6) δ 167.7, 159.9 (d, $^{1}J_{CF}$ = 249.6 Hz), 147.2, 145.1, 132.3 (d, $^{3}J_{CF}$ = 9.1 Hz), 131.2, 129.0, 128.2, 125.1, 122.9 (d, $^{2}J_{CF}$ = 28.3 Hz), 121.4 and 107.5 (d, $^{2}J_{CF}$ =23.2 Hz); ^{19}F

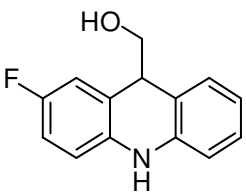
NMR (376.56 MHz, DMSO-d_6) δ = -110.15; *m/z* [ES^-]: $[M-H]^+$ 240, $[2M-H]^-$ 481; Found: m/z, 240.0461; $C_{14}H_7FNO_2$ $[M-H]^+$ req. *m/z*, 240.0421; ν_{max} (cm^{-1}) (ground solid) 3367 (m), 1188 (s), 825, 758; m.p. 254 °C.



2-[(4-Fluorophenyl)amino]benzoic acid 12: Isolated as a by-product from the preceding reaction: dark orange solid; ^{1}H NMR (400MHz, DMSO-d_6) δ 13.01 (br s, 1 H), 9.54 (br s, 1 H), 7.91 (dd, *J* = 1.5, 8.0 Hz, 1 H), 7.37 (ddd, *J* = 1.6, 7.1, 8.5 Hz, 1 H), 7.32 - 7.24 (m, 2 H), 7.23 - 7.14 (m, 2 H), 7.07 (d, *J* = 8.4 Hz, 1 H), 6.79 - 6.74 (m, 1 H); ^{13}C NMR (100.13 MHz, DMSO-d_6) δ 169.9, 158.4 (d, $^1J_{CF}$ = 240.1 Hz), 147.6, 136.7 (d, $^4J_{CF}$ = 2.4 Hz), 134.2, 131.8, 124.2 (d, $^3J_{CF}$ = 8.0 Hz), 117.1, 116.0 (d, $^2J_{CF}$ = 22.4 Hz), 133.2, 112.2; ^{19}F NMR (376.56 MHz, DMSO-d_6) δ -199.29; *m/z* [CI+NH_3] 232; Found: m/z, 232.0777; $C_{13}H_{11}FNO_2$ $[M+H]^+$ req. m/z, 232.0774; m.p. 148-150 °C



2-Fluoroacridine-9-carboxylic acid methyl ester 13: Using standard Schlenk techniques, 2-fluoroacridine-9-carboxylic acid (2.30 g, 9.45 mmol) was dissolved in freshly distilled thionyl chloride (70 mL). The solution was then heated to 80 °C, and stirred under an inert atmosphere for 14 hours. The thionyl chloride was removed *in vacuo* and the residue dissolved in methanol and left to stir for 2 h at room temperature in an inert atmosphere, then the methanol was removed: the residue was dissolved in CH_2Cl_2 and washed with saturated aq. $NaHCO_3$, water and brine. The organic extract was dried over sodium sulphate, filtered and evaporated. The crude methyl ester was isolated pure after column chromatography in ether/hexane (1:2) as a beige solid (1.69 g, 70 %); ^{1}H NMR (400MHz, DMSO-d_6) δ 8.27 (dd, 1 H, *J* = 9.4, 5.5 Hz), 8.25 (d, 1 H, *J* = 8.8 Hz), 8.03 (d, 1 H, *J* = 8.7 Hz), 7.80 (ddd, 1 H, *J* = 8.7, 6.7, 1.4 Hz) and 7.66-7.60 (m, 3H), 4.21 (s, 3H); ^{13}C NMR (100.13 MHz, DMSO-d_6) δ 167.5, 160.5 (d $^1J_{CF}$ = 251.5 Hz), 148.1 (d, $^4J_{CF}$ = 2.23 Hz), 146.1, 135.8 (d, J_{CF} = 7.9 Hz), 132.8 (d, *J* = 9.4 Hz), 130.1 (d, *J* = 12.6 Hz), 127.8, 124.8, 122.8 (d, *J* = 10.4 Hz), 122.7, 122.3, 122.0, 107.4 (d, *J* = 23.8 Hz) and 53.1; ^{19}F NMR (376.56 MHz, DMSO-d_6) δ -109.99; *m/z* [CI + NH_3] 256, 198; Found: m/z, 256.0777; $C_{15}H_{11}FNO_2$ (MH^+) req. m/z, 256.0774; Found: C, 70.44 ; H, 4.01; N, 5.44; $C_{15}H_{10}FNO_2$ req. C 70.58; H, 3.95; N, 5.49 %; ν_{max} (cm^{-1}) [ground solid] 1720 (s), 1462 (m), 1215 (s), 1171 (s), 827 (m), 760 (m); m.p. 147 °C.



(2-Fluoro-9,10-dihydroacridin-9-yl)methanol 14: 2-Fluoroacridine-9-carboxylic acid methyl ester (1.05 g, 4.12 mmol) was dissolved in anhydrous

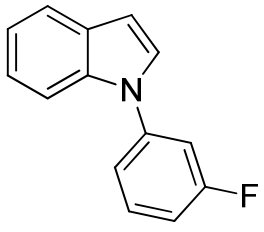
THF (60 mL) to which $LiAlH_4$ (1 M in THF, 5.15 mL) was added dropwise under an inert atmosphere. The reaction was then slowly heated to 80 °C and maintained at that temperature for 3 h. The reaction was then quenched by addition of H_2O (0.4 mL) followed by 15% aq. NaOH (0.4 mL) and further H_2O (1.2 mL). The resulting precipitate was filtered off, then the filtrate was diluted with EtOAc, washed with water and sat. aq. $NaHCO_3$ followed by drying over sodium sulphate, filtration and evaporation to yield the crude product. Purification by column chromatography (ethyl acetate/hexane, 1:4) yielded the alcohol as a pale, rather air-sensitive yellow solid (0.89 g, 92 %); ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.18 (dq, *J* = 7.5, 1.1 Hz, 2 H), 6.97 - 6.92 (m, 2 H), 6.88 (dt, *J* = 8.4, 2.8 Hz, 1 H), 6.75 (dd, *J* = 7.9, 1.0 Hz, 1 H), 6.68 (dd, *J* = 8.6, 4.6 Hz, 1 H), 6.08 (br s, 1 H), 4.07 (t, *J* = 6.7 Hz, 1 H) and 3.62 (d, *J* = 6.6 Hz, 2 H); ^{13}C NMR (100.13 MHz, DMSO-d_6) δ 157.7 (d, $^1J_{CF}$ = 238.4 Hz), 139.8, 136.01 (d, $^4J_{CF}$ = 1.8 Hz), 129.1, 127.9, 121.86 (d, $^3J_{CF}$ = 6.9 Hz), 120.97, 119.34, 115.5 (d, $^2J_{CF}$ = 22.4 Hz), 114.3 (d, $^2J_{CF}$ = 22.9 Hz), 114.2 (d, $^3J_{CF}$ = 7.8 Hz), 113.7, 67.4 and 45.5; ^{19}F NMR (376.56 MHz, DMSO-d_6) δ -123.84; *m/z* (CI) $[M+H]^+$ 230, 212, 198; Found: m/z, 230.0981; $C_{14}H_{13}FNO$ $[MH^+]$ req. m/z, 230.0981; ν_{max} (cm^{-1}) [ground solid] 3291 (m), 1485 (s), 1313 (m), 1227 (m), 814 (m), 748 (m); m.p. 130 °C.

Characterisation of compound **15** is given below.

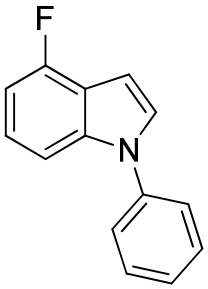
General experimental procedure for the synthesis of *N*-aryl Indoles.

N-Aryl indoles were prepared with modification of the procedure reported by Ma *et al*[2] as follows:

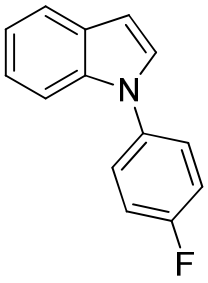
The appropriate indole (2.2 mmol), K_2CO_3 (5.0 mmol), CuI (0.1 mmol) and L-proline (0.2 mmol) were dissolved in DMSO (4 mL). The mixture was heated gently to 100 °C (± 5 °C) under an inert atmosphere for 10 min, then iodobenzene (2.0 mmol) was added dropwise over 20 min and the reaction left to stir for 24 h. Upon completion the cooled solution was partitioned between EtOAc and H_2O and the aqueous layer extracted with EtOAc (×2); the combined organic phases were washed with brine and dried over Na_2SO_4, filtered and concentrated. The crude material was subsequently purified by column chromatography to give the pure product.



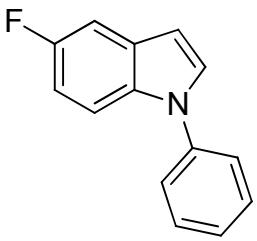
1-(3-Fluorophenyl)-1*H*-indole (NAI-3´-F): Pale yellow oil, 78 %; (400 MHz, $CDCl_3$) δ 7.69-7.67 (m, 1H, H), 7.59-7.57 (m, 1H), 7.42 (dt, *J*=8.2, 6.2 Hz, 1H), 7.31 (d, *J*=3.3 Hz, 1H), 7.30-7.15 (m, 4H), 7.03 (tdd, *J* = 8.3, 2.5, 0.9 Hz, 1H) and 6.69 (d, *J*= 3.3, 0.8Hz, 1H); ^{13}C NMR [100.62 MHz, $CDCl_3$] δ 163.5 (d, $^1J_{CF}$ = 247.5 Hz), 141.6 (d, $^3J_{CF}$ = 10.0 Hz), 135.9, 131.2 (d, *J* = 9.3 Hz), 129.8, 127.9, 123.0, 121.6, 121.0, 120.0 (d, $^4J_{CF}$=3.1 Hz), 113.5 (d, 2*J*CF = 21.1 Hz), 111.8 (d, $^2J_{CF}$ = 23.8 Hz), 110.7 and 104.6; ^{19}F NMR [376.46 MHz, $CDCl_3$] δ -111.23 (s); Found: C, 79.69; H, 4.81; N, 6.52; $C_{14}H_{10}FN$ req. C, 79.60; H, 4.77; N, 6.63 %; Found: m/z, 212.0872; $C_{14}H_{11}FN$ $[M + H]^+$ req. m/z, 212.0870; ν_{max} (cm^{-1}, neat) 1546.63 (s), 1461.78 (m) and 1203.36 (m).



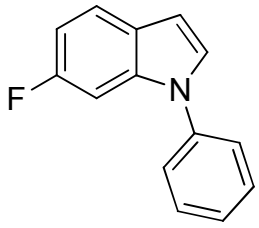
4-Fluoro-1-phenyl-1*H*-indole (NAI-4-F): Pale yellow oil, 70 %; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.4 - 7.5 (m, 4 H), 7.3 - 7.4 (m, 1 H), 7.3 (dd, *J*=8.3, 0.4 Hz, 1 H), 7.3 (d, *J*=3.3 Hz, 1 H), 7.1 (dt, *J*=8.1, 5.2 Hz, 1 H), 6.8 (ddd, *J*=10.2, 7.9, 0.5 Hz, 1 H) and 6.8 (dd, *J*=3.3, 0.8 Hz, 1 H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.4 (d, *J*=248.8 Hz), 139.4 (s), 138.4 (d, *J*=11.1 Hz), 129.6 (s), 127.9 (s), 126.8 (s), 124.4 (s), 122.8 (d, *J*=7.7 Hz), 118.3 (d, *J*=24.5 Hz), 106.6 (d, *J*=3.5 Hz), 105.2 (s), 105.0 (s), 99.5 (s) and 99.4 (s); ^{19}F NMR (376 MHz, $CDCl_3$) δ -122.2 (s); Found: C, 79.73; H, 4.91; N, 6.14; $C_{14}H_{10}FN$ req. C, 79.60; H, 4.77; N, 6.63 %.



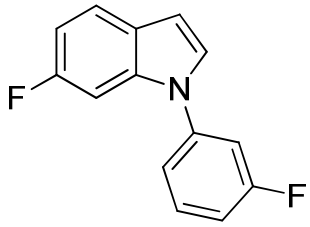
1-(4-Fluorophenyl)-1*H*-indole (NAI-4´-F) 18: Colourless oil, 81 %**;** ^{1}H NMR [400.13 MHz, $CDCl_3$] δ 7.67-7.65 (m, 1H), 7.44-7.42 (m, 1H) 7.40-7.35 (m, 2H), 7.21-7.10 (m, 5H) and 6.64 (dd, *J* =3.3, 0.7 Hz, 1H); ^{13}C NMR [100.62 MHz, $CDCl_3$] δ 161.3 (d, $^{1}J_{CF}$ = 246.2 Hz, $C^{4'}$), 136.4 (s), 136.2 (d, $^{4}J_{CF}$ = 3.0 Hz, $C^{1'}$), 129.5 (s), 128.3 (s, C^{2}), 126.4 (d, $^{3}J_{CF}$ = 8.4 Hz, $C^{2',6'}$), 122.8 (s), 121.5 (s), 120.7 (s), 116.7 (d, $^{2}J_{CF}$ = 22.7 Hz, $C^{3',5'}$), 110.5 (s) and 103.9 (s); ^{19}F NMR [376.46 MHz, $CDCl_3$] δ -115.59 (s); Found: C, 79.73; H, 4.91; N, 6.14; $C_{14}H_{10}FN$ req. C, 79.60; H, 4.77; N, 6.63 %; Found: m/z, 212.0873; $C_{14}H_{11}FN$ [MH^+] req. m/z, 212.0870.



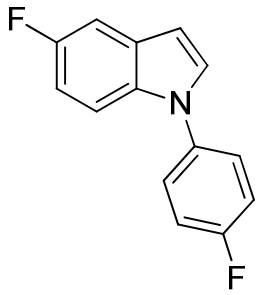
5-Fluoro-1-phenyl-1*H*-indole (NAI-5-F): Pale yellow oil, 76 %; ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.54- 7.43 (m, 5 H), 7.38 - 7.30 (m, 3 H), 6.95 (dt, *J* = 2.5, 9.1 Hz, 1 H) and 6.63 (dd, *J* = 0.6, 3.2 Hz, 1 H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.1 (d, $^{1}J_{CF}$ =234.6 Hz), 139.6, 132.5, 129.7, 129.6 (d, $^{3}J_{CF}$ =13.8 Hz), 129.4, 126.7, 124.3, 111.2 (d, $^{3}J_{CF}$ =9.6 Hz), 110.6 (d, $^{2}J_{CF}$ =26.1 Hz), 105.8 (d, $^{2}J_{CF}$ =23.4 Hz) and 103.4 (d, $^{4}J_{CF}$ = 4.6 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -122.40; Found: C, 79.70; H, 4.82; N, 6.72; $C_{14}H_{10}FN$ req. C, 79.60; H, 4.77; N, 6.63 %; Found: m/z, 212.0868; $C_{14}H_{11}FN$ [MH^+] req. m/z, 212.0870.



6-Fluoro-1-phenyl-1*H*-indole (NAI-6-F): Pale yellow oil, 83 %; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (dd, *J* = 5.4, 8.7 Hz, 1 H), 7.55 - 7.45 (m, 4 H), 7.37 (t, *J* = 7.4 Hz, 1 H), 7.31 (d, *J* = 3.3 Hz, 1 H), 7.25 - 7.21 (m, 1 H), 6.93 (dt, *J* = 2.3, 9.0 Hz, 1 H) and 6.65 (d, *J* = 3.3 Hz, 1 H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.2 (d, $^{1}J_{CF}$ =236.5 Hz), 139.4, 135.8 (d, $^{3}J_{CF}$ =12.3 Hz), 129.7, 128.4 (d, $^{4}J_{CF}$ =3.8 Hz), 126.7, 125.6, 124.2, 121.8 (d, $^{3}J_{CF}$ =10.0 Hz), 109.1 (d, $^{2}J_{CF}$ =24.9 Hz), 103.6 and 97.0 (d, $^{2}J_{CF}$ =26.5 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -120.65; Found: C, 79.48; H, 4.85; N, 6.7; $C_{14}H_{10}FN$ req. C, 79.60; H, 4.77; N, 6.63 %; Found: m/z, 212.0869; $C_{14}H_{11}FN$ [MH^+] req. m/z, 212.0870.



6-Fluoro-1-(3-fluorophenyl)-1*H*-indole (NAI-3´,6-F): Pale yellow oil, 75 %; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (dd, *J* = 5.4, 8.7 Hz, 1 H), 7.45 (dt, *J* = 6.3, 8.2 Hz, 1 H), 7.29 - 7.20 (m, 3 H), 7.17 (td, *J* = 2.3, 9.7 Hz, 1 H), 7.05 (ddt, *J* = 0.9, 2.5, 8.3 Hz, 1 H), 6.94 (ddd, *J* = 2.3, 8.8, 9.3 Hz, 1 H) and 6.64 (dd, *J* = 0.8, 3.3 Hz, 1 H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.2 (d, $^{1}J_{CF}$ =248.1 Hz), 160.3 (d, $^{1}J_{CF}$ =238.5 Hz), 140.9 (d, $^{3}J_{CF}$ =10.0 Hz), 135.6 (d, $^{3}J_{CF}$ =12.3 Hz), 131.0 (d, $^{3}J_{CF}$ =9.2 Hz), 128.0 (d, $^{4}J_{CF}$ =3.5 Hz), 125.8 (s), 122.0 (d, $^{3}J_{CF}$ =10.0 Hz), 119.5 (d, $^{4}J_{CF}$ =3.1 Hz), 113.5 (d, $^{2}J_{CF}$ =21.1 Hz), 111.3 (d, $^{2}J_{CF}$ =23.8 Hz), 109.4 (d, $^{2}J_{CF}$ =24.5 Hz), 104.3 (s) and 97.0 (d, $^{2}J_{CF}$ =27.2 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -110.8, -119.9; Found: C, 73.37; H, 4.03; N, 5.94 ; $C_{14}H_9F_2N$ req. C, 73.36; H, 3.96; N, 6.11 %; Found: m/z, 230.0772; $C_{14}H_{10}F_2N$ [MH^+] req. m/z, 230.0776.

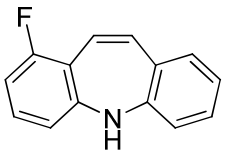


5-Fluoro-1-(4-fluorophenyl)-1*H*-indole (NAI-4´,5-F) 19: Pale yellow oil, 85% ; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38- 7.43 (m, 2H), 7.27 - 7.36 (m, 3H), 7.15 - 7.22 (m, 2H), 6.94 (td, *J*=9.1, 2.6 Hz, 1H), 6.61 (dd, *J*=3.2 and 0.7 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.9 (d, $^{1}J_{CF}$ =247.7 Hz), 157.7 (d, $^{1}J_{CF}$ =235.4 Hz), 135.6 (d, $^{4}J_{CF}$ =2.7 Hz), 132.7, 129.5, 129.4, 126.1 (d, $^{3}J_{CF}$ =8.4 Hz), 116.5 (d, $^{2}J_{CF}$ =23.4 Hz), 110.9 (d, $^{4}J_{CF}$ =6.5 Hz), 110.7 (d, $^{2}J_{CF}$ =23.0 Hz), 105.9 (d, $^{2}J_{CF}$ =23.4 Hz) and 103.4 (d, $^{4}J_{CF}$ =4.6 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -115.3, -124.5; $C_{14}H_9F_2N$ req. C, 73.36; H, 3.96; N 6.11 %; Found: m/z, 230.0777; $C_{14}H_{10}F_2N$ [MH^+] req. m/z, 230.0776.

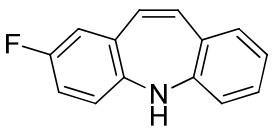
General experimental procedures for the synthesis of iminostilbenes.[3, 4]

Method A: (*For the acridinemethanol route only*): A suspension of P_2O_5 (0.9 g, 6.34 mmol) in xylene (30 mL) was placed under an inert atmosphere and heated to 150 °C with stirring. (2-fluoro-9,10-dihydro-acridin-9-yl) methanol **14** (0.205 g, 0.895 mmol) was dissolved in xylene (50 mL) and added to the reaction over 2 h via a pressure equalizing dropping funnel. After addition was complete, the reaction mixture was stirred for a further 15 min, cooled to room temperature, poured into an ice/water slurry (300 mL) and vigorously stirred for 10 min. The reaction mixture was then extracted with ethyl acetate (2 × 60 mL) and the combined organic extracts washed with water, saturated aqueous $NaHCO_3$ and brine. The crude extract was then purified by column chromatography with 1:9 EtOAc/hexane to deliver **15** (0.11g, 58%).

Method B (For the N-aryl indoles): Polyphosphoric acid (1 mL per 100 mg aryl indole) was purged with argon and heated to 100 °C for 30 min. The N-aryl indole was then added to the gently stirring reaction mixture via a syringe and the reaction mixture left to stir at 110 °C (± 5 °C) for 36 to 72 h, with monitoring of reaction progress by partition TLC. Once judged to have reached completion the reaction mixture was allowed to cool slowly to 35 °C, poured cautiously into an ice-cold, saturated, aqueous $NaHCO_3$ solution and vigorously stirred for 1 h. The crude product was extracted with dichloromethane (2×100 mL) then the combined organic phases were washed with water, $NaHCO_3$ and brine. After concentration *in vacuo*, the combined crude material was purified by column chromatography using EtOAc/hexane 1:9.

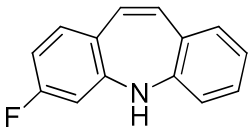


1-Fluoro-5*H*-dibenz[*b,f*]azepine 22: Prepared by method B using 4-fluoro-1-phenyl-1*H*-indole (1.012 g, 4.77 mmol) and hot polyphosphoric acid (10.152 g, 5.06 mL). The product was isolated as orange/yellow solid (0.245 g, 24 %); when starting from 1-(3-fluorophenyl)-1*H*-indole (1.219 g, 5.59 mmol), the product was formed as a mixture with 3-fluoro-5*H*-dibenz[*b,f*]azepine and was separated by gradient elution with hexane → 1:4 EtOAc/hexane (0.223 g, 18 %); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.03 - 7.10 (m, 1 H), 6.98 (td, *J*=8.1, 6.1 Hz, 1 H), 6.84 - 6.93 (m, 2 H), 6.48 - 6.60 (m, 3 H), 6.43 (d, *J*=1.0 Hz, 1 H), 6.31 (d, *J*=7.4 Hz, 1 H) and 5.03 (br s, 1 H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.7 (d, $^1J_{CF}$ =248.4 Hz), 151.0 (d, $^3J_{CF}$ =5.4 Hz), 148.0 (s), 133.1 (d, $^4J_{CF}$=1.5 Hz), 130.6 (s), 130.1 (d, $^3J_{CF}$=10.7 Hz), 129.8 (s), 129.6 (s), 123.7 (d, $^3J_{CF}$=8.4 Hz), 123.4 (s), 119.6 (s), 118.0 (d, $^2J_{CF}$=14.6 Hz), 114.8 (d, $^4J_{CF}$=2.7 Hz) and 109.7 (d, $^2J_{CF}$=23.0 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -116.99; Found: m/z, 211.0807; $C_{14}H_{10}FN$ [M^+] requires m/z, 211.0797; m/z 212 [MH^+]. Combined yield with **23**, 42%.

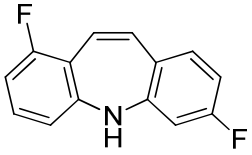


2-Fluoro-5*H*-dibenz[*b,f*]azepine 15: Prepared by method A, orange solid (v. s.; 0.110 g, 58 %) and method B, by two independent routes, also isolated as an orange solid. From1-(4-fluorophenyl)-1*H*-indole (2.018 g, 9.56 mmol) was obtained after purification **15** (0.810 g, 40.1 %); from 5-fluoro-1-phenyl-1*H*-indole (1.144 g, 5.42

mmol) was obtained after purification **15** (0.534 g, 47 %); ^{1}H NMR (400 MHz ,$CDCl_3$) δ 7.08 (dt, *J* = 1.9, 7.4 Hz, 1 H), 6.95 - 6.86 (m, 2 H), 6.76 (dt, *J* = 2.8, 8.3 Hz, 1 H), 6.62 (dd, *J* = 2.9, 9.2 Hz, 1 H), 6.55 (dd, *J* = 0.4, 7.8 Hz, 1 H), 6.49 (dd, *J* = 4.8, 8.6 Hz, 1 H), 6.44 (d, A of AB *J* = 11.8 Hz, 1 H), 6.30 (d, B of AB, *J* = 11.8 Hz, 1H) and 4.94 (br s, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ = 240.2 (d, $^{1}J_{CF}$ = 240.2 Hz), 148.8, 144.5 (d, $^{4}J_{CF}$ = 2.3 Hz), 133.8, 131.9 (d, $^{3}J_{CF}$=7.6), 131.2 (d, $^{4}J_{CF}$ = 1.7), 130.9, 130.1, 129.9, 123.6, 120.6 (d, $^{3}J_{CF}$= 8.2 Hz), 119.7, 116.7 (d, $^{2}J_{CF}$= 22.8 Hz) and 115.8 (d, $^{2}J_{CF}$ = 22.5 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ = -122.78; Found: C, 79.73; H, 4.81; N, 6.60; $C_{14}H_{10}FN$ requires C, 79.60; H 4.77; N, 6.63 %; Found: m/z, 212.0879; $C_{14}H_{11}FN$ $[M+H]^+$ requires m/z, 212.0876.

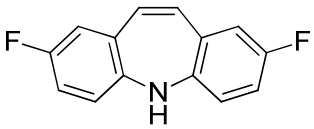


3-Fluoro-5*H*-dibenz[*b*,*f*]azepine 23: Prepared by method B: 6-fluoro-1-phenyl-1*H*-indole (1.311 g, 6.01 mmol) yielded the product as an orange oil (0.624 g, 48 %). 1-(3-Fluorophenyl)-1*H*-indole (1.219 g, 5.59 mmol) yielded the product as a mixture with 1-fluoro-5*H*-dibenz[*b*,*f*]azepine and **23** was separated by gradient elution with hexane → 1:4 EtOAc/hexane, 0.271 g (22 %); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.00 (ddt, *J*=11.4, 7.9, 4.5, Hz, 1 H), 6.80 (d, *J*=4.2 Hz, 2 H), 6.80 (dd, *J*=8.4, 6.5 Hz, 1 H), 6.50 (td, *J*=8.3, 2.4 Hz, 1 H), 6.50 (d, *J*=7.8 Hz, 1 H), 6.20 (s, 2 H), 6.20 (dd, *J*=9.7, 2.5 Hz, 1 H) and 4.9 (br s, 1 H);^{13}C NMR (101 MHz, $CDCl_3$) δ 163.9 (d, $^{1}J_{CF}$ = 247.7 Hz), 150.0 (d, $^{3}J_{CF}$ = 9.2 Hz), 147.3 (s), 131.8 (d, $^{3}J_{CF}$ = 9.6 Hz), 131.2 (s), 131.1 (s), 130.5 (s), 129.6 (s), 129.5 (s), 125.8 (d, $^{4}J_{CF}$ = 3.5 Hz), 123.4 (s), 119.3 (s), 109.3 (d, $^{2}J_{CF}$=21.1 Hz) and 106.5 (d, $^{2}J_{CF}$ = 24.5 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ ppm -114.32; Found: m/z, 211.0793; $C_{14}H_{10}FN$ $[M^+]$ requires m/z, 211.0797; m/z 212 $[MH^+]$. The combined yield with **22**, when starting from 1-(3-fluorophenyl)-1*H*-indole, was 40%.

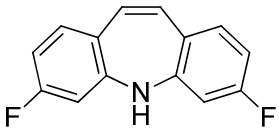


1,7-Difluoro-5*H*-dibenz[*b*,*f*]azepine 25: 6-fluoro-1-(3-fluorophenyl)-1*H*-indole (1.008 g, 4.4 mmol) yielded the product as a mixture with 3,7-difluoro-5*H*-dibenz[*b*,*f*]azepine **24** and yielded, after isolation by column chromatography, **25** (0.166 g, 16 %) together with **24** (35%, v. i.);^{1}H NMR (400 MHz, $CDCl_3$) δ 6.98 (td, *J*=8.1, 6.1 Hz, 1 H) 6.82 (dd, *J*=8.4, 6.4 Hz, 1 H) 6.52 - 6.62 (m, 2 H) 6.48 (d, *J*=1.0 Hz, 1 H) 6.34 (d, *J*=1.0 Hz, 1 H) 6.21 - 6.29 (m, 2 H) and 5.01 (br s, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ164.0 (d, $^{1}J_{CF}$ = 248.7 Hz), 160.60 (d, $^{1}J_{CF}$ = 248.4), 149.9 (d, $^{4}J_{CF}$ = 5.2 Hz), 149.6 (d, $^{3}J_{CF}$ = 9.1 Hz), 132.11 (s), 131.9 (d, $^{3}J_{CF}$ = 9.7 Hz), 130.2 (d, $^{3}J_{CF}$ = 10.8 Hz), 125.8 (d, $^{4}J_{CF}$ = 3.3 Hz), 122.8 (d, $^{3}J_{CF}$ = 8.2 Hz), 122.8 (d, $^{3}J_{CF}$ = 8.8 Hz), 118.0 (d, $^{2}J_{CF}$ = 14.7 Hz), 114.8 (d, $^{4}J_{CF}$ = 2.8 Hz), 110.1 (d, $^{2}J_{CF}$ = 23.1 Hz), 109.9 (d, $^{2}J_{CF}$ = 21.2 Hz) and 106.9 (d, $^{2}J_{CF}$ = 24.0 Hz); ^{19}F NMR

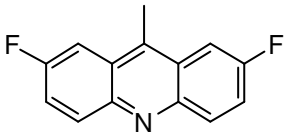
(376 MHz, $CDCl_3$) δ ppm -113.87, -116.84; Found: C, 73.25; H, 3.9; N, 6.0; $C_{14}H_9F_2N$ requires C, 73.40; H, 3.9; N, 6.1%; Found: m/z, 229.0709; $C_{14}H_9F_2N$ $[M^+]$ requires m/z, 229.0703.



2,8-Difluoro-5*H*-dibenz[*b*,*f*]azepine 20: 5-fluoro-1-(4-fluorophenyl)-1*H*-indole (1.214 g, 5.34 mmol) yielded the product as an orange solid after purification (0.797 g, 66 %); ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.77 (ddd, *J* = 8.5, 8.0, 2.9 Hz, 2 H), 6.63 (dd, *J* = 9.1, 2.9 Hz, 2 H), 6.49 (dd, *J* = 8.6, 4.8 Hz, 2 H), 6.38 (s, 2 H) and 4.86 (br s, 1 H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 159.2 (d, $^1J_{CF}$ = 240.8 Hz), 144.2 (d, $^4J_{CF}$ = 2.4 Hz) 132.1 (d, $^4J_{CF}$ = 1.9 Hz), 131.2 (d, $^3J_{CF}$ = 7.7 Hz), 120.3 (d, $^2J_{CF}$ = 8.1 Hz), 116.4 (d, $^2J_{CF}$ = 22.9 Hz) and 115.8 (d, $^2J_{CF}$ = 22.5 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -122.31; Found: C, 73.25; H, 3.9; N, 6.0; $C_{14}H_9F_2N$ requires C, 73.40; H, 3.9; N, 6.1%; Found: m/z, 230.0779; $C_{14}H_{10}F_2N$ $[M+H]^+$ requires m/z, 230.0781.



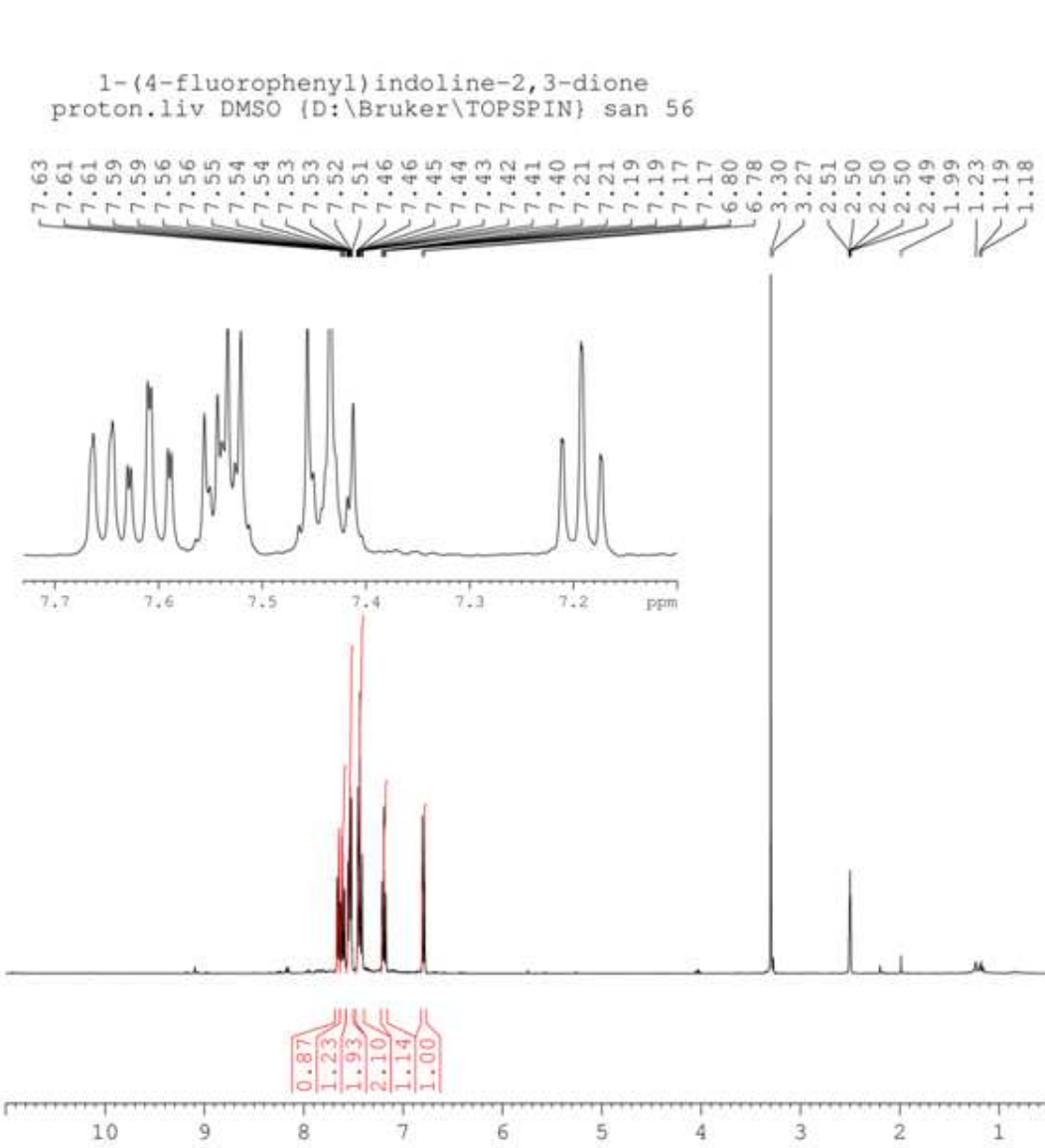
3,7-Difluoro-5*H*-dibenz[*b*,*f*]azepine 24: 6-fluoro-1-(3-fluorophenyl)-1*H*-indole (1.008 g, 4.4 mmol) yielded the product as a mixture with 1,7-difluoro-5*H*-dibenz[*b*,*f*]azepine **25**; after isolation by column chromatography there was obtained **24** (0.351 g (35 %); ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.77 (dd, *J*=8.4, 6.4 Hz, 2 H), 6.53 (dd, *J*=18.9, 2.5 Hz, 2 H), 6.21 (dd, *J*=9.7, 2.5 Hz, 2 H), 6.16 (s, 2 H) and 4.89 (br s, 1 H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.9 (d, $^1J_{CF}$ = 248.1 Hz), 152.2 (d, $^4J_{CF}$ = 3.0 Hz), 149.0 (d, $^3J_{CF}$ = 10.0 Hz), 131.8 (d, $^3J_{CF}$ = 9.6 Hz), 130.2 (s), 109.7 (d, $^2J_{CF}$ = 21.1 Hz) and 106.7 (d, $^2J_{CF}$ = 24.2 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ = -114.06; Found: C, 73.30; H, 3.8; N, 5.95; $C_{14}H_9F_2N$ requires C, 73.40; H, 3.9; N, 6.1%; combined yield with **25**, 51%.

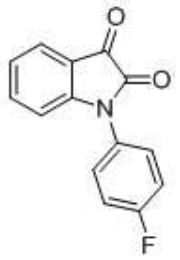


2,7-Difluoro-9-methylacridine 21: Isolated as a by-product from the preparation of **20**; yield variable, see text; ^{1}H NMR (400 MHz , $CDCl_3$) δ = 8.21 (dd, *J* = 5.7, 9.7 Hz, 2 H), 7.76 (dd, *J* = 2.8, 10.6 Hz, 2 H), 7.56 (ddd, *J* = 9.6, 7.3, 2.7 Hz, 2 H) and 2.98 (s, 3 H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 160.1 (d, $^1J_{CF}$ = 257.6 Hz), 145.4 (s), 140.5 (s), 133.2 (d, $^3J_{CF}$ = 8.4 Hz), 125.9 (d, $^3J_{CF}$ =10.0 Hz), 121.3 (d, $^2J_{CF}$ = 28.4 Hz), 106.5 (d, $^2J_{CF}$ = 23.0 Hz) and 14.1 (s); ^{19}F NMR (376 MHz, $CDCl_3$) δ = -111.72; Found: m/z, 230.0777; $C_{14}H_{10}F_2N$ $[M+H]^+$ requires m/z, 230.0781.

3. NMR Spectroscopic Data.

1-(4-fluorophenyl)indoline-2,3-dione
proton.liv DMSO {D:\Bruker\TOPSPIN} san 56





10

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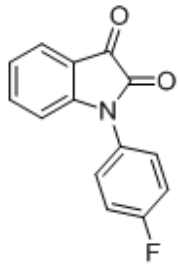
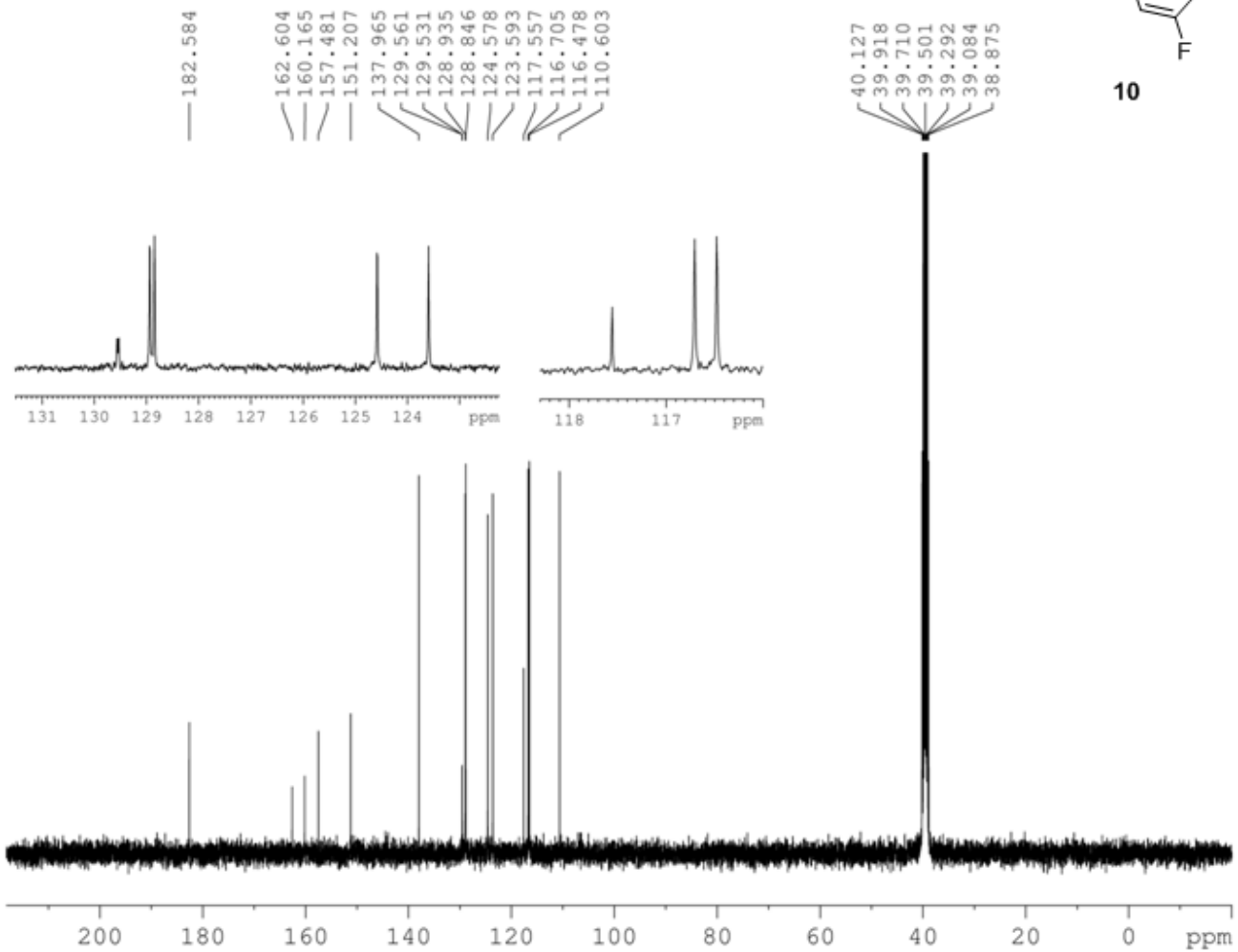
INSTRUM	spect	
PROBHD	5 mm QNP 1H/13	
PULPROG	zg	
TD	32768	
SOLVENT	DMSO	
NS	16	
DS	2	
SWH	6218.905	Hz
FIDRES	0.189786	Hz
AQ	2.6345973	sec
RG	114	
DW	80.400	usec
DE	6.00	usec
TE	303.2	K
D1	1.00000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	1H	
P1	10.40	usec
PL1	-3.00	dB
SFO1	400.1325018	MHz
SI	32768	
SF	400.1300026	MHz
WDW	EM	
SSB	0	
LB	0.10	Hz
GB	0	
PC	1.00	

1-(4-fluorophenyl)indoline-2,3-dione
carbon.liv DMSO {D:\Bruker\TOPSPIN} san 56



10



NAME	ISA-4'-F	
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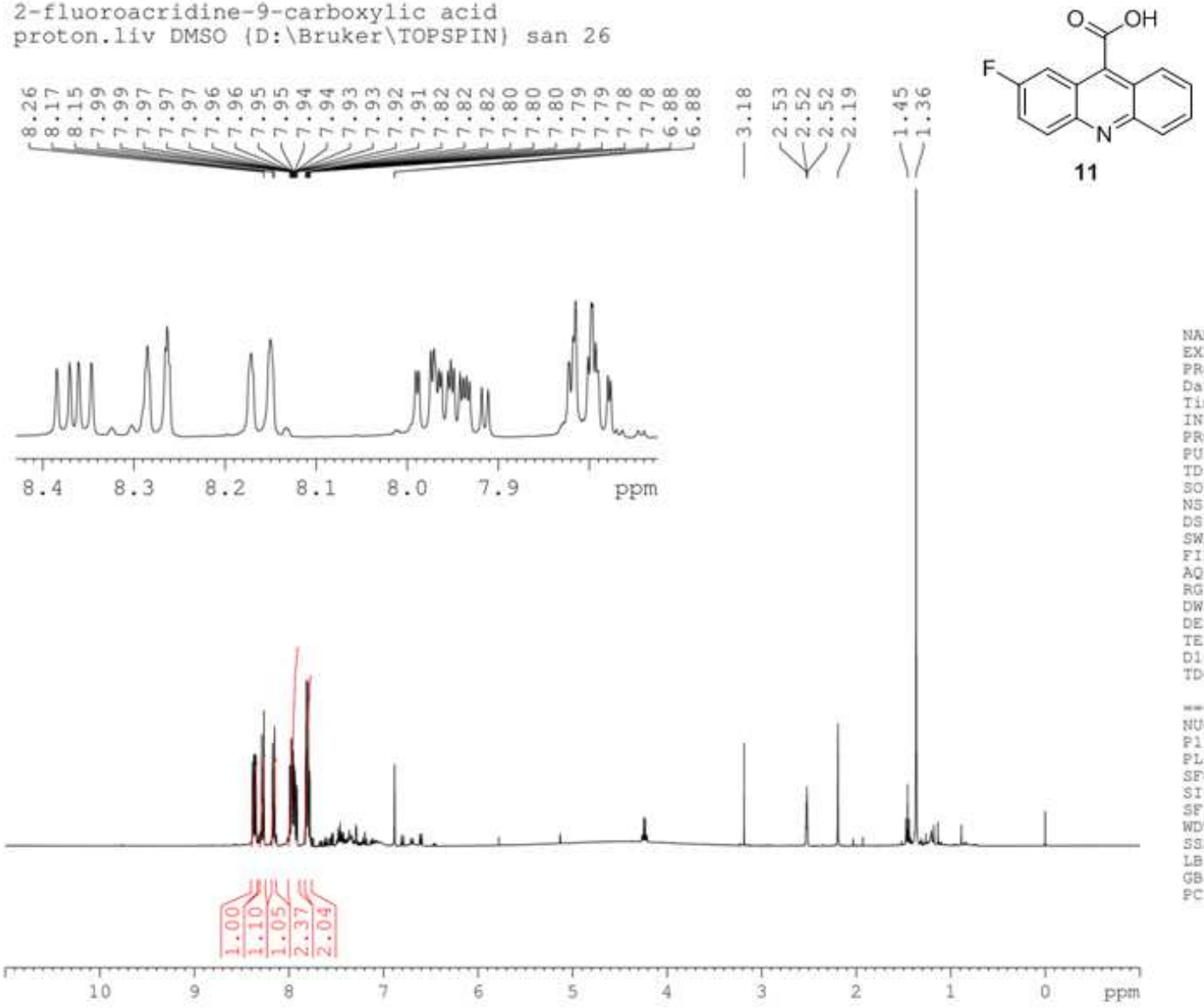
PULPROG	zgpg30	
TD	32768	
SOLVENT	DMSO	
NS	1024	
DS	4	
SWH	23980.814	Hz
FIDRES	0.731836	Hz
AQ	0.6832628	sec
RG	1824.6	
DW	20.850	usec
DE	6.00	usec
TE	303.2	K
D1	0.50000000	sec
d11	0.03000000	sec
DELTA	0.40000001	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	13C	
P1	11.12	usec
PL1	5.00	dB
SFO1	100.6227898	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	80.00	usec
PL2	-3.00	dB
PL12	16.37	dB
PL13	18.00	dB
SFO2	400.1316005	MHz
SI	32768	
SF	100.6128244	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	

2-fluoroacridine-9-carboxylic acid
proton.liv DMSO (D:\Bruker\TOPSPIN) san 26



11

NAME	ACRCOOH-2-F
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PROCNO	1
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SOLVENT	DMSO
NS	16
DS	2
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FIDRES	0.189786 Hz
AQ	2.6345973 sec
RG	71.8
DW	80.400 usec
DE	6.00 usec
TE	292.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
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WDW	EM
SSB	0
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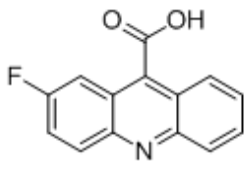
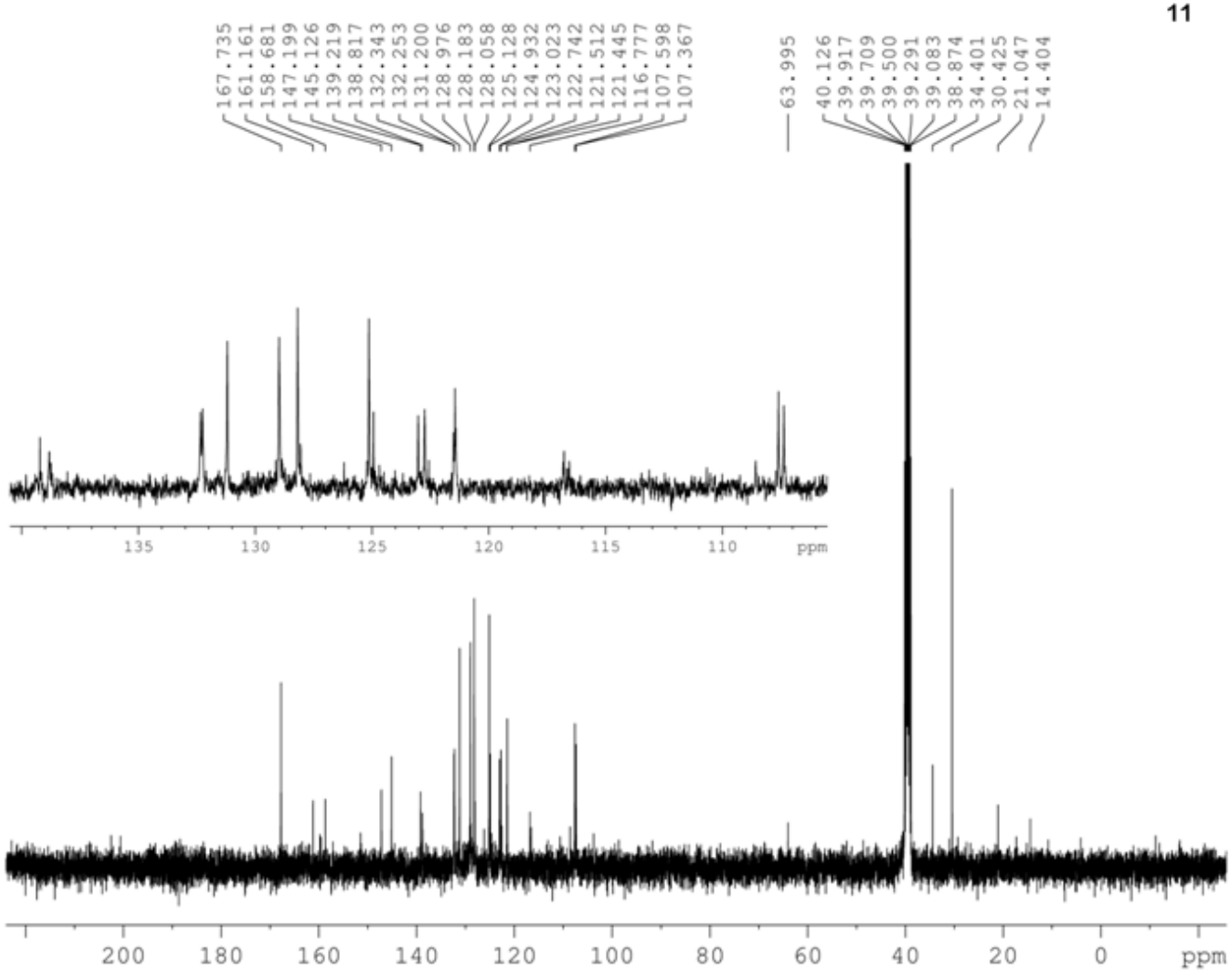
GB	0
PC	1.00

2-fluoroacridine-9-carboxylic acid
carbon.liv DMSO {D:\Bruker\TOPSPIN} san 26

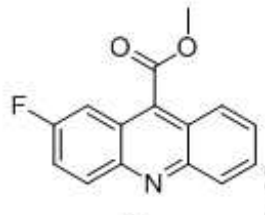


11



NAME	ACRCOOH-2-F
EXPNO	262
PROCNO	1
Date_	20070914
Time	13.31
INSTRUM	spect
PROBHD	5 mm QNP 1H/13
PULPROG	zgpg30
TD	32768
SOLVENT	DMSO
NS	1024
DS	4
SWH	25125.629 Hz
FIDRES	0.766773 Hz
AQ	0.6521332 sec
RG	13004
DW	19.900 usec
DE	6.00 usec
TE	294.0 K
D1	0.50000000 sec
d11	0.03000000 sec
DELTA	0.40000001 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	5.85 usec
PL1	-6.00 dB
SFO1	100.6227898 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-3.00 dB
PL12	16.37 dB
PL13	18.00 dB
SFO2	400.1316005 MHz
SI	32768
SF	100.6128133 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

methyl 2-fluoroacridine-9-carboxylate
proton.liv CDCl3 (D:\Bruker\TOPSPIN) san 18



13

8.27 8.26 8.26 8.25 8.25 8.23 8.04 8.02 7.82 7.80 7.80 7.80 7.78 7.78 7.66 7.66 7.64 7.64 7.63 7.63 7.62 7.62 7.62 7.62 7.61 7.61 7.60 7.60 7.59 7.59 7.27

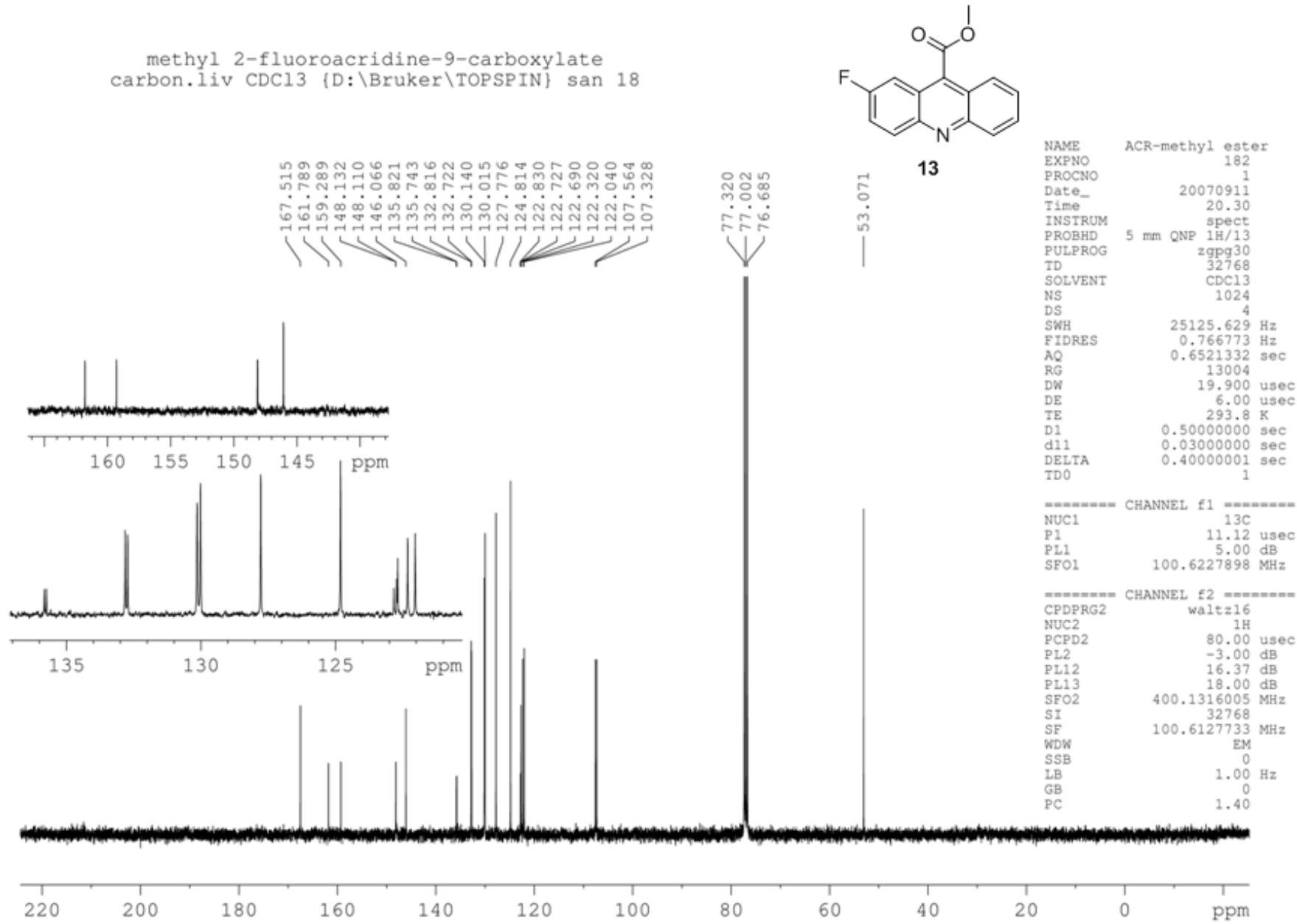
4.21 1.25 0.00

8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 ppm

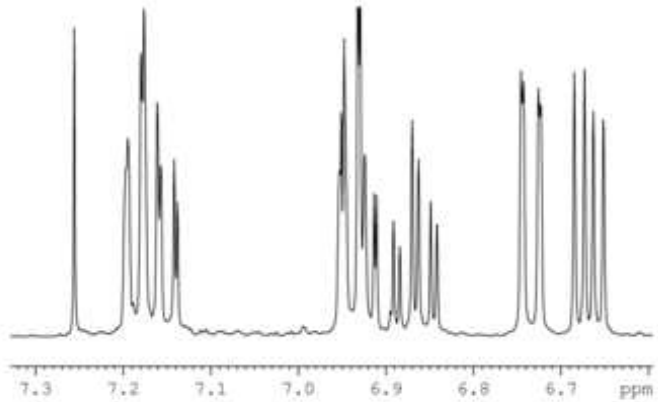
NAME	ACR-methyl ester
EXPNO	180
PROCNO	1
Date_	20070911
Time	20.03
INSTRUM	spect
PROBHD	5 mm QNP 1H/13
PULPROG	zg
TD	32768
SOLVENT	CDCl3
NS	16
DS	2
SWH	6218.905 Hz
FIDRES	0.189786 Hz
AQ	2.6345973 sec
RG	80.6
DW	80.400 usec
DE	6.00 usec
TE	292.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	13.25 usec
PL1	3.00 dB
SFO1	400.1325018 MHz
SI	32768
SF	400.1300053 MHz
WDW	EM
SSB	0
LB	0.10 Hz
GB	0
PC	1.00

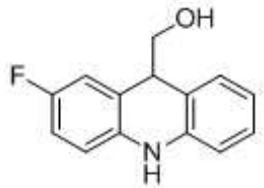
1.61 0.84 1.00 2.57 3.12

10 9 8 7 6 5 4 3 2 1 0 ppm


methyl 2-fluoroacridine-9-carboxylate
carbon.liv CDCl3 {D:\Bruker\TOPSPIN} san 18
13
167.515
161.789
159.289
148.132
148.110
146.066
135.821
135.743
132.816
132.722
130.140
130.015
127.776
124.814
122.830
122.727
122.690
122.320
122.040
107.564
107.328
77.320
77.002
76.685
53.071
160 155 150 145 ppm
135 130 125 ppm
220 200 180 160 140 120 100 80 60 40 20 0 ppm
NAME ACR-methyl ester
EXPNO 182
PROCNO 1
Date_ 20070911
Time 20.30
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1024
DS 4
SWH 25125.629 Hz
FIDRES 0.766773 Hz
AQ 0.6521332 sec
RG 13004
DW 19.900 usec
DE 6.00 usec
TE 293.8 K
D1 0.50000000 sec
d11 0.03000000 sec
DELTA 0.40000001 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 11.12 usec
PL1 5.00 dB
SFO1 100.6227898 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 16.37 dB
PL13 18.00 dB
SFO2 400.1316005 MHz
SI 32768
SF 100.6127733 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

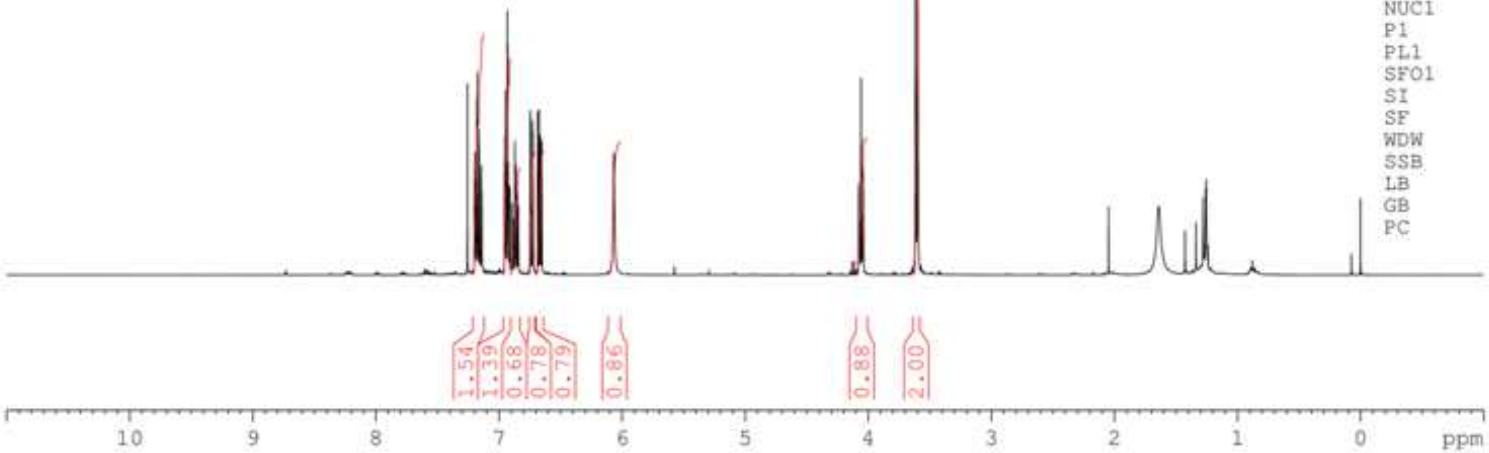
(2-fluoroacridin-9-yl)methanol
proton.liv CDCl3 (D:\Bruker\TOPSPIN) san 19



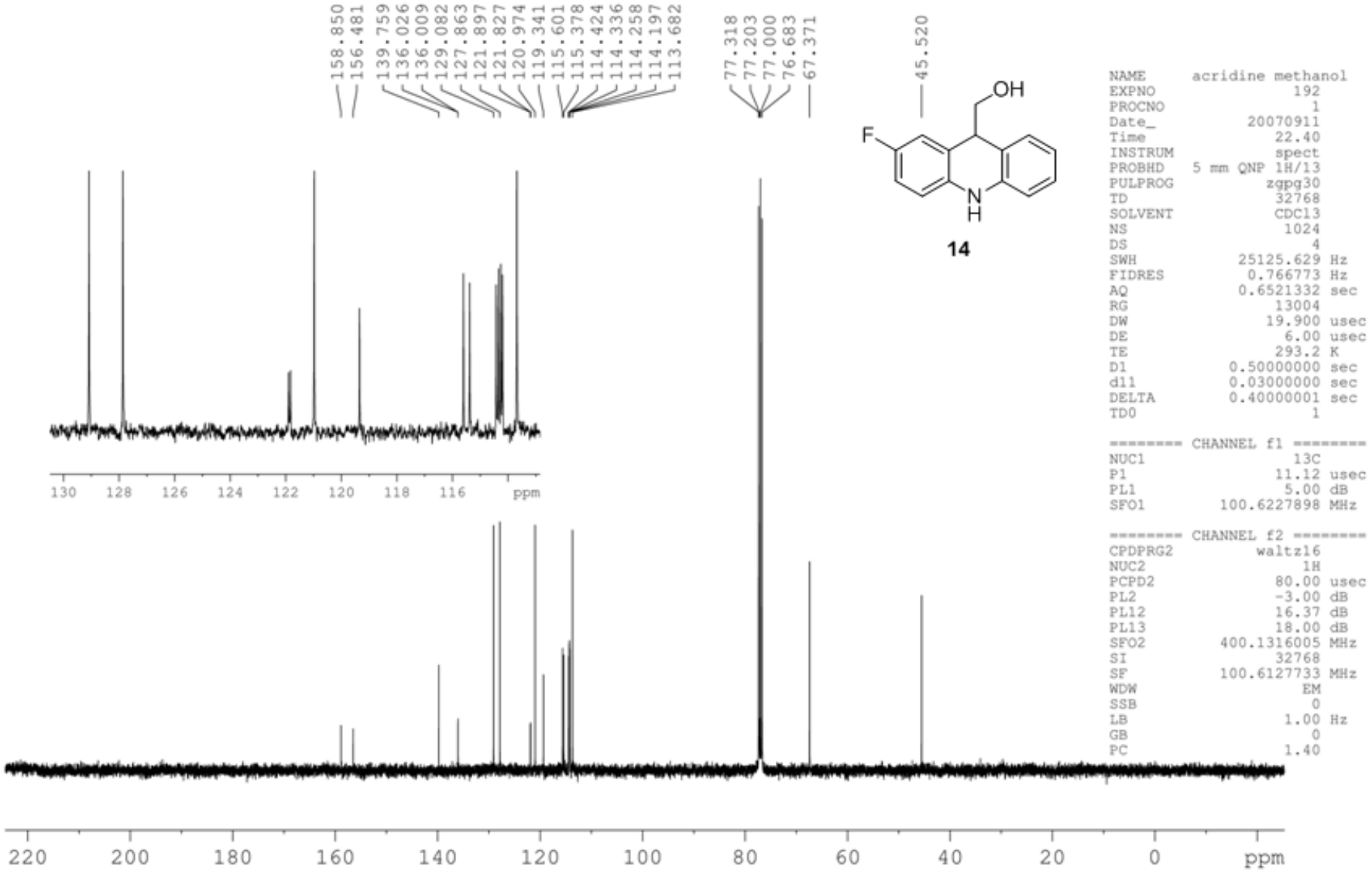


14

NAME	acridine methanol
EXPNO	190
PROCNO	1
Date_	20070911
Time	22.13
INSTRUM	spect
PROBHD	5 mm QNP 1H/13
PULPROG	zg
TD	32768
SOLVENT	CDCl3
NS	16
DS	2
SWH	6218.905 Hz
FIDRES	0.189786 Hz
AQ	2.6345973 sec
RG	90.5
DW	80.400 use
DE	6.00 use
TE	292.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 =======	
NUC1	1H
P1	13.25 use
PL1	3.00 dB
SFO1	400.1325018 MHz
SI	32768
SF	400.1300110 MHz
WDW	EM
SSB	0
LB	0.10 Hz
GB	0
PC	1.00



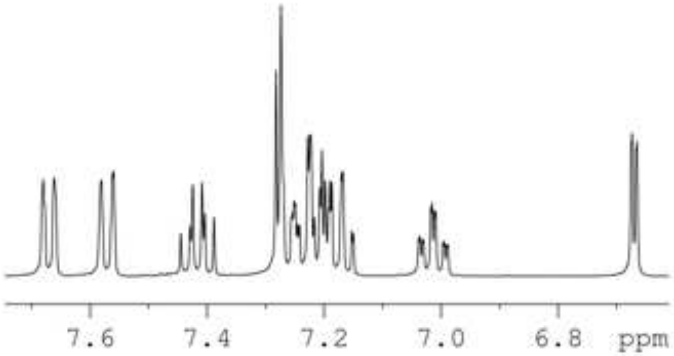
(2-fluoroacridin-9-yl)methanol
carbon.liv CDCl3 {D:\Bruker\TOPSPIN} san 19



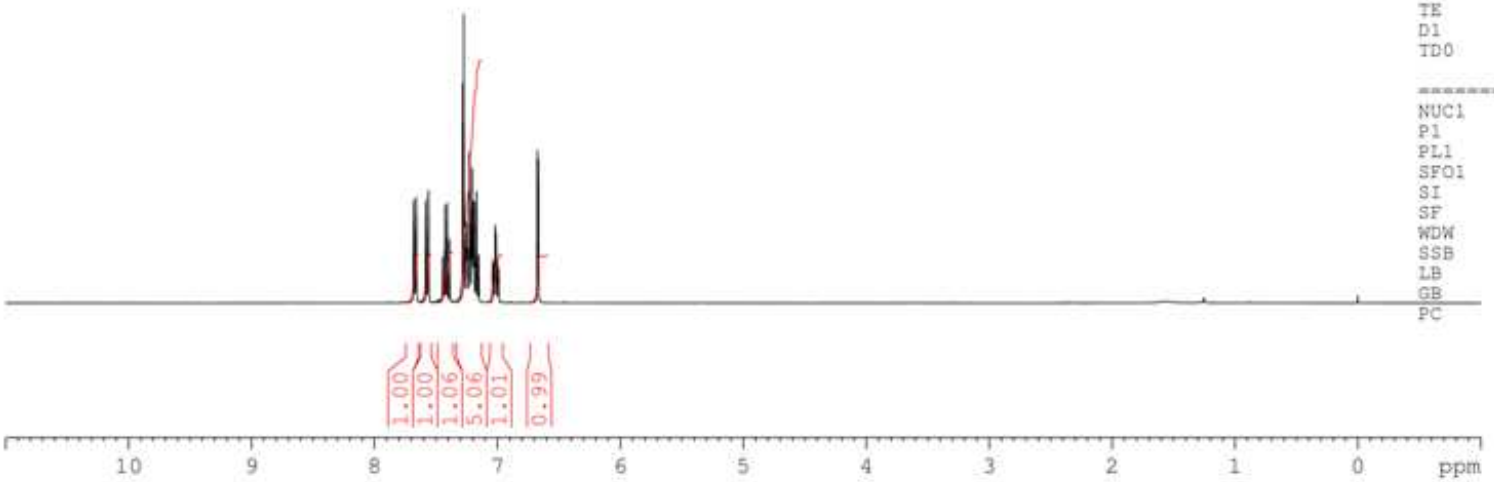
14

NAME	acridine methanol	
EXPNO	192	
PROCNO	1	
Date_	20070911	
Time	22.40	
INSTRUM	spect	
PROBHD	5 mm QNP 1H/13	
PULPROG	zgpg30	
TD	32768	
SOLVENT	CDCl3	
NS	1024	
DS	4	
SWH	25125.629	Hz
FIDRES	0.766773	Hz
AQ	0.6521332	sec
RG	13004	
DW	19.900	usec
DE	6.00	usec
TE	293.2	K
D1	0.50000000	sec
d11	0.03000000	sec
DELTA	0.40000001	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	13C	
P1	11.12	usec
PL1	5.00	dB
SFO1	100.6227898	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	80.00	usec
PL2	-3.00	dB
PL12	16.37	dB
PL13	18.00	dB
SFO2	400.1316005	MHz
SI	32768	
SF	100.6127733	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	

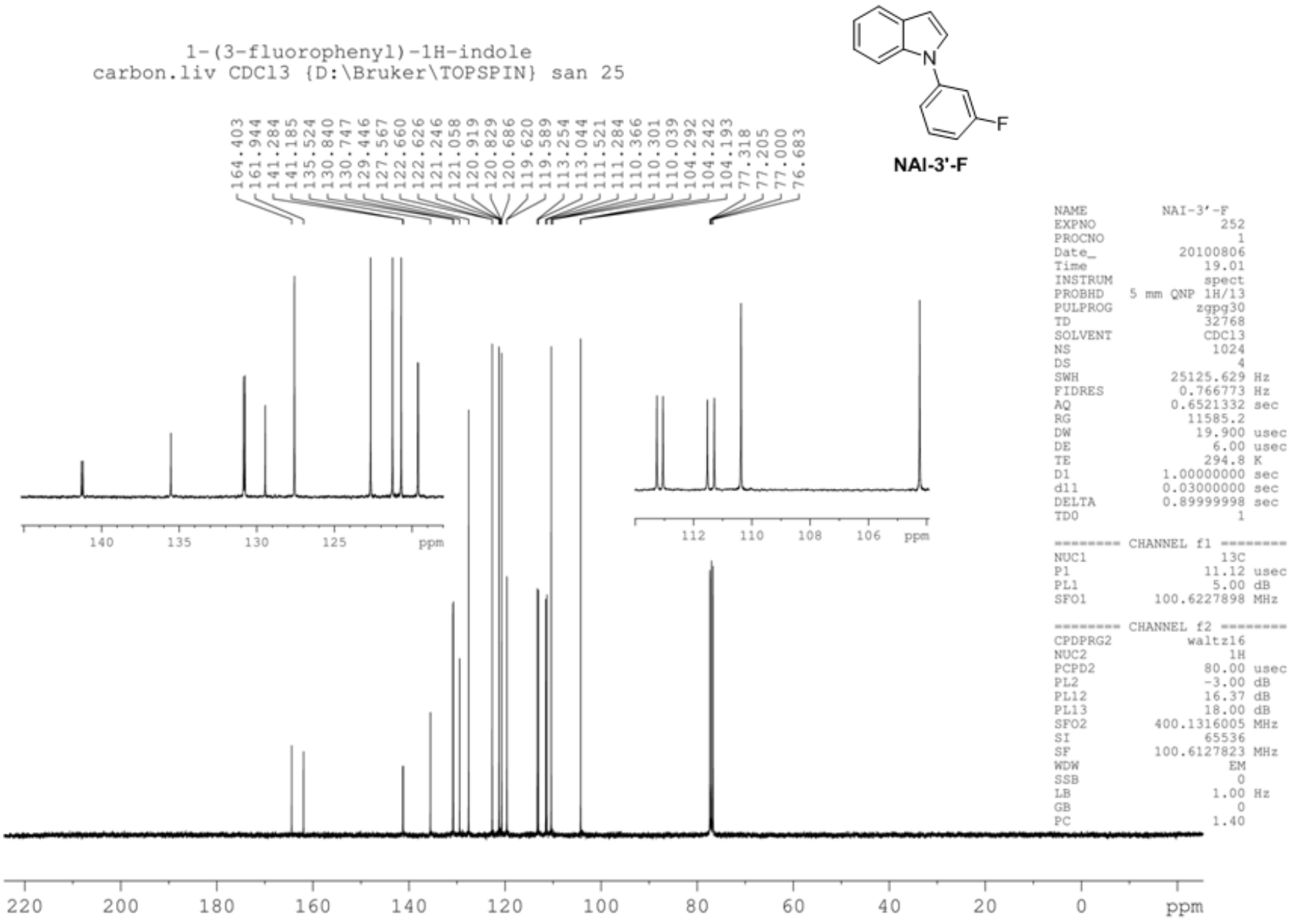
1-(3-fluorophenyl)-1H-indole
proton.liv CDCl3 (D:\Bruker\TOPSPIN) san 25



NAME	NAI-3'-F
EXPNO	250
PROCNO	1
Date_	20100806
Time	18.26
INSTRUM	spect
PROBHD	5 mm QNP 1H/13
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	64
DS	2
SWH	6218.905 Hz
FIDRES	0.094893 Hz
AQ	5.2691445 sec
RG	64
DW	80.400 usec
DE	6.00 usec
TE	293.1 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	13.25 usec
PL1	3.00 dB
SFO1	400.1325018 MHz
SI	131072
SF	400.1300465 MHz
WDW	EM
SSB	0
LB	0.20 Hz
GB	0
PC	1.00



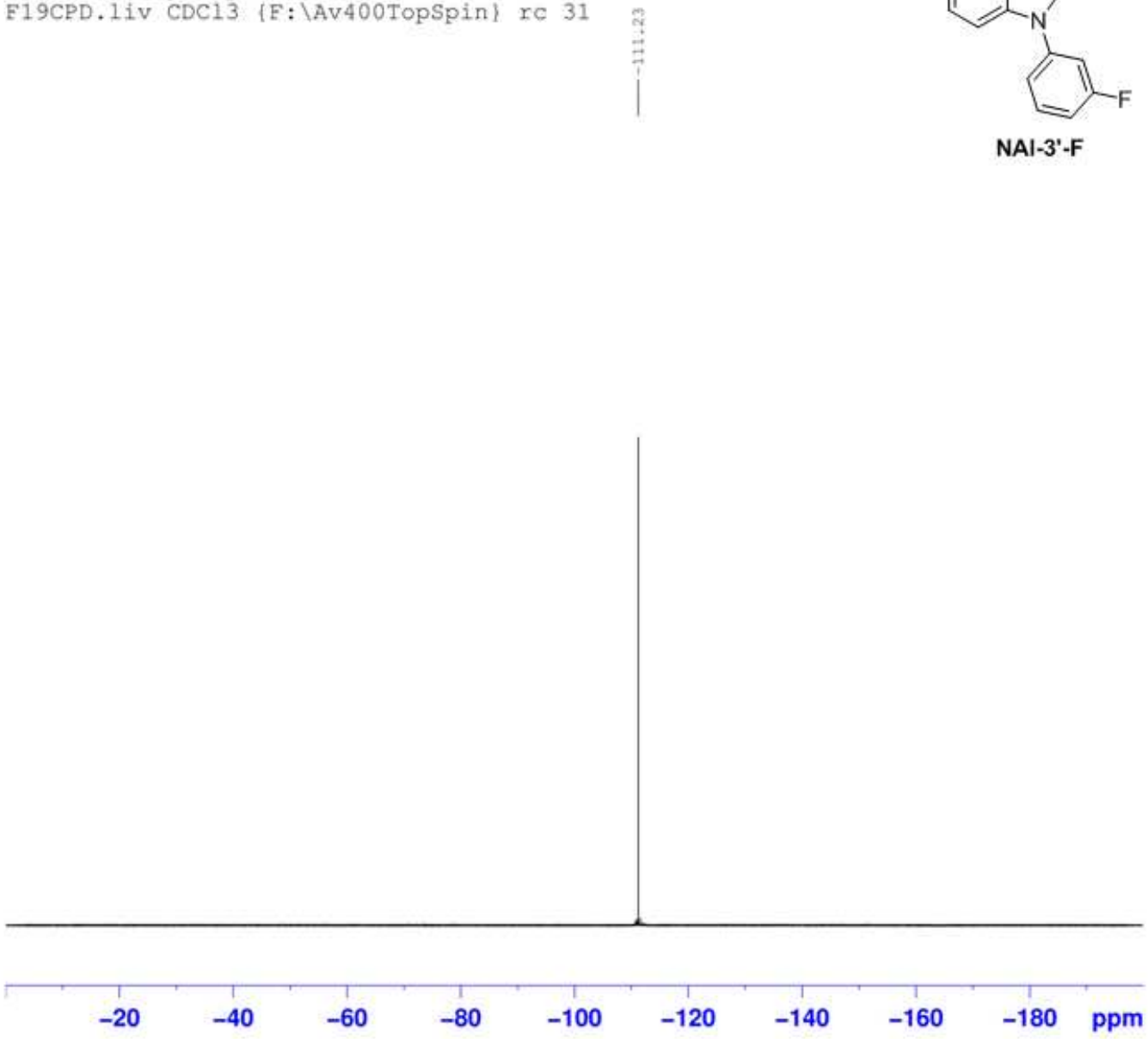
1-(3-fluorophenyl)-1H-indole
carbon.liv CDCl3 {D:\Bruker\TOPSPIN} san 25



NAI-3'-F

NAME	NAI-3'-F	
EXPNO	252	
PROCNO	1	
Date_	20100806	
Time	19.01	
INSTRUM	spect	
PROBHD	5 mm QNP 1H/13	
PULPROG	zgpg30	
TD	32768	
SOLVENT	CDCl3	
NS	1024	
DS	4	
SWH	25125.629	Hz
FIDRES	0.766773	Hz
AQ	0.6521332	sec
RG	11585.2	
DW	19.900	usec
DE	6.00	usec
TE	294.8	K
D1	1.00000000	sec
d11	0.03000000	sec
DELTA	0.89999998	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	13C	
P1	11.12	usec
PL1	5.00	dB
SFO1	100.6227898	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	80.00	usec
PL2	-3.00	dB
PL12	16.37	dB
PL13	18.00	dB
SFO2	400.1316005	MHz
SI	65536	
SF	100.6127823	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	

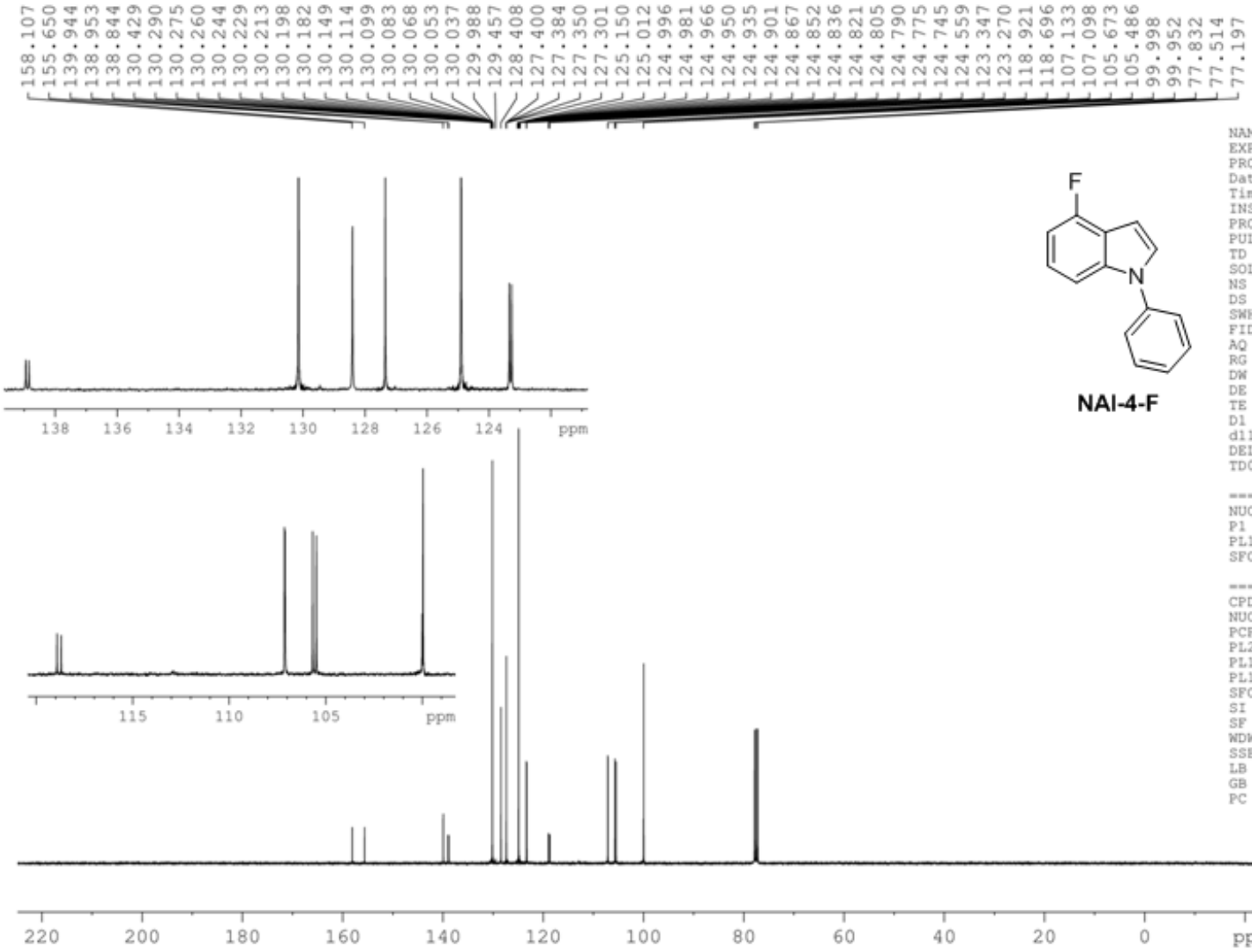
1-(3-fluoropheny)-1H lndole
F19CPD.liv CDC13 {F:\Av400TopSpin} rc 31



NAI-3'-F

NAME	NAI-3'-F	
EXPNO	313	
PROCNO	1	
Date_	20110113	
Time	15.05	
INSTRUM	spect	
PROBHD	5 mm QNP 1H/13	
PULPROG	zgfhigqn	
TD	131072	
SOLVENT	CDC13	
NS	16	
DS	4	
SWH	75187.969	Hz
FIDRES	0.573639	Hz
AQ	0.8716788	sec
RG	4597.6	
DW	6.650	usec
DE	6.00	usec
TE	296.7	K
D1	1.00000000	sec
d11	0.03000000	sec
d12	0.00002000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	19F	
P1	18.00	usec
PL1	-6.00	dB
SFO1	376.4608844	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	80.00	usec
PL2	-3.00	dB
PL12	16.37	dB
SFO2	400.1316005	MHz
SI	65536	
SF	376.4985340	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	

4-fluoro-1-phenyl-1H-indole
carbon.liv CDCl3 {D:\Bruker\TOPSPIN} san 26

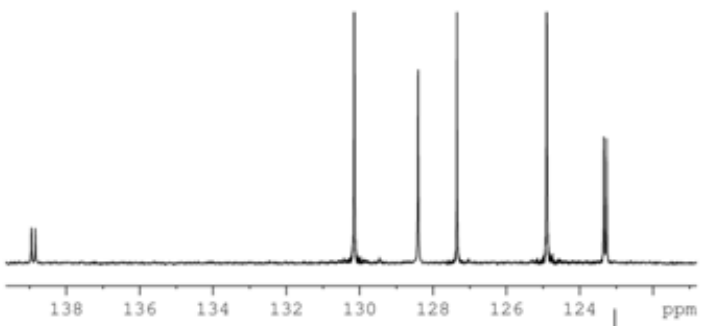


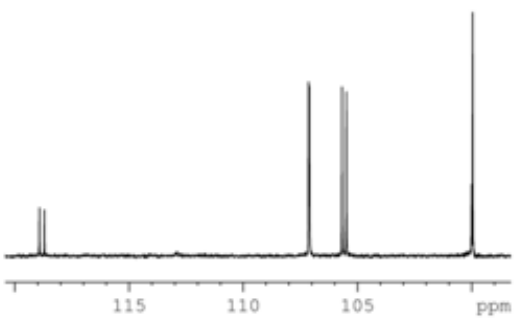
NAI-4-F

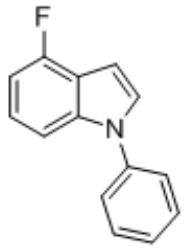
NAME	NAI-4-F	
EXPNO	262	
PROCNO	1	
Date_	20100807	
Time	1.41	
INSTRUM	spect	
PROBHD	5 mm QNP 1H/13	
PULPROG	zgpg30	
TD	32768	
SOLVENT	CDCl3	
NS	1024	
DS	4	
SWH	25125.629	Hz
FIDRES	0.766773	Hz
AQ	0.6521332	sec
RG	13004	
DW	19.900	usec
DE	6.00	usec
TE	294.5	K
D1	1.00000000	sec
d11	0.03000000	sec
DELTA	0.89999998	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	13C	
P1	11.12	usec
PL1	5.00	dB
SFO1	100.6227898	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	80.00	usec
PL2	-3.00	dB
PL12	16.37	dB
PL13	18.00	dB
SFO2	400.1316005	MHz
SI	65536	
SF	100.6127290	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	

4-fluoro-1-phenyl-1H-indole
carbon.liv CDCl3 {D:\Bruker\TOPSPIN} san 26

158.107
155.650
139.944
138.953
138.844
130.429
130.290
130.275
130.260
130.244
130.229
130.213
130.198
130.182
130.149
130.114
130.099
130.083
130.068
130.053
130.037
129.988
129.457
128.408
127.400
127.384
127.350
127.301
125.150
125.012
124.996
124.981
124.966
124.950
124.935
124.901
124.867
124.852
124.836
124.821
124.805
124.790
124.775
124.745
124.559
123.347
123.270
118.921
118.696
107.133
107.098
105.673
105.486
99.998
99.952
77.832
77.514
77.197



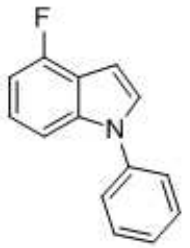




NAI-4-F

NAME	NAI-4-F
EXPNO	262
PROCNO	1
Date_	20100807
Time	1.41
INSTRUM	spect
PROBHD	5 mm QNP 1H/13
PULPROG	zgpg30
TD	32768
SOLVENT	CDCl3
NS	1024
DS	4
SWH	25125.629 Hz
FIDRES	0.766773 Hz
AQ	0.6521332 sec
RG	13004
DW	19.900 usec
DE	6.00 usec
TE	294.5 K
D1	1.00000000 sec
d11	0.03000000 sec
DELTA	0.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	11.12 usec
PL1	5.00 dB
SFO1	100.6227898 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-3.00 dB
PL12	16.37 dB
PL13	18.00 dB
SFO2	400.1316005 MHz
SI	65536
SF	100.6127290 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

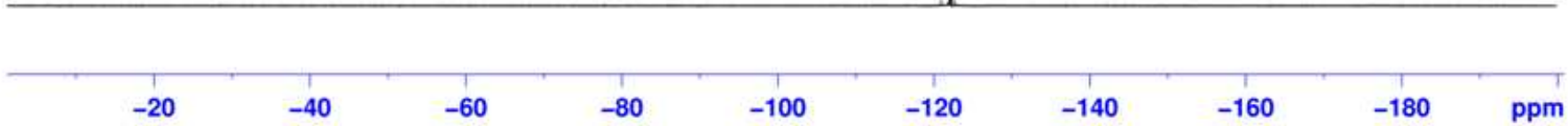
4-fluoro-1-phenyl-1H-indole
F19CPD.liv CDCl3 (F:\Av400TopSpin) rc 13



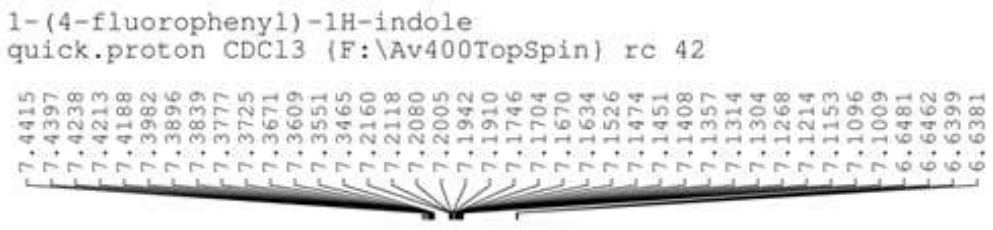
NAI-4-F

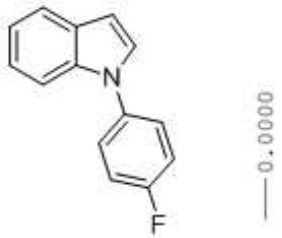
-122.24

NAME	NAI-4-F
EXPNO	130
PROCNO	1
Date_	20110218
Time	13.42
INSTRUM	spect
PROBHD	5 mm QNP 1H/13
PULPROG	zgfhigqn
TD	131072
SOLVENT	CDCl3
NS	16
DS	4
SWH	75187.969 Hz
FIDRES	0.573639 Hz
AQ	0.8716788 sec
RG	5160.6
DW	6.650 usec
DE	6.00 usec
TE	294.1 K
D1	1.00000000 sec
d11	0.03000000 sec
d12	0.00002000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	19F
P1	18.00 usec
PL1	-6.00 dB
SFO1	376.4608844 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-3.00 dB
PL12	16.37 dB
SFO2	400.1316005 MHz
SI	65536
SF	376.4985340 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



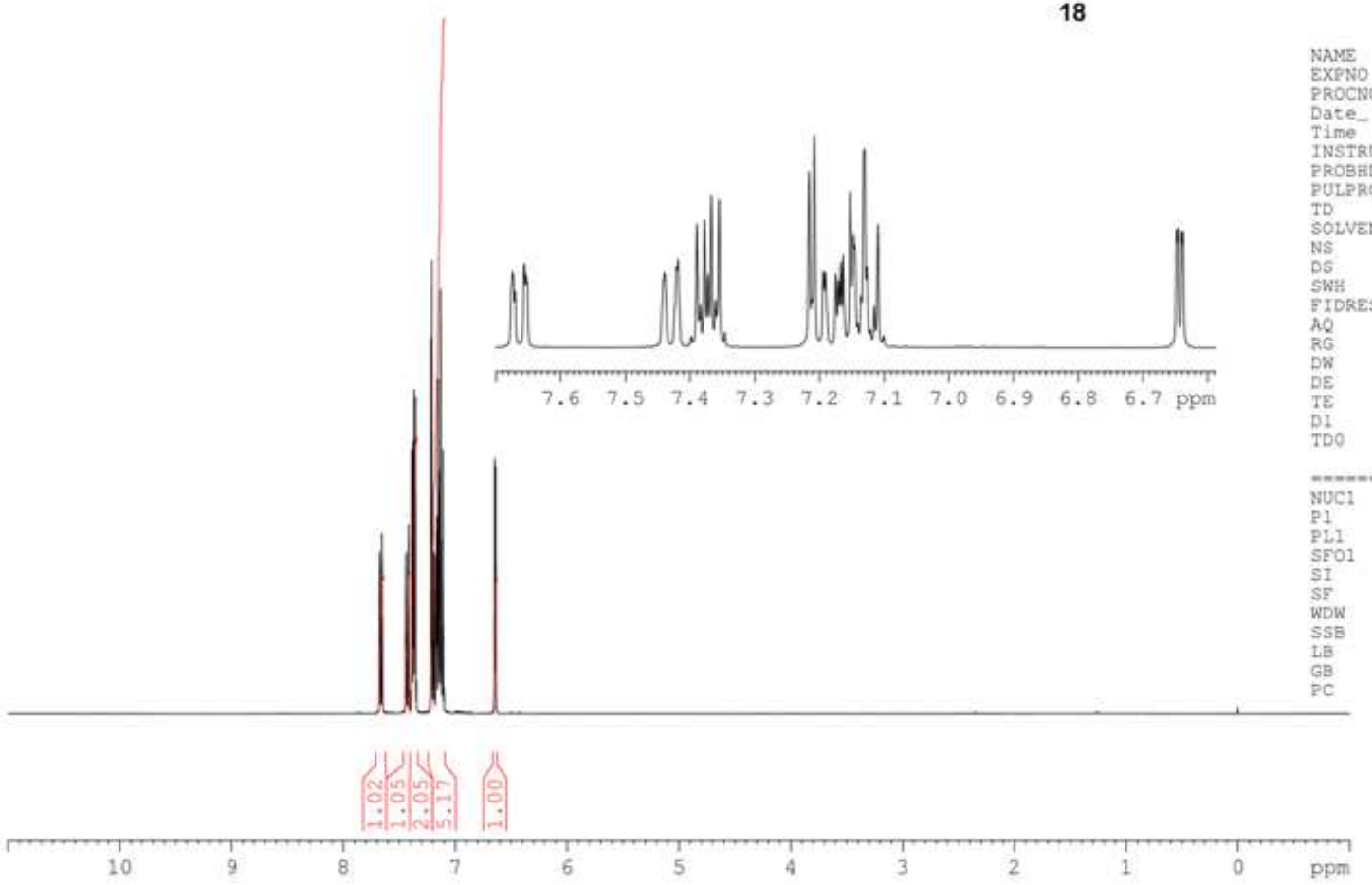
1-(4-fluorophenyl)-1H-indole
quick.proton CDCl3 (F:\Av400TopSpin) rc 42





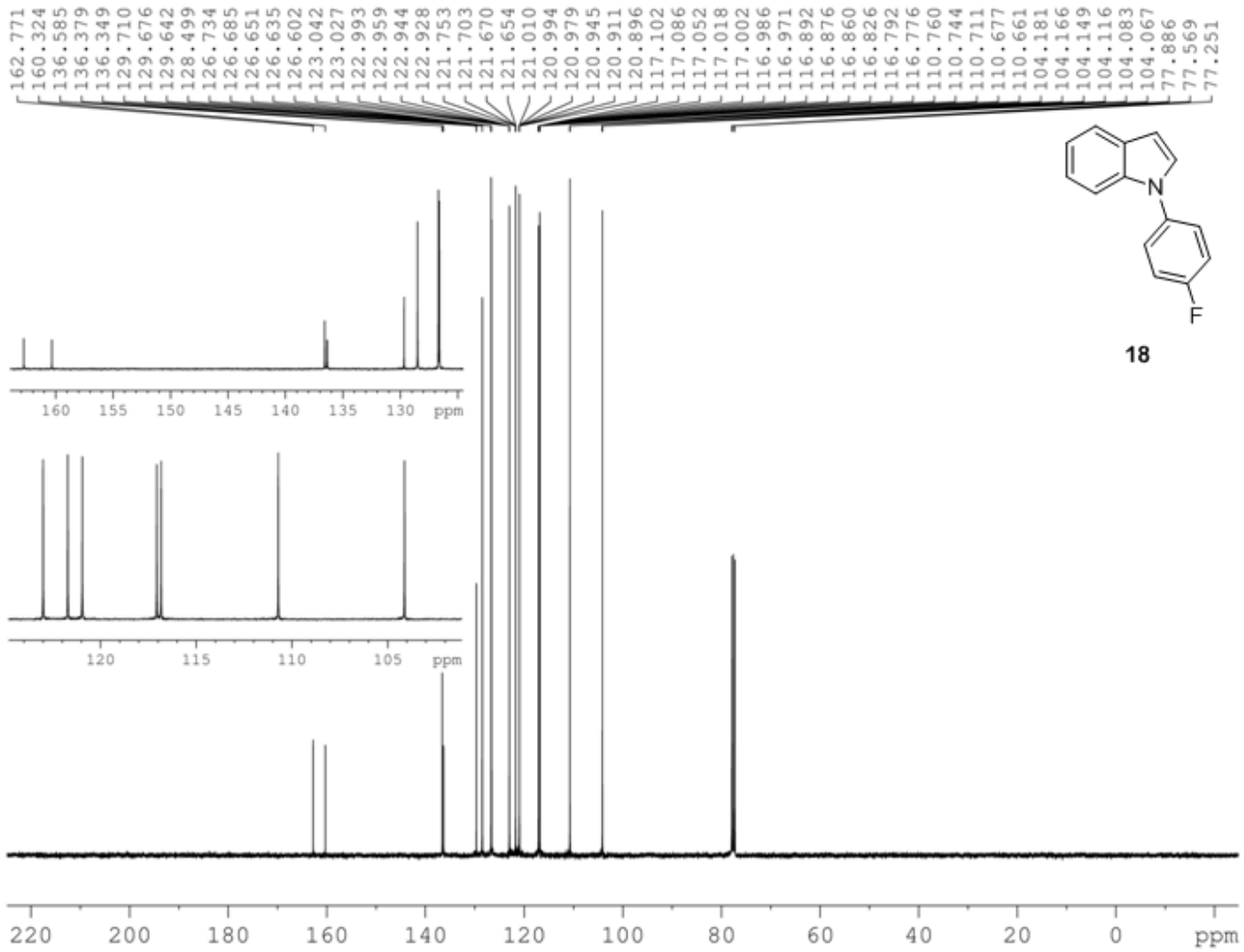
0.0000

18



NAME	NAI-4'-F
EXPNO	420
PROCNO	1
Date_	20110114
Time	5.18
INSTRUM	spect
PROBHD	5 mm QNP 1H/13
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	6218.905 Hz
FIDRES	0.094893 Hz
AQ	5.2691445 sec
RG	45.3
DW	80.400 usec
DE	6.00 usec
TE	296.7 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	13.25 usec
PL1	3.00 dB
SFO1	400.1325018 MHz
SI	131072
SF	400.1300629 MHz
WDW	EM
SSB	0
LB	0.20 Hz
GB	0
PC	1.00

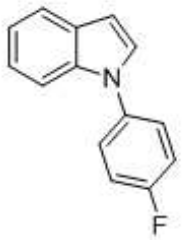
1-(4-fluorophenyl)-1H-indole
carbon.liv CDCl3 {F:\Av400TopSpin} rc 42



18

NAME	NAI-4'-F	
EXPNO	421	
PROCNO	1	
Date_	20110114	
Time	5.48	
INSTRUM	spect	
PROBHD	5 mm QNP 1H/13	
PULPROG	zgpg30	
TD	32768	
SOLVENT	CDCl3	
NS	1024	
DS	4	
SWH	25125.629	Hz
FIDRES	0.766773	Hz
AQ	0.6521332	sec
RG	13004	
DW	19.900	usec
DE	6.00	usec
TE	297.1	K
D1	1.00000000	sec
d11	0.03000000	sec
DELTA	0.89999998	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	13C	
P1	11.12	usec
PL1	5.00	dB
SFO1	100.6227898	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	80.00	usec
PL2	-3.00	dB
PL12	16.37	dB
PL13	18.00	dB
SFO2	400.1316005	MHz
SI	65536	
SF	100.6127290	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	

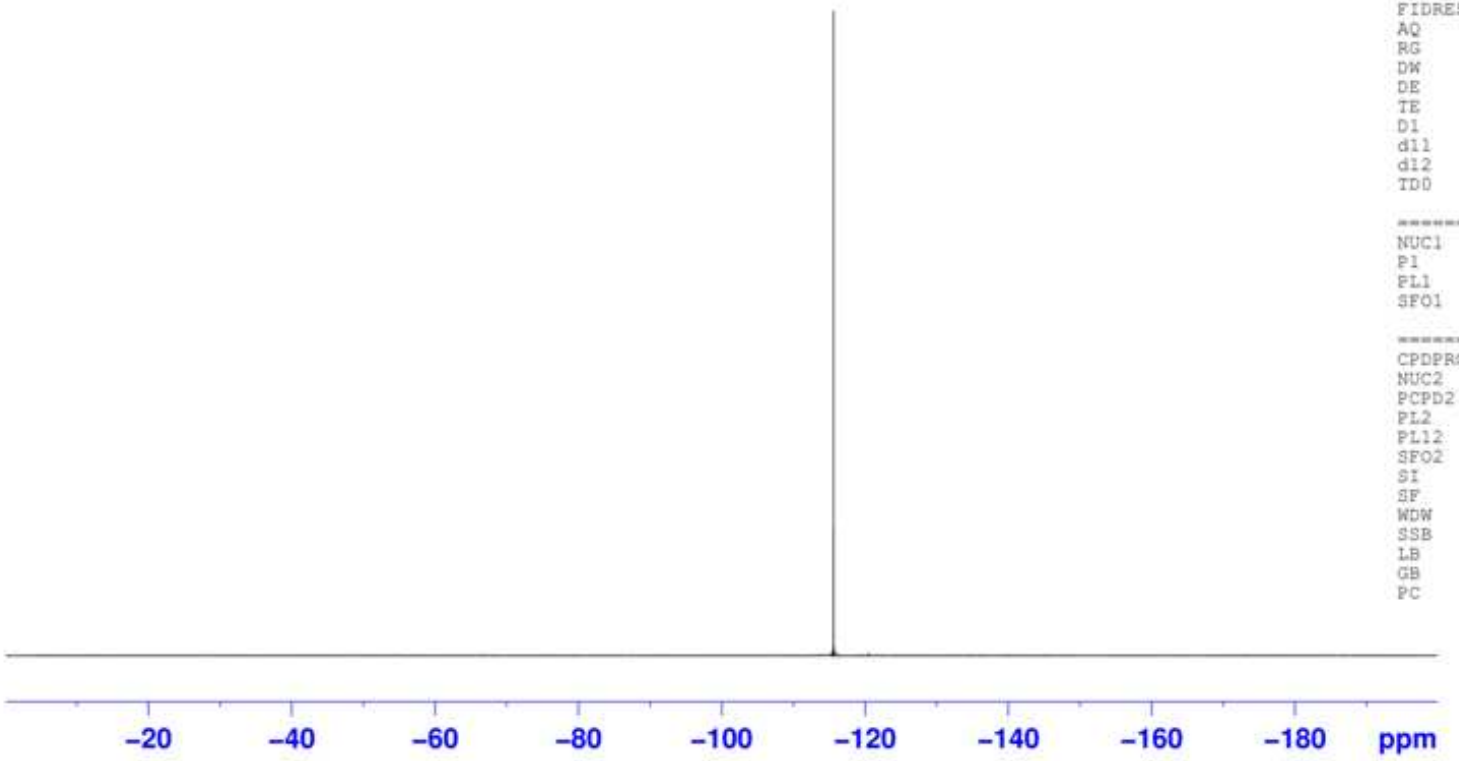
1-(4-fluorophenyl)-1H-indole
F19CPD.liv CDCl3 (F:\Av400TopSpin) rc 42

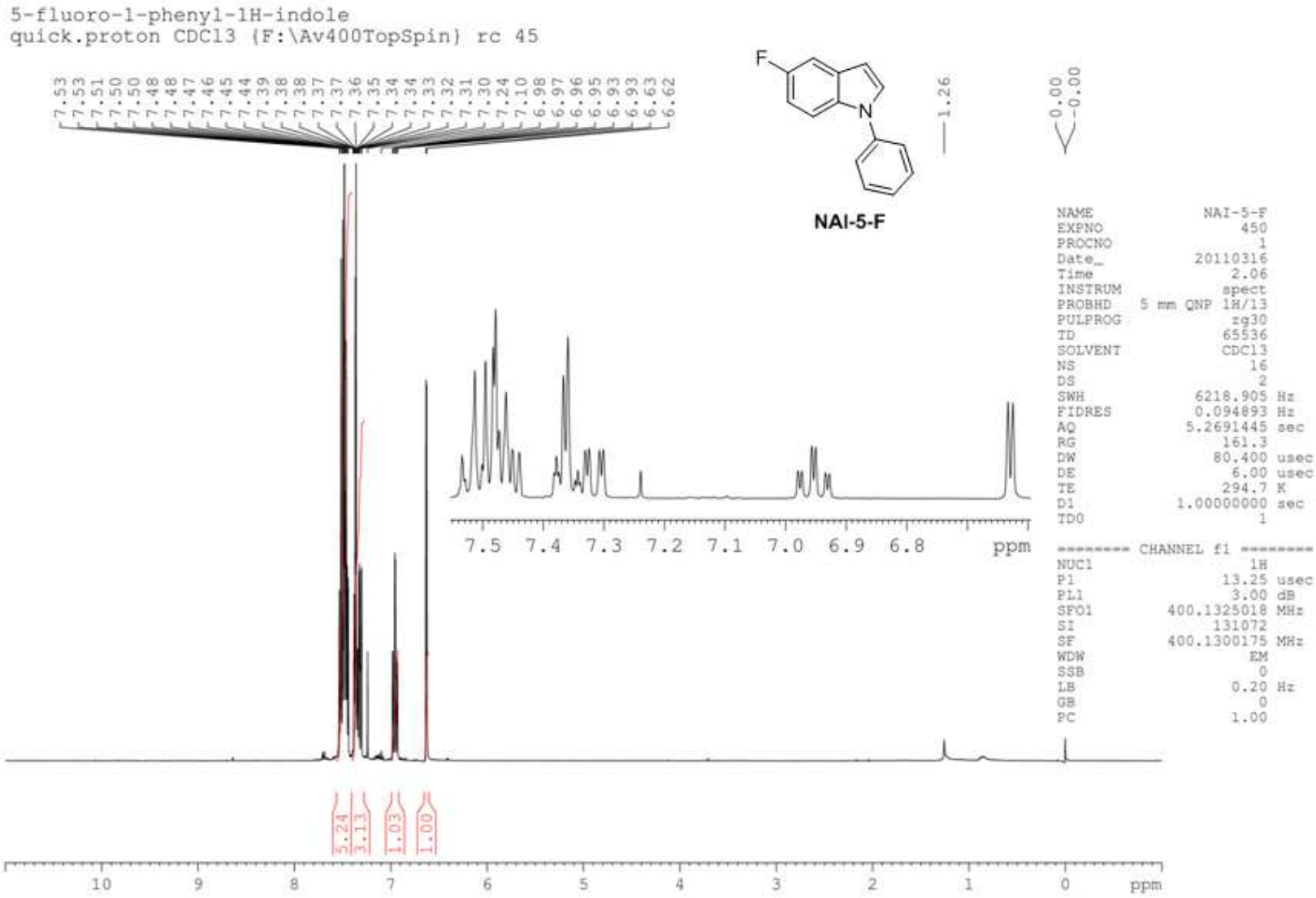


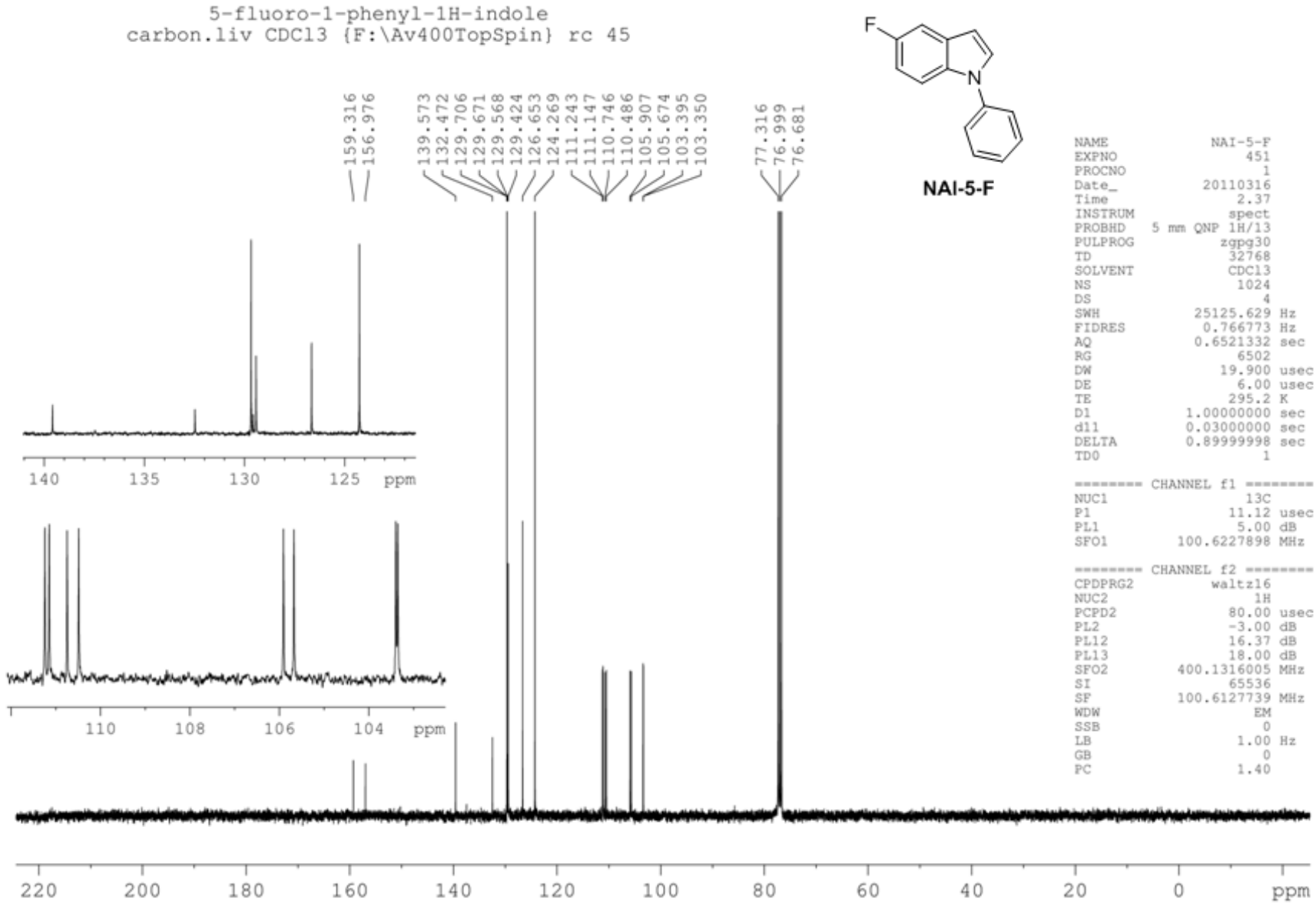
18

-115.59

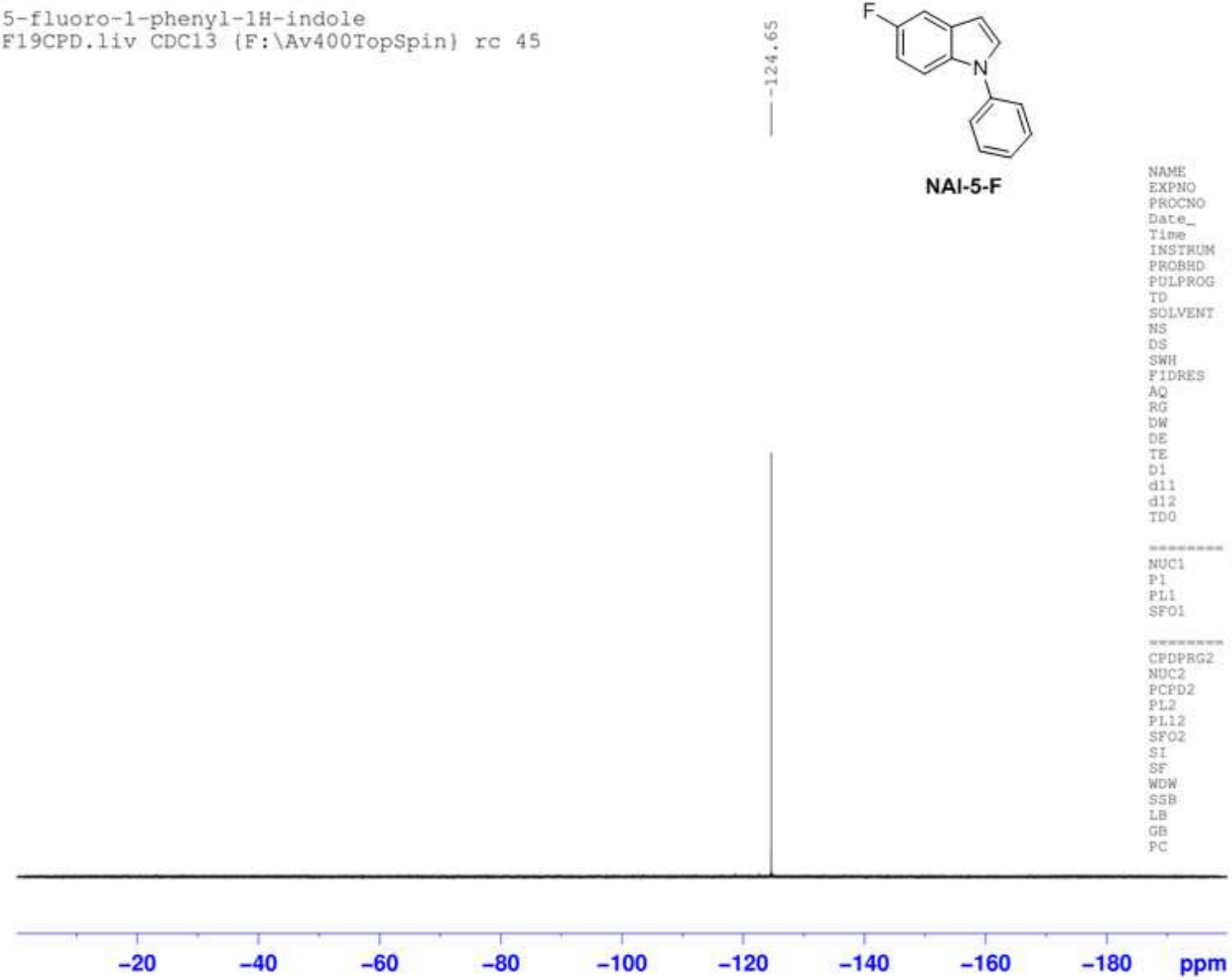
NAME	NAI-4'-F
EXPNO	423
PROCNO	1
Date_	20110113
Time	16.48
INSTRUM	spect
PROBHD	5 mm QNP 1H/13
PULPROG	zgfhigqn
TD	131072
SOLVENT	CDCl3
NS	16
DS	4
SWH	75187.969 Hz
FIDRES	0.573639 Hz
AQ	0.8716788 sec
RG	3649.1
DW	6.650 usec
DE	6.00 usec
TE	296.7 K
D1	1.00000000 sec
d11	0.03000000 sec
d12	0.00002000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	19F
P1	18.00 usec
PL1	-6.00 dB
SFO1	376.4608844 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-3.00 dB
PL12	16.37 dB
SFO2	400.1316005 MHz
SI	65536
SF	376.4985340 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00




5-fluoro-1-phenyl-1H-indole
quick.proton CDCl3 (F:\Av400TopSpin) rc 45
7.53 7.53 7.51 7.50 7.50 7.48 7.48 7.47 7.46 7.45 7.44 7.39 7.38 7.38 7.37 7.37 7.36 7.35 7.34 7.34 7.33 7.32 7.31 7.30 7.24 7.10 6.98 6.97 6.96 6.95 6.93 6.93 6.63 6.62
F
N
NAI-5-F
1.26
0.00
0.00
7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 ppm
5.24
3.13
1.03
1.00
10 9 8 7 6 5 4 3 2 1 0 ppm
NAME NAI-5-F
EXPNO 450
PROCNO 1
Date_ 20110316
Time 2.06
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6218.905 Hz
FIDRES 0.094893 Hz
AQ 5.2691445 sec
RG 161.3
DW 80.400 usec
DE 6.00 usec
TE 294.7 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.25 usec
PL1 3.00 dB
SFO1 400.1325018 MHz
SI 131072
SF 400.1300175 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.00

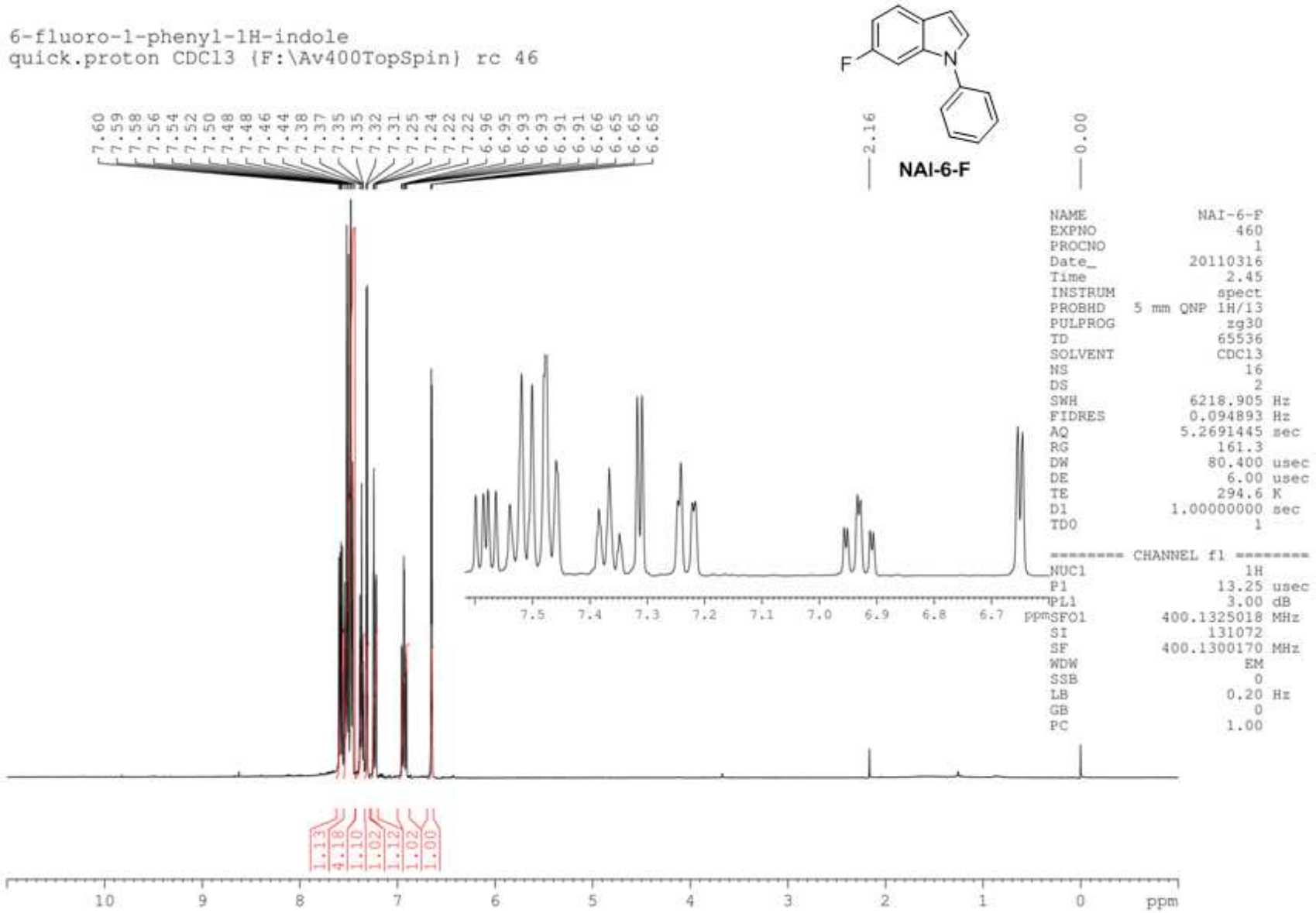

5-fluoro-1-phenyl-1H-indole
carbon.liv CDCl3 {F:\Av400TopSpin} rc 45
159.316
156.976
139.573
132.472
129.706
129.671
129.568
129.424
126.653
124.269
111.243
111.147
110.746
110.486
105.907
105.674
103.395
103.350
77.316
76.999
76.681
F
N
NAI-5-F
NAME NAI-5-F
EXPNO 451
PROCNO 1
Date_ 20110316
Time 2.37
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1024
DS 4
SWH 25125.629 Hz
FIDRES 0.766773 Hz
AQ 0.6521332 sec
RG 6502
DW 19.900 usec
DE 6.00 usec
TE 295.2 K
D1 1.00000000 sec
d11 0.03000000 sec
DELTA 0.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 11.12 usec
PL1 5.00 dB
SFO1 100.6227898 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 16.37 dB
PL13 18.00 dB
SFO2 400.1316005 MHz
SI 65536
SF 100.6127739 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
140 135 130 125 ppm
110 108 106 104 ppm
220 200 180 160 140 120 100 80 60 40 20 0 ppm

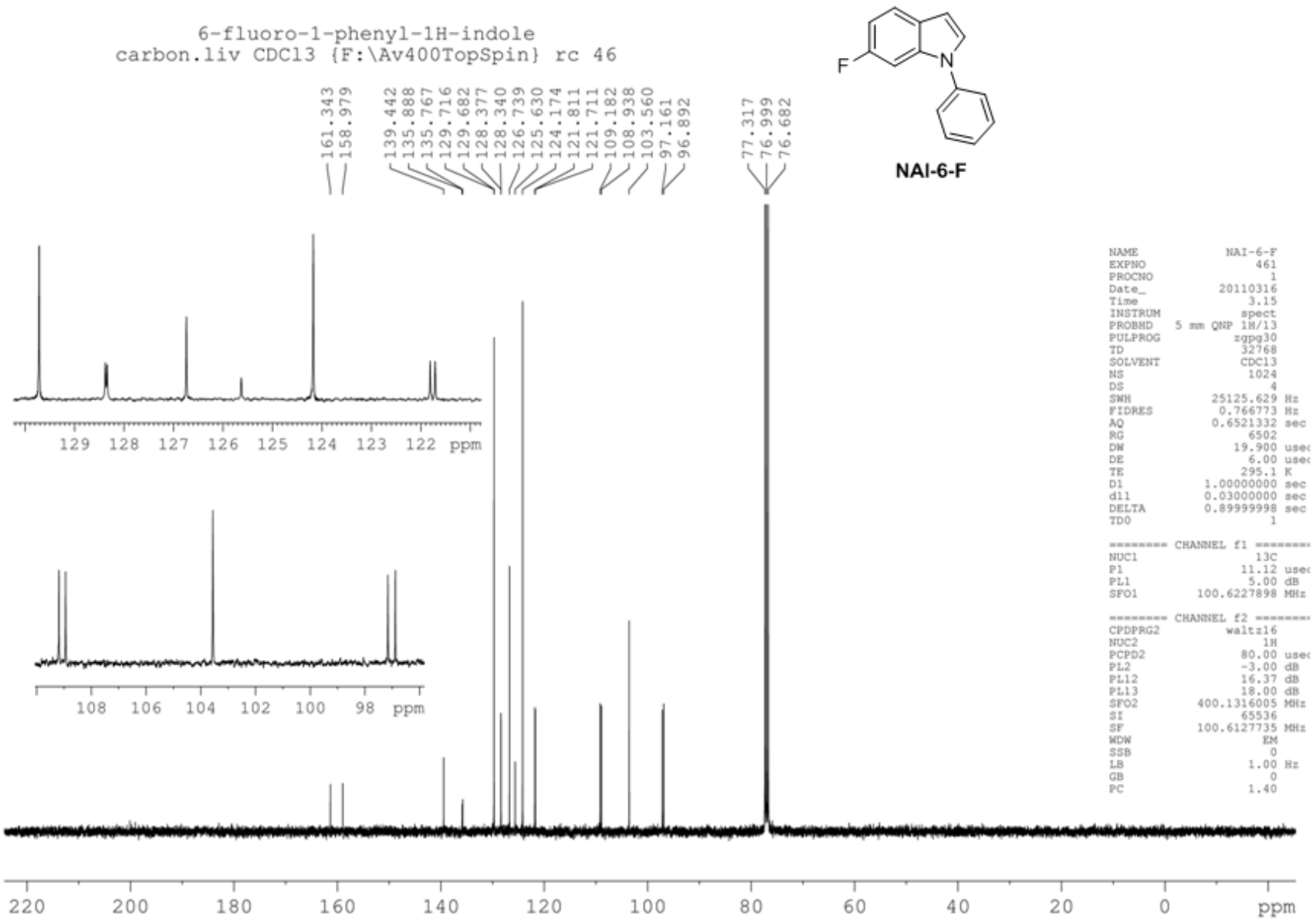
5-fluoro-1-phenyl-1H-indole
F19CPD.liv CDCl3 (F:\Av400TopSpin) rc 45



NAI-5-F

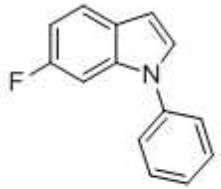
NAME	NAI-5-F	
EXPNO	452	
PROCNO	1	
Date_	20110316	
Time	2.38	
INSTRUM	spect	
PROBHD	5 mm QNP 1H/13	
PULPROG	zgfhigqn	
TD	131072	
SOLVENT	CDCl3	
NS	16	
DS	4	
SWH	75187.969	Hz
FIDRES	0.573639	Hz
AQ	0.8716788	sec
RG	9195.2	
DW	6.650	usec
DE	6.00	usec
TE	295.0	K
D1	1.00000000	sec
d11	0.03000000	sec
d12	0.00002000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	19F	
P1	18.00	usec
PL1	-6.00	dB
SFO1	376.4608844	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	80.00	usec
PL2	-3.00	dB
PL12	16.37	dB
SFO2	400.1316005	MHz
SI	65536	
SF	376.4985340	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	


6-fluoro-1-phenyl-1H-indole
quick.proton CDCl3 (F:\Av400TopSpin) rc 46
NAI-6-F
NAME NAI-6-F
EXPNO 460
PROCNO 1
Date_ 20110316
Time 2.45
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6218.905 Hz
FIDRES 0.094893 Hz
AQ 5.2691445 sec
RG 161.3
DW 80.400 usec
DE 6.00 usec
TE 294.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.25 usec
PL1 3.00 dB
SFO1 400.1325018 MHz
SI 131072
SF 400.1300170 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.00
ppm

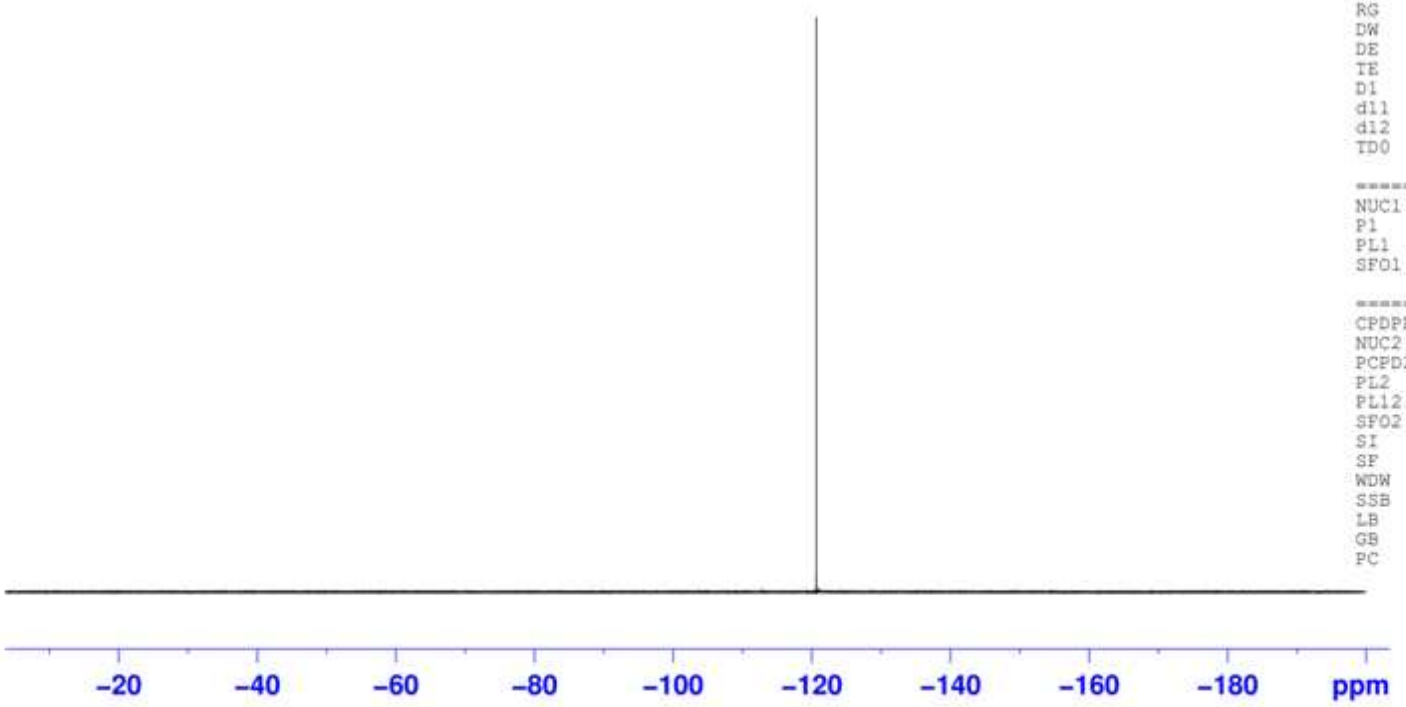

6-fluoro-1-phenyl-1H-indole
carbon.liv CDCl3 {F:\Av400TopSpin} rc 46
161.343
158.979
139.442
135.888
135.767
129.716
129.682
128.377
128.340
126.739
125.630
124.174
121.811
121.711
109.182
108.938
103.560
97.161
96.892
77.317
76.999
76.682
F
N
NAI-6-F
129 128 127 126 125 124 123 122 ppm
108 106 104 102 100 98 ppm
NAME NAI-6-F
EXPNO 461
PROCNO 1
Date_ 20110316
Time 3.15
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1024
DS 4
SWH 25125.629 Hz
FIDRES 0.766773 Hz
AQ 0.6521332 sec
RG 6502
DW 19.900 usec
DE 6.00 usec
TE 295.1 K
D1 1.00000000 sec
d11 0.03000000 sec
DELTA 0.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 11.12 usec
PL1 5.00 dB
SFO1 100.6227898 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 16.37 dB
PL13 18.00 dB
SFO2 400.1316005 MHz
SI 65536
SF 100.6127735 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
220 200 180 160 140 120 100 80 60 40 20 0 ppm

6-fluoro-1-phenyl-1H-indole
F19CPD.liv CDC13 (F:\Av400TopSpin) rc 46

-120.65

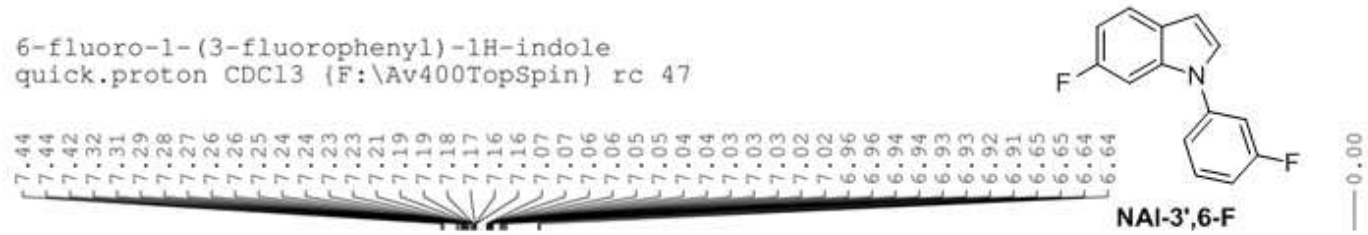


NAI-6-F

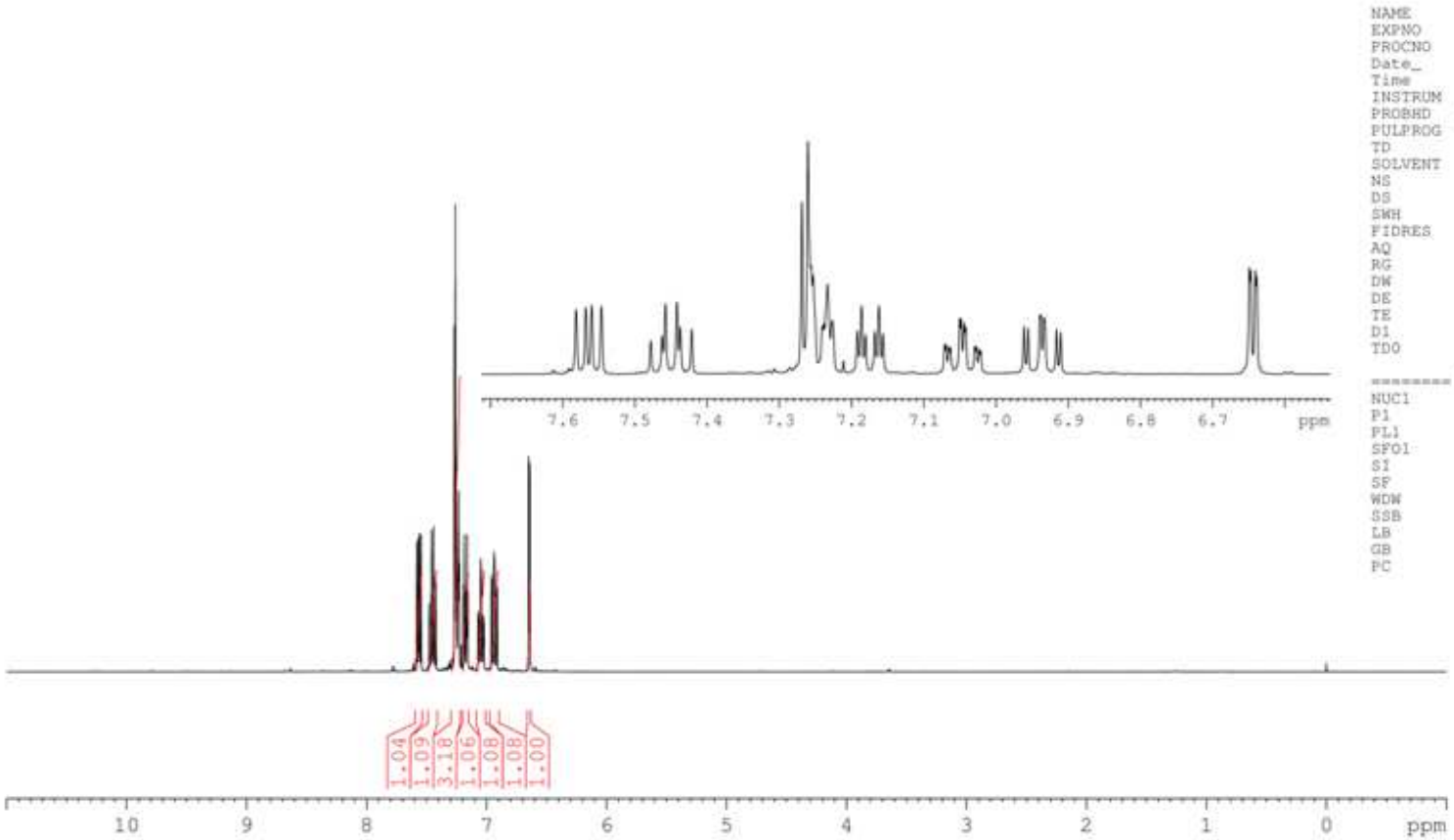


NAME	NAI-6-F
EXPNO	462
PROCNO	1
Date_	20110316
Time	3.17
INSTRUM	spect
PROBHD	5 mm QNP 1H/13
PULPROG	zgfhigqn
TD	131072
SOLVENT	CDC13
NS	16
DS	4
SWH	75187.969 Hz
FIDRES	0.573639 Hz
AQ	0.8716788 sec
RG	7298.2
DW	6.650 usec
DE	6.00 usec
TE	294.9 K
D1	1.00000000 sec
d11	0.03000000 sec
d12	0.00002000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	19F
P1	18.00 usec
PL1	-6.00 dB
SFO1	376.4608844 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-3.00 dB
PL12	16.37 dB
SFO2	400.1316005 MHz
SI	65536
SF	376.4985340 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

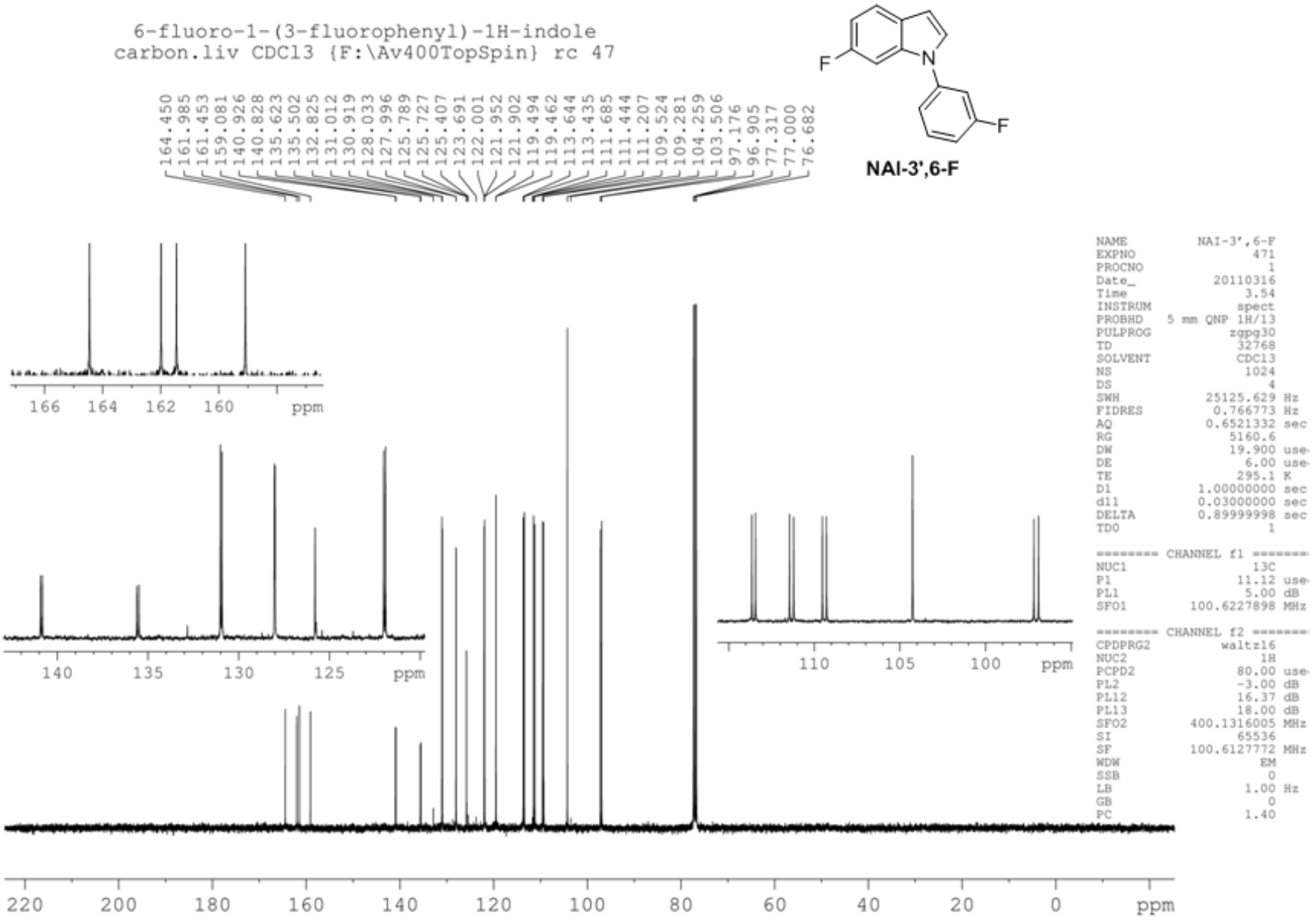
6-fluoro-1-(3-fluorophenyl)-1H-indole
quick.proton CDCl3 (F:\Av400TopSpin) rc 47



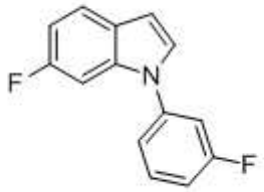
NAI-3',6-F



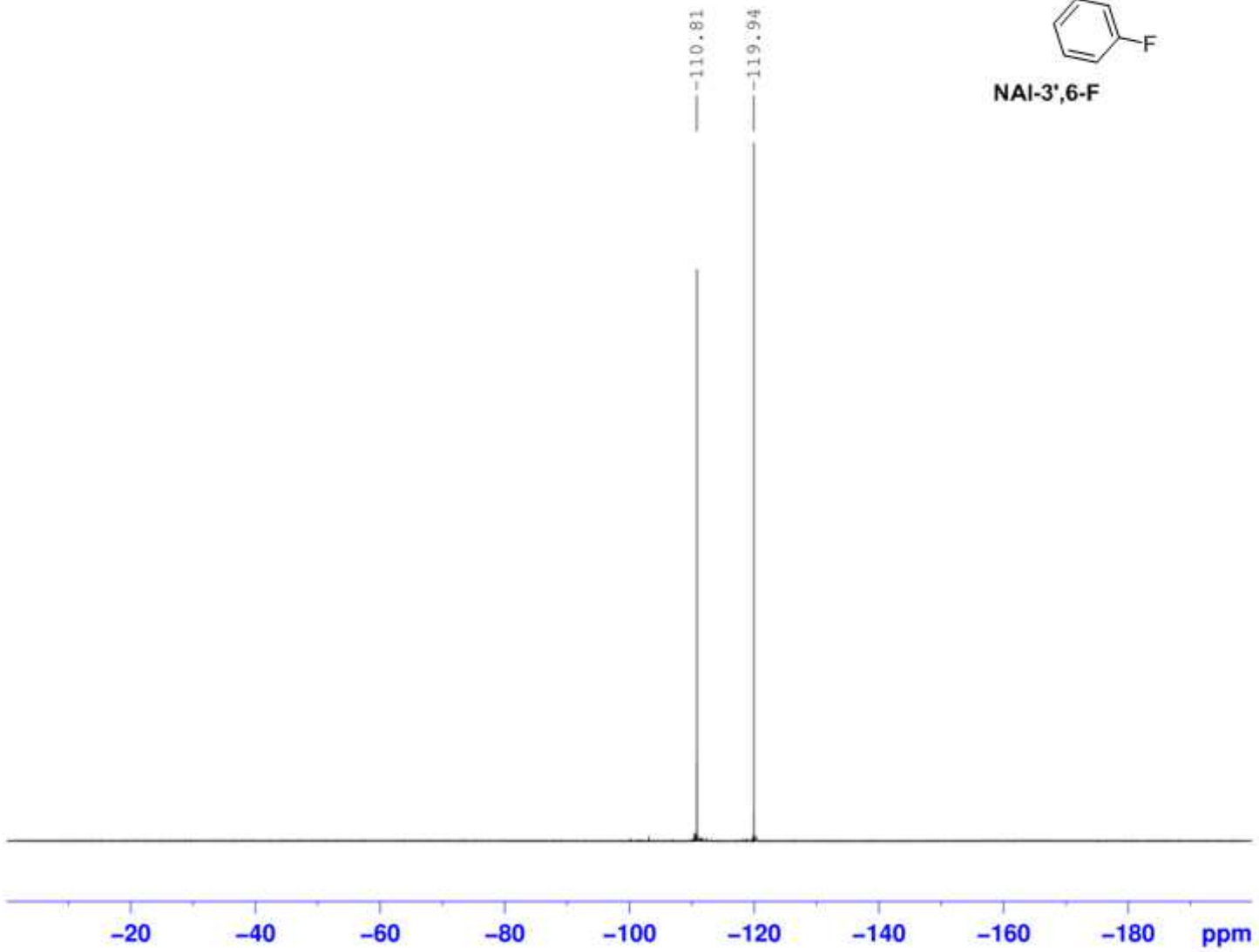
NAME	NAI-3',6-F
EXPNO	470
PROCNO	1
Date_	20110316
Time	3.24
INSTRUM	spect
PROBHD	5 mm QNP 1H/13
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	6218.905 Hz
FIDRES	0.094893 Hz
AQ	5.2691445 sec
RG	80.6
DW	80.400 usec
DE	6.00 usec
TE	294.5 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	13.25 usec
PL1	3.00 dB
SFO1	400.1325018 MHz
SI	131072
SF	400.1300286 MHz
WDW	EM
SSB	0
LB	0.20 Hz
GB	0
PC	1.00


6-fluoro-1-(3-fluorophenyl)-1H-indole
carbon.liv CDCl3 {F:\Av400TopSpin} rc 47
164.450
161.985
161.453
159.081
140.926
140.828
135.623
135.502
132.825
131.012
130.919
128.033
127.996
125.789
125.727
125.407
123.691
122.001
121.952
121.902
119.494
119.462
113.644
113.435
111.685
111.444
111.207
109.524
109.281
104.259
103.506
97.176
96.905
77.317
77.000
76.682
F
N
F
NAI-3',6-F
166 164 162 160 ppm
140 135 130 125 ppm
110 105 100 ppm
220 200 180 160 140 120 100 80 60 40 20 0 ppm
NAME NAI-3',6-F
EXPNO 471
PROCNO 1
Date_ 20110316
Time 3.54
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1024
DS 4
SWH 25125.629 Hz
FIDRES 0.766773 Hz
AQ 0.6521332 sec
RG 5160.6
DW 19.900 use
DE 6.00 use
TE 295.1 K
D1 1.00000000 sec
d11 0.03000000 sec
DELTA 0.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 11.12 use
PL1 5.00 dB
SFO1 100.6227898 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 use
PL2 -3.00 dB
PL12 16.37 dB
PL13 18.00 dB
SFO2 400.1316005 MHz
SI 65536
SF 100.6127772 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

6-fluoro-1-(3-fluorophenyl)-1H-indole
F19CPD.liv CDCl3 (F:\Av400TopSpin) rc 47

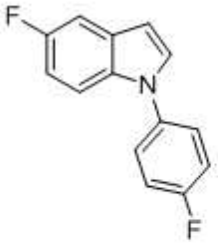


NAI-3',6-F



NAME	NAI-3',6-F
EXPNO	472
PROCNO	1
Date_	20110316
Time	3.56
INSTRUM	spect
PROBHD	5 mm QNP 1H/13
PULPROG	zgfhigqn
TD	131072
SOLVENT	CDCl3
NS	16
DS	4
SWH	75187.969 Hz
FIDRES	0.573639 Hz
AQ	0.8716788 sec
RG	3649.1
DW	6.650 use
DE	6.00 use
TE	294.9 K
D1	1.00000000 sec
d11	0.03000000 sec
d12	0.00002000 sec
TD0	1
======== CHANNEL f1 =======	
NUC1	19F
P1	18.00 use
PL1	-6.00 dB
SFO1	376.4608844 MHz
======== CHANNEL f2 =======	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 use
PL2	-3.00 dB
PL12	16.37 dB
SFO2	400.1316005 MHz
SI	65536
SF	376.4985340 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

5-fluoro-1-(4-fluorophenyl)-1H-indole
quick.proton CDCl3 (F:\Av400TopSpin) rc 48

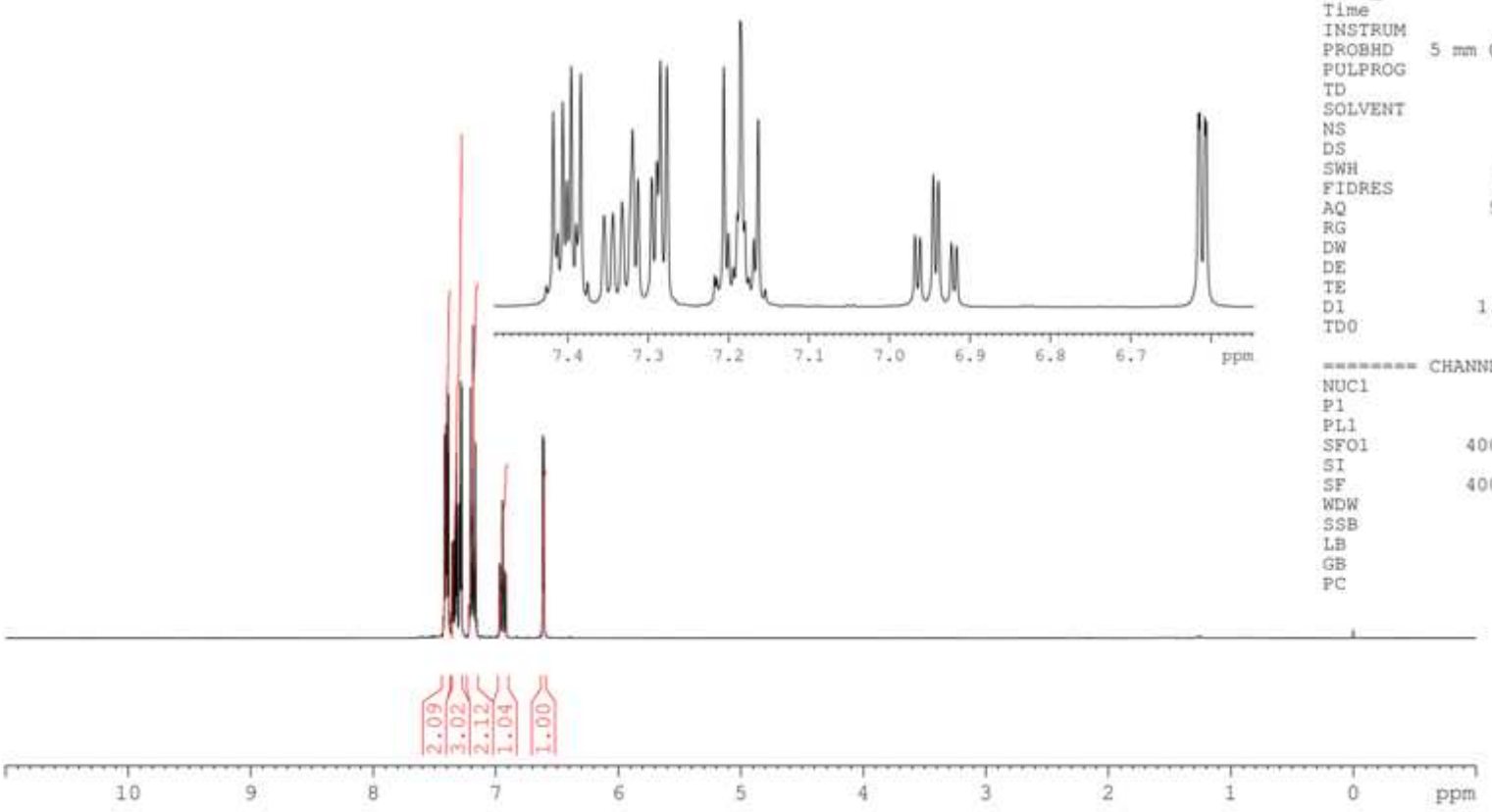


19

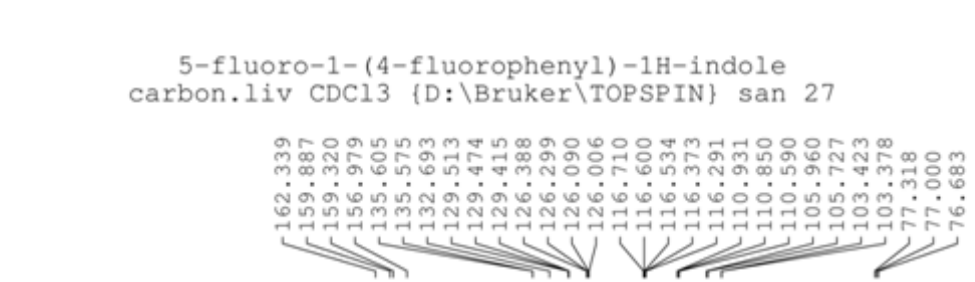
7.42 7.41 7.41 7.40 7.40 7.39 7.38 7.38 7.35 7.34 7.33 7.32 7.31 7.30 7.29 7.28 7.28 7.27 7.22 7.21 7.21 7.20 7.19 7.19 7.19 7.18 7.17 7.17 7.16 7.15 6.97 6.96 6.95 6.94 6.92 6.92 6.62 6.61 6.61 6.61

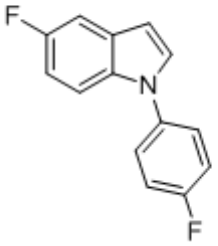
0.00

NAME	NAI-4',5-F
EXPNO	480
PROCNO	1
Date_	20110316
Time	4.03
INSTRUM	spect
PROBHD	5 mm QNP 1H/13
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	6218.905 Hz
FIDRES	0.094893 Hz
AQ	5.2691445 sec
RG	90.5
DW	80.400 usec
DE	6.00 usec
TE	294.5 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	13.25 usec
PL1	3.00 dB
SFO1	400.1325018 MHz
SI	131072
SF	400.1300263 MHz
WDW	EM
SSB	0
LB	0.20 Hz
GB	0
PC	1.00



5-fluoro-1-(4-fluorophenyl)-1H-indole
carbon.liv CDCl3 {D:\Bruker\TOPSPIN} san 27





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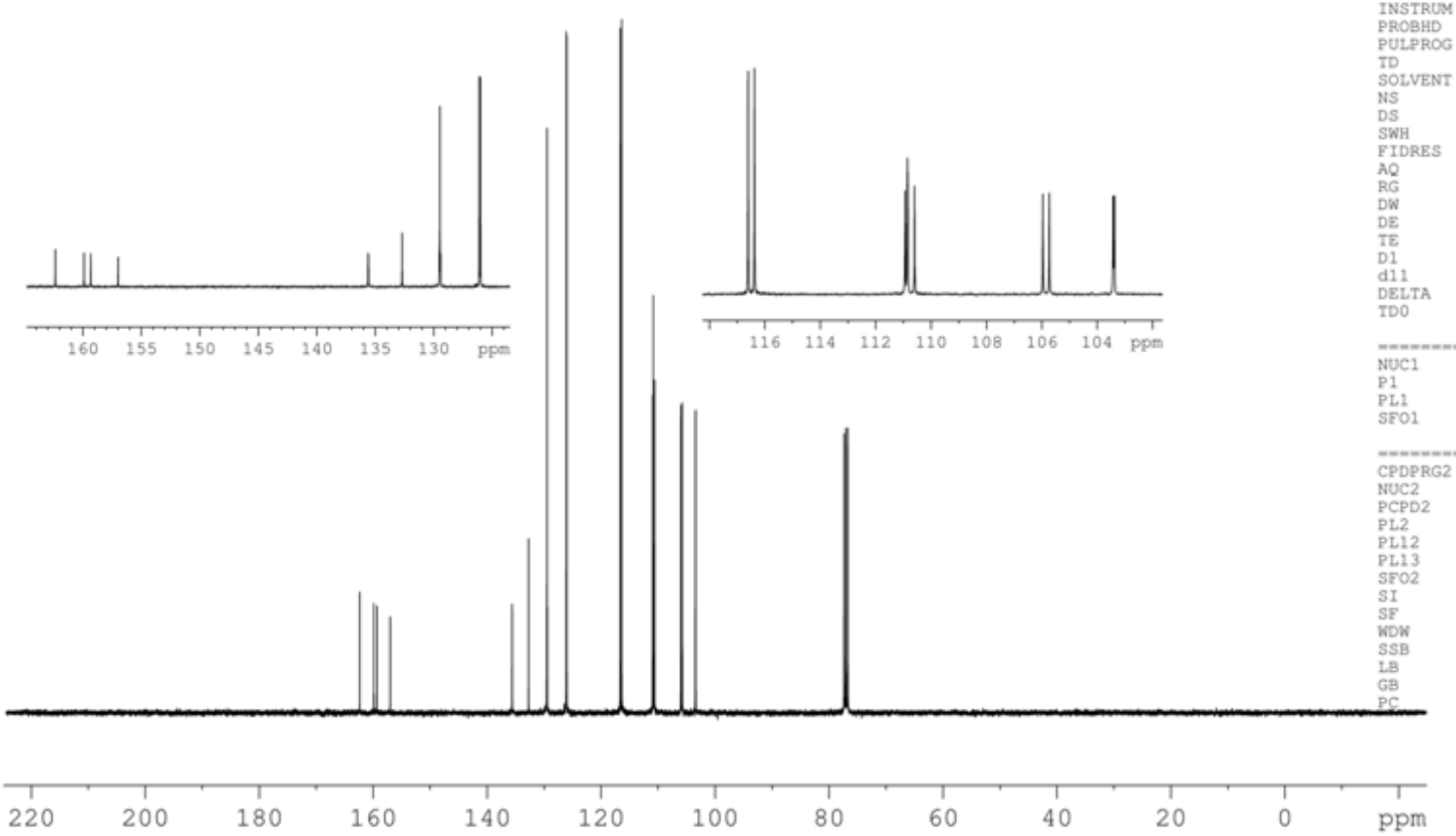
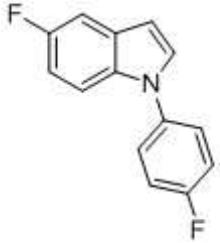
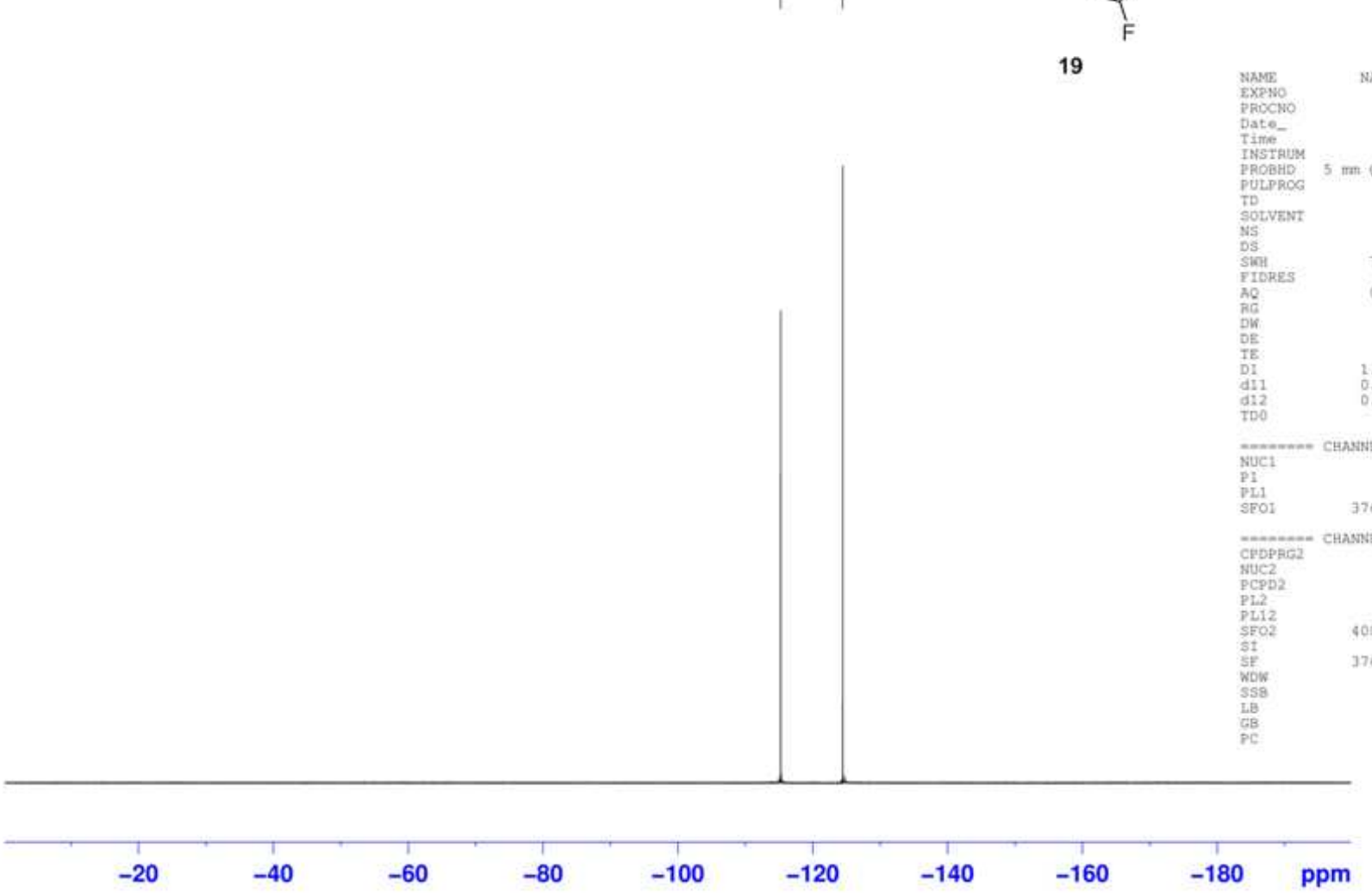


NAME	NAI-4',5-F	
EXPNO	272	
PROCNO	1	
Date_	20100806	
Time	20.37	
INSTRUM	spect	
PROBHD	5 mm QNP 1H/13	
PULPROG	zgpg30	
TD	32768	
SOLVENT	CDCl3	
NS	1024	
DS	4	
SWH	25125.629	Hz
FIDRES	0.766773	Hz
AQ	0.6521332	sec
RG	6502	
DW	19.900	use
DE	6.00	use
TE	296.2	K
D1	1.00000000	sec
d11	0.03000000	sec
DELTA	0.89999998	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	13C	
P1	11.12	use
PL1	5.00	dB
SFO1	100.6227898	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	80.00	use
PL2	-3.00	dB
PL12	16.37	dB
PL13	18.00	dB
SFO2	400.1316005	MHz
SI	65536	
SF	100.6127801	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	

5-fluoro-1-(4-fluorophenyl)-1H-indole
F19CPD.liv CDCl3 {F:\Av400TopSpin} rc 48

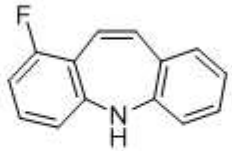


19

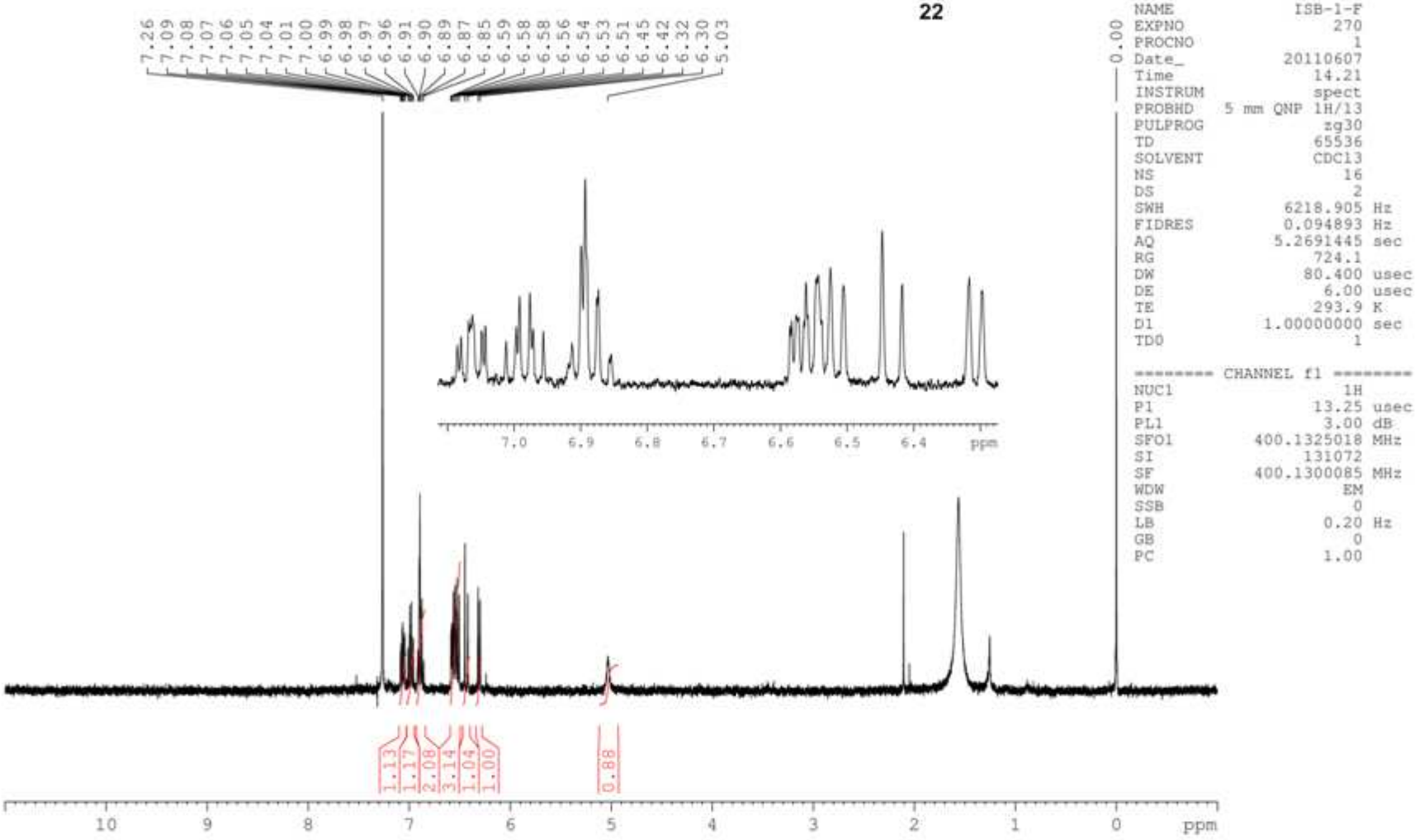


NAME	NAI-4',5-F
EXPNO	482
PROCNO	1
Date_	20110316
Time	4.34
INSTRUM	spect
PROBHD	5 mm QNP 1H/13
PULPROG	zgfhigqn
TD	131072
SOLVENT	CDCl3
NS	16
DS	4
SWH	75187.969 Hz
FIDRES	0.573639 Hz
AQ	0.8716788 sec
RG	3649.1
DW	6.650 usec
DE	6.00 usec
TE	294.9 K
D1	1.00000000 sec
d11	0.03000000 sec
d12	0.00002000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	19F
P1	18.00 usec
PL1	-6.00 dB
SFO1	376.4608844 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-3.00 dB
PL12	16.37 dB
SFO2	400.1316005 MHz
SI	65536
SF	376.4985340 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

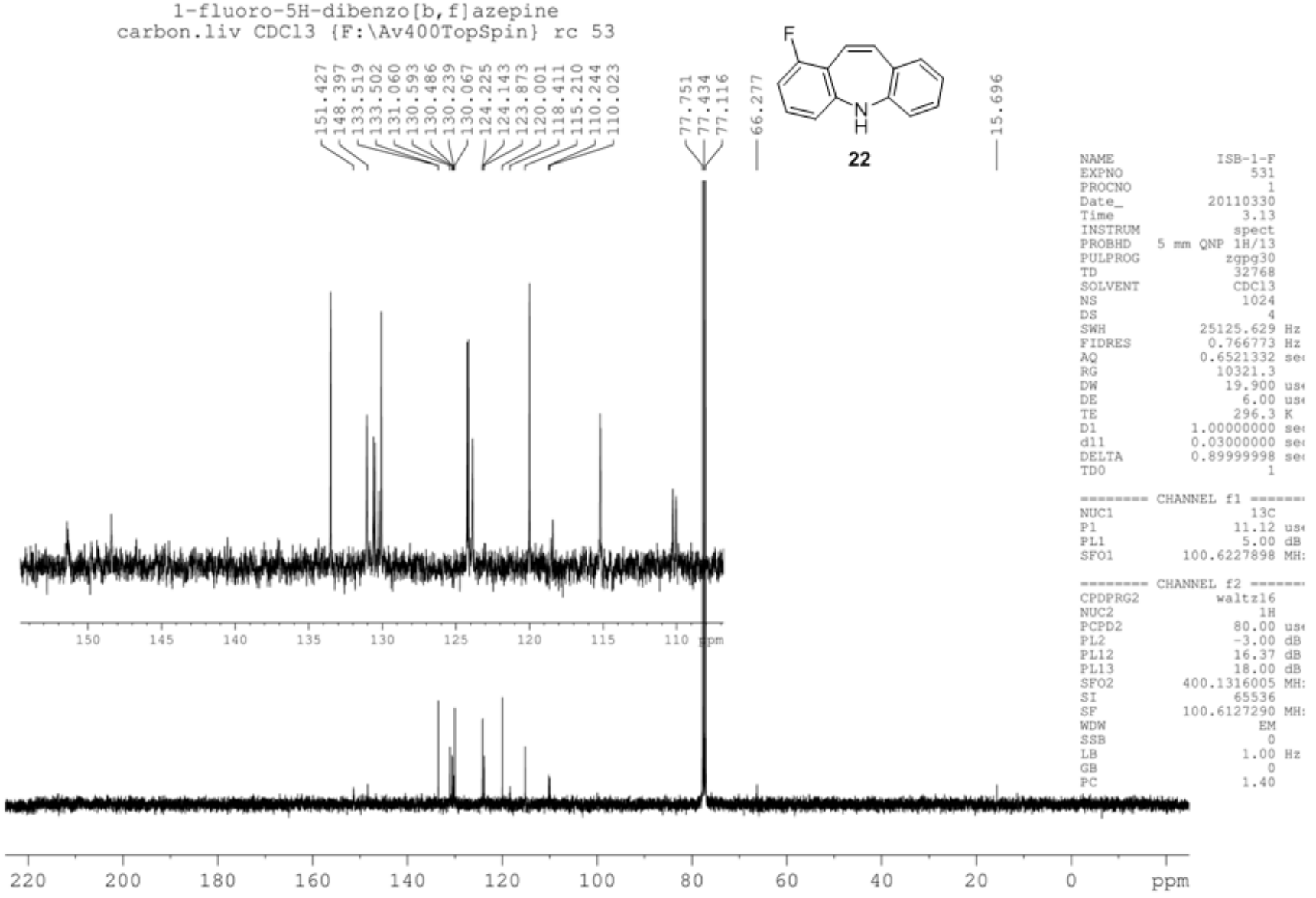
1-fluoro-5H-dibenzo[b,f]azepine
quick.proton CDCl3 (F:\Av400TopSpin) rc 27



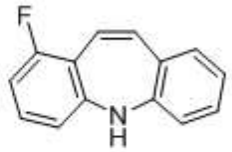
22



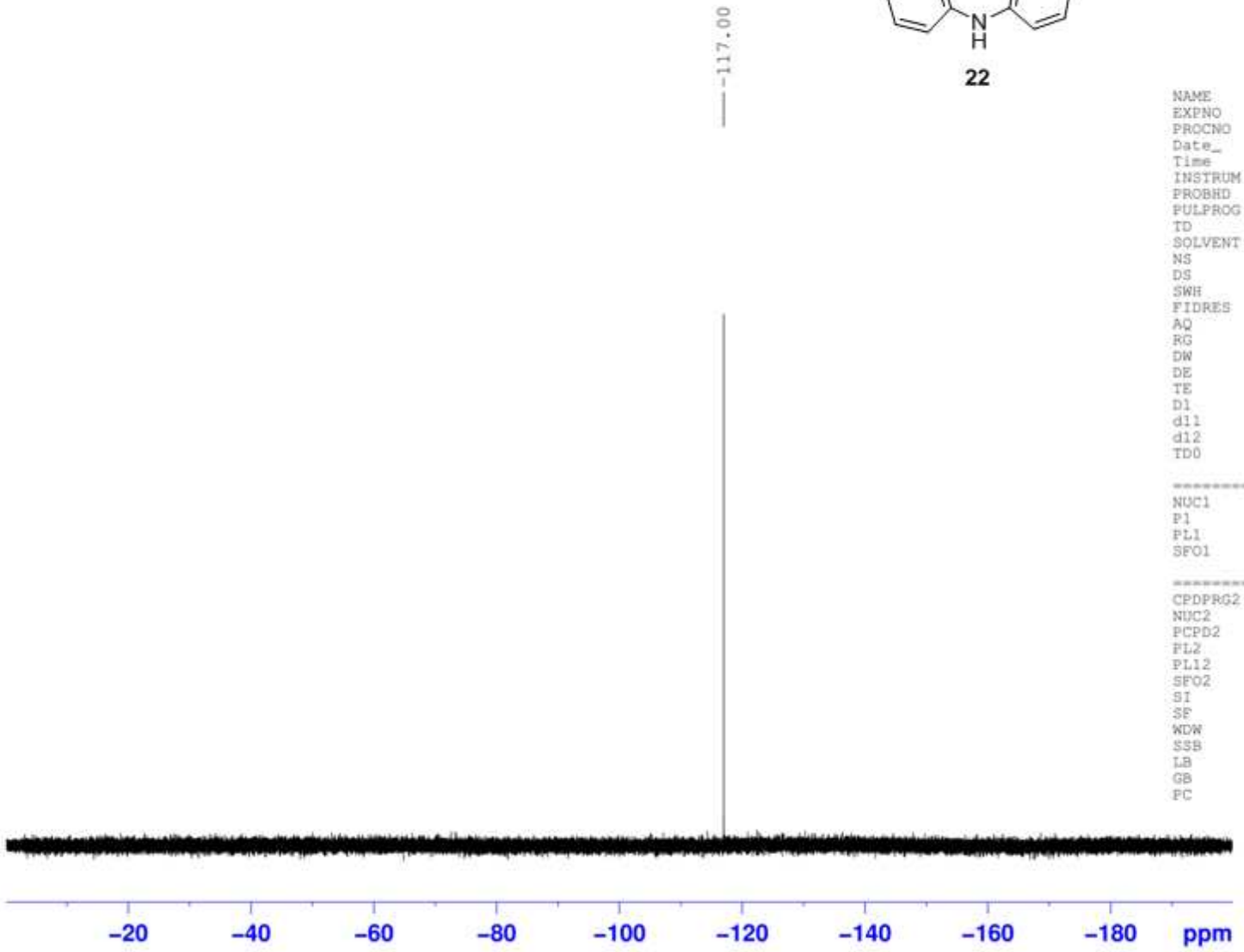
NAME	ISB-1-F
EXPNO	270
PROCNO	1
Date_	20110607
Time	14.21
INSTRUM	spect
PROBHD	5 mm QNP 1H/13
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	6218.905 Hz
FIDRES	0.094893 Hz
AQ	5.2691445 sec
RG	724.1
DW	80.400 usec
DE	6.00 usec
TE	293.9 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	13.25 usec
PL1	3.00 dB
SFO1	400.1325018 MHz
SI	131072
SF	400.1300085 MHz
WDW	EM
SSB	0
LB	0.20 Hz
GB	0
PC	1.00


1-fluoro-5H-dibenzo[b,f]azepine
carbon.liv CDCl3 {F:\Av400TopSpin} rc 53
151.427
148.397
133.519
133.502
131.060
130.593
130.486
130.239
130.067
124.225
124.143
123.873
120.001
118.411
115.210
110.244
110.023
77.751
77.434
77.116
66.277
15.696
F
N
H
22
NAME ISB-1-F
EXPNO 531
PROCNO 1
Date_ 20110330
Time 3.13
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1024
DS 4
SWH 25125.629 Hz
FIDRES 0.766773 Hz
AQ 0.6521332 se
RG 10321.3
DW 19.900 us
DE 6.00 us
TE 296.3 K
D1 1.00000000 se
d11 0.03000000 se
DELTA 0.89999998 se
TD0 1
======== CHANNEL f1 =======
NUC1 13C
P1 11.12 us
PL1 5.00 dB
SFO1 100.6227898 MH
======== CHANNEL f2 =======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 us
PL2 -3.00 dB
PL12 16.37 dB
PL13 18.00 dB
SFO2 400.1316005 MH
SI 65536
SF 100.6127290 MH
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
150 145 140 135 130 125 120 115 110 ppm
220 200 180 160 140 120 100 80 60 40 20 0 ppm

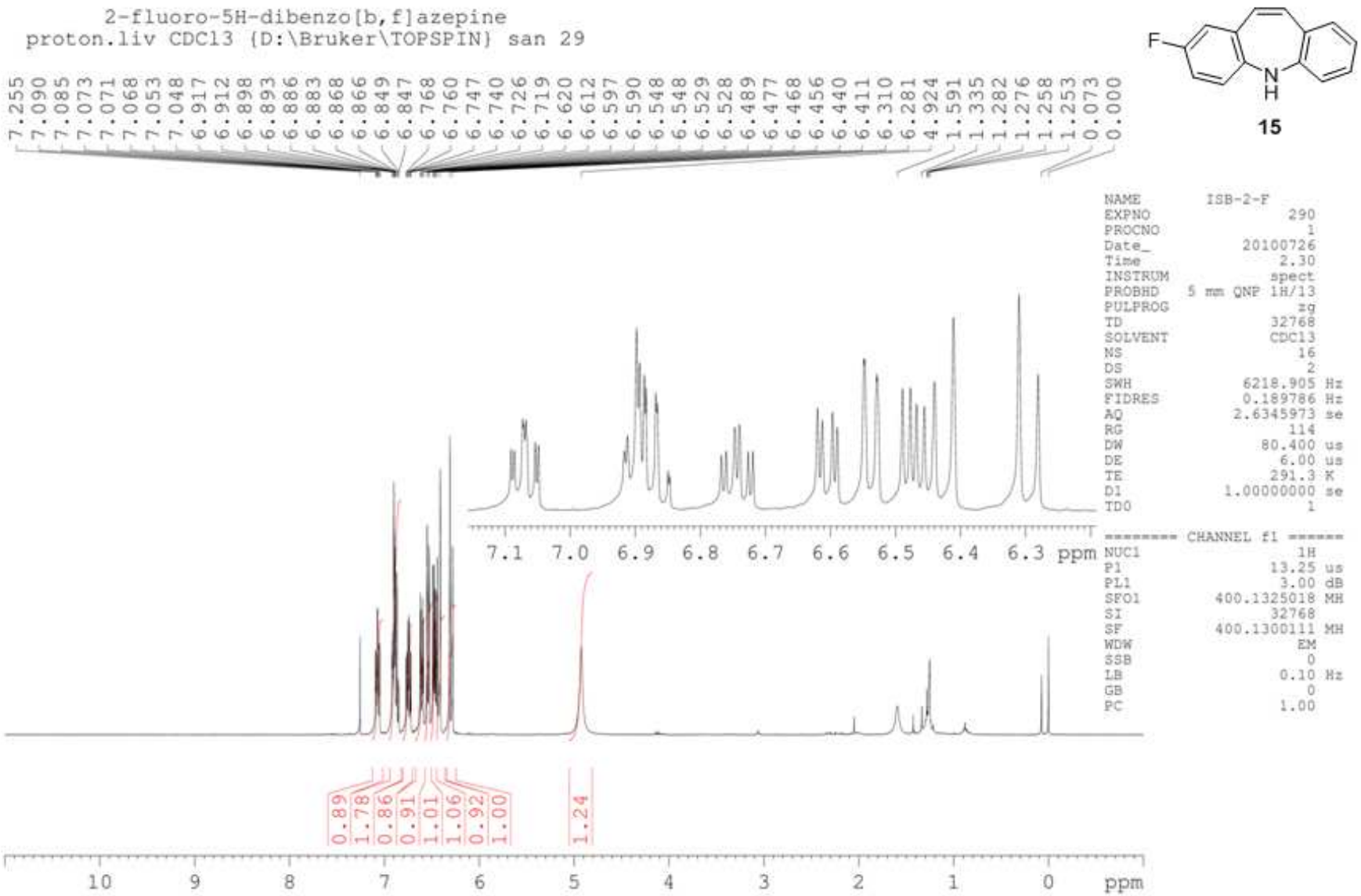
1-fluoro-5H-dibenzo[b,f]azepine
F19CPD.liv CDCl3 (F:\Av400TopSpin) rc 34



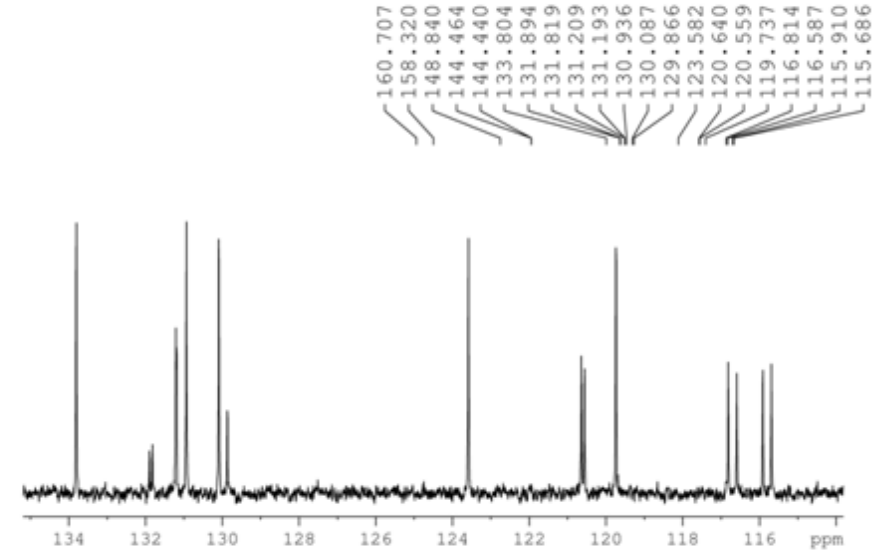
22

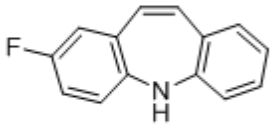


NAME	ISB-1-F	
EXPNO	341	
PROCNO	1	
Date_	20110511	
Time	16.37	
INSTRUM	spect	
PROBHD	5 mm QNP 1H/13	
PULPROG	zgfhigqn	
TD	131072	
SOLVENT	CDCl3	
NS	16	
DS	4	
SWH	75187.969	Hz
FIDRES	0.573639	Hz
AQ	0.8716788	sec
RG	7298.2	
DW	6.650	usec
DE	6.00	usec
TE	297.8	K
D1	1.00000000	sec
d11	0.03000000	sec
d12	0.00002000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	19F	
P1	18.00	usec
PL1	-6.00	dB
SFO1	376.4608844	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	80.00	usec
PL2	-3.00	dB
PL12	16.37	dB
SFO2	400.1316005	MHz
SI	65536	
SF	376.4985340	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	


2-fluoro-5H-dibenzo[b,f]azepine
proton.liv CDCl3 (D:\Bruker\TOPSPIN) san 29
7.255 7.090 7.085 7.073 7.071 7.068 7.053 7.048 6.917 6.912 6.898 6.893 6.886 6.883 6.868 6.866 6.849 6.847 6.768 6.760 6.747 6.740 6.726 6.719 6.620 6.612 6.597 6.590 6.548 6.548 6.529 6.528 6.489 6.477 6.468 6.456 6.440 6.411 6.310 6.281 4.924 1.591 1.335 1.282 1.276 1.258 1.253 0.073 0.000
F
N
H
15
NAME ISB-2-F
EXPNO 290
PROCNO 1
Date_ 20100726
Time 2.30
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 6218.905 Hz
FIDRES 0.189786 Hz
AQ 2.6345973 se
RG 114
DW 80.400 us
DE 6.00 us
TE 291.3 K
D1 1.00000000 se
TD0 1
======== CHANNEL f1 ======
NUC1 1H
P1 13.25 us
PL1 3.00 dB
SFO1 400.1325018 MH
SI 32768
SF 400.1300111 MH
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
7.1 7.0 6.9 6.8 6.7 6.6 6.5 6.4 6.3 ppm
0.89 1.78 0.86 0.91 1.01 1.06 0.92 1.00 1.24
10 9 8 7 6 5 4 3 2 1 0 ppm

2-fluoro-5H-dibenzo[b,f]azepine
carbon.liv CDCl3 {D:\Bruker\TOPSPIN} san 29

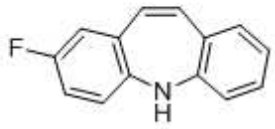




15

NAME	ISB-2-F	
EXPNO	292	
PROCNO	1	
Date_	20100726	
Time	2.56	
INSTRUM	spect	
PROBHD	5 mm QNP 1H/13	
PULPROG	zgpg30	
TD	32768	
SOLVENT	CDCl3	
NS	1024	
DS	4	
SWH	25125.629	Hz
FIDRES	0.766773	Hz
AQ	0.6521332	sec
RG	13004	
DW	19.900	usec
DE	6.00	usec
TE	291.7	K
D1	0.50000000	sec
d11	0.03000000	sec
DELTA	0.40000001	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	13C	
P1	11.12	usec
PL1	5.00	dB
SFO1	100.6227898	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	80.00	usec
PL2	-3.00	dB
PL12	16.37	dB
PL13	18.00	dB
SFO2	400.1316005	MHz
SI	32768	
SF	100.6127379	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	

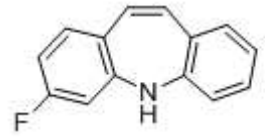
2-fluoro-5H-dibenzo[b,f]azepine
F19CPD.liv CDCl3 (F:\Av400TopSpin) rc 18



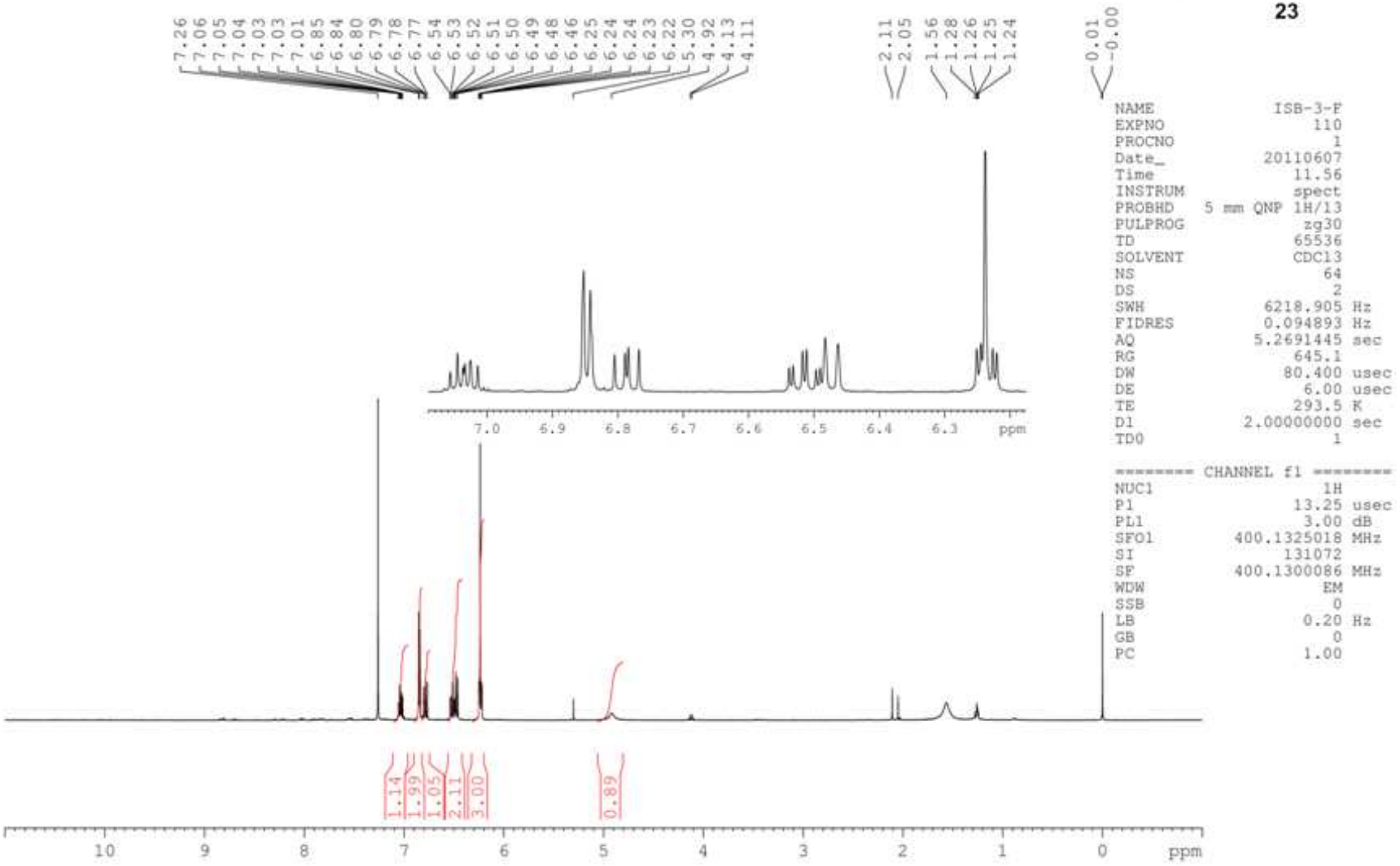
15

NAME	ISB-2-F	
EXPNO	181	
PROCNO	1	
Date_	20110606	
Time	15.28	
INSTRUM	spect	
PROBHD	5 mm QNP 1H/13	
PULPROG	zgfhigqn	
TD	131072	
SOLVENT	CDCl3	
NS	16	
DS	4	
SWH	75187.969	Hz
FIDRES	0.573639	Hz
AQ	0.8716788	sec
RG	8192	
DW	6.650	usec
DE	6.00	usec
TE	294.5	K
D1	1.00000000	sec
d11	0.03000000	sec
d12	0.00002000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	19F	
P1	18.00	usec
PL1	-6.00	dB
SFO1	376.4608844	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	80.00	usec
PL2	-3.00	dB
PL12	16.37	dB
SFO2	400.1316005	MHz
SI	65536	
SF	376.4985340	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	

3-fluoro-5H-dibenzo[b,f]azepine
proton.liv CDCl3 (F:\Av400TopSpin) rc 11

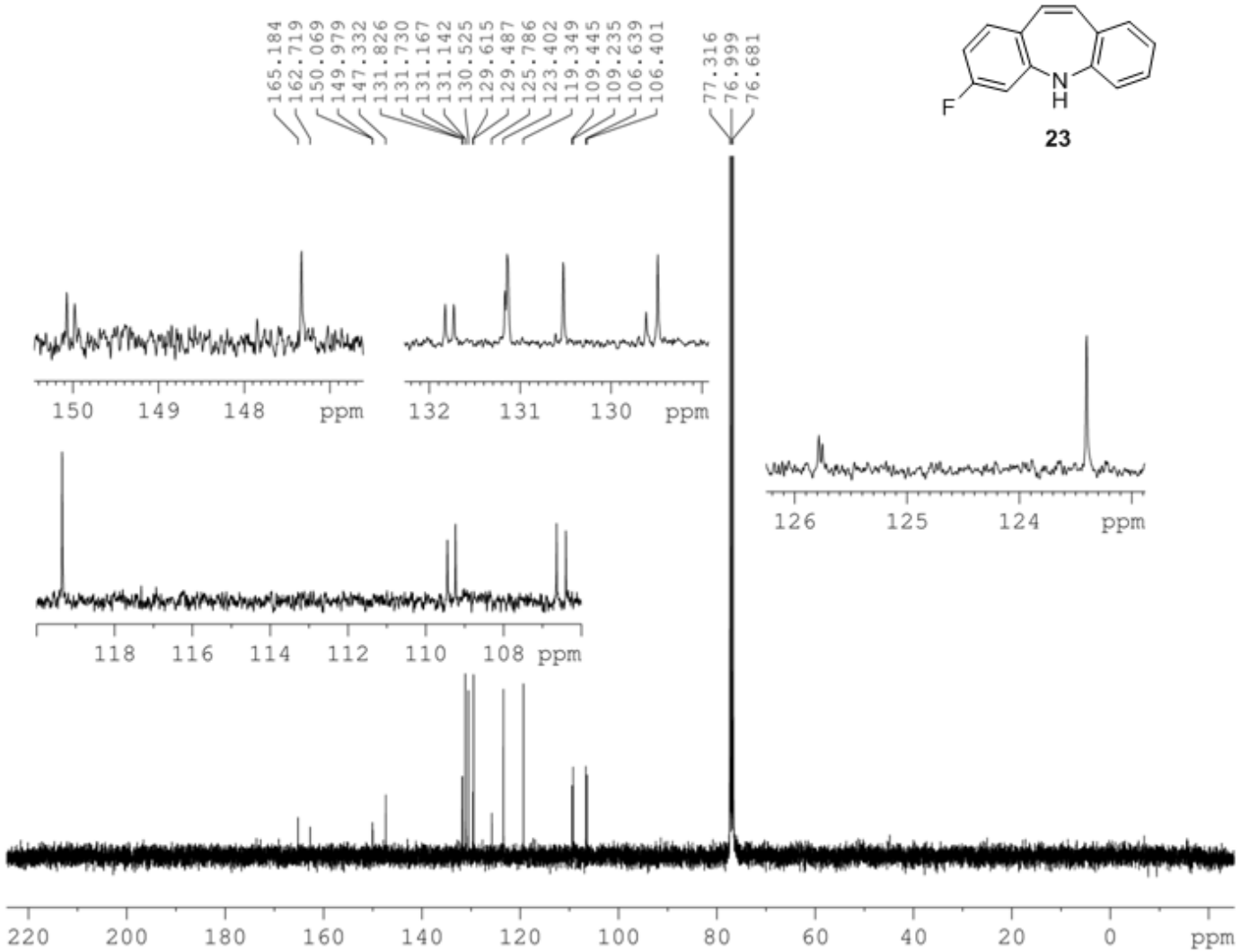


23



NAME	ISB-3-F
EXPNO	110
PROCNO	1
Date_	20110607
Time	11.56
INSTRUM	spect
PROBHD	5 mm QNP 1H/13
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	64
DS	2
SWH	6218.905 Hz
FIDRES	0.094893 Hz
AQ	5.2691445 sec
RG	645.1
DW	80.400 usec
DE	6.00 usec
TE	293.5 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	13.25 usec
PL1	3.00 dB
SFO1	400.1325018 MHz
SI	131072
SF	400.1300086 MHz
WDW	EM
SSB	0
LB	0.20 Hz
GB	0
PC	1.00

3-fluoro-5H-dibenzo[b,f]azepine
carbon.liv CDCl3 {F:\Av400TopSpin} rc 12

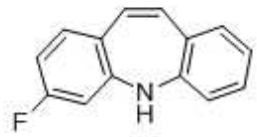


23

NAME	ISB-3-F	
EXPNO	122	
PROCNO	1	
Date_	20110614	
Time	20.38	
INSTRUM	spect	
PROBHD	5 mm QNP 1H/13	
PULPROG	zgpg30	
TD	32768	
SOLVENT	CDCl3	
NS	2048	
DS	4	
SWH	25125.629	H
FIDRES	0.766773	H
AQ	0.6521332	s
RG	6502	
DW	19.900	u
DE	6.00	u
TE	297.0	K
D1	1.00000000	s
d11	0.03000000	s
DELTA	0.89999998	s
TD0	1	
======== CHANNEL f1 =====		
NUC1	13C	
P1	11.12	u
PL1	5.00	d
SFO1	100.6227898	M
======== CHANNEL f2 =====		
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	80.00	u
PL2	-3.00	d
PL12	16.37	d
PL13	18.00	d
SFO2	400.1316005	M
SI	65536	
SF	100.6127712	M
WDW	EM	
SSB	0	
LB	1.00	H
GB	0	
PC	1.40	

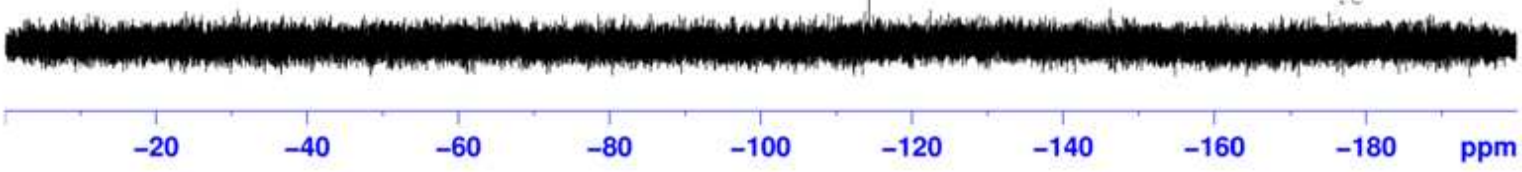
3-fluoro-5H-dibenzo[b,f]azepine
F19CPD.liv CDC13 {F:\Av400TopSpin} rc 11

-114.34

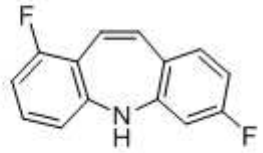


23

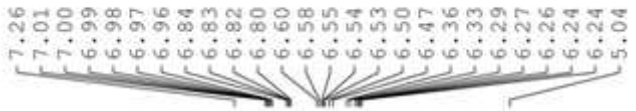
NAME	ISB-3-F
EXPNO	111
PROCNO	1
Date_	20110607
Time	11.57
INSTRUM	spect
PROBHD	5 mm QNP 1H/13
PULPROG	zgfhigqn
TD	131072
SOLVENT	CDC13
NS	16
DS	4
SWH	75187.969 Hz
FIDRES	0.573639 Hz
AQ	0.8716788 sec
RG	8192
DW	6.650 usec
DE	6.00 usec
TE	293.6 K
D1	1.00000000 sec
d11	0.03000000 sec
d12	0.00002000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	19F
P1	18.00 usec
PL1	-6.00 dB
SFO1	376.4608844 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-3.00 dB
PL12	16.37 dB
SFO2	400.1316005 MHz
SI	65536
SF	376.4985340 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



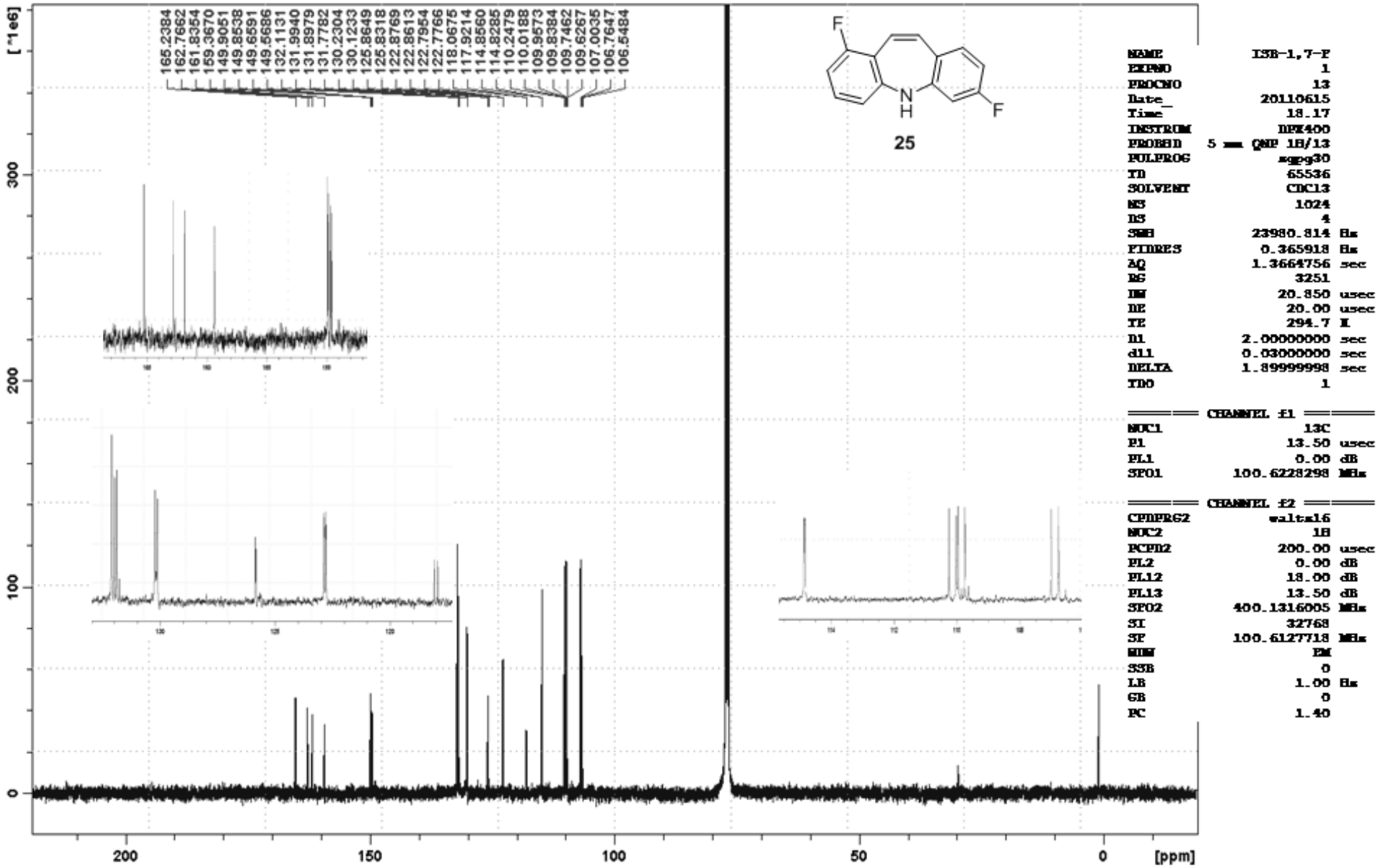
1,7-difluoro-5H-dibenzo[b,f]azepine
quick.proton CDCl3 (F:\Av400TopSpin) rc 40



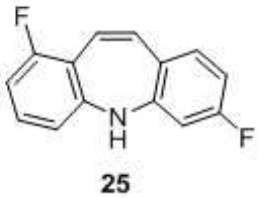
25



NAME	ISB-1,7-F
EXPNO	400
PROCNO	1
Date_	20110607
Time	16.50
INSTRUM	spect
PROBHD	5 mm QNP 1H/13
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	6218.905 Hz
FIDRES	0.094893 Hz
AQ	5.2691445 sec
RG	456.1
DW	80.400 usec
DE	6.00 usec
TE	294.1 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	13.25 usec
PL1	3.00 dB
SFO1	400.1325018 MHz
SI	131072
SF	400.1300090 MHz
WDW	EM
SSB	0
LB	0.20 Hz
GB	0
PC	1.00


165.2384
162.7662
161.8354
159.3670
149.9051
149.8538
149.6591
149.5686
132.1131
131.9940
131.8979
131.7782
130.2304
130.1233
125.8649
125.8318
122.8769
122.8613
122.7954
122.7766
118.0675
117.9214
114.8560
114.8285
110.2479
110.0188
109.9573
109.8384
109.7462
109.6267
107.0035
106.7647
106.5484
F
N
H
F
25
NAME ISB-1,7-F
EXPNO 1
PROCNO 13
Date_ 20110615
Time 18.17
INSTRUM DPX400
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 3251
DW 20.850 usec
DE 20.00 usec
TE 294.7 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
CHANNEL f1
NUC1 13C
P1 13.50 usec
PL1 0.00 dB
SFO1 100.6228298 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 200.00 usec
PL2 0.00 dB
PL12 18.00 dB
PL13 13.50 dB
SFO2 400.1316005 MHz
SI 32768
SF 100.6127718 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
[*1e6]
300
200
100
0
200
150
100
50
0
[ppm]

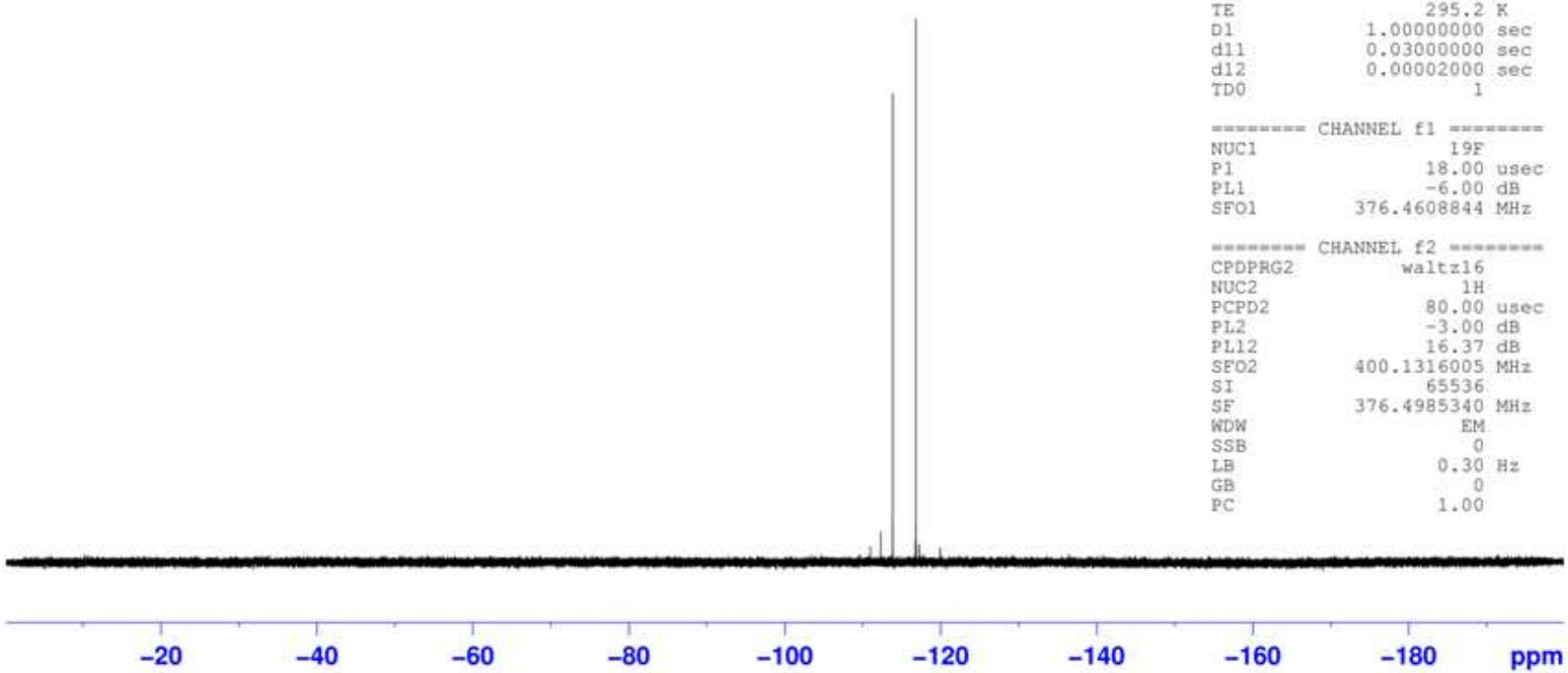
1,7-difluoro-5H-dibenzo[b,f]azepine
F19CPD.liv CDCl3 (F:\Av400TopSpin) rc 43



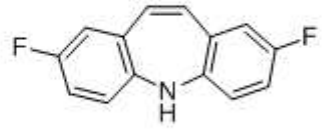
25

-113.84
-116.82

NAME	ISB-1,7-F
EXPNO	432
PROCNO	1
Date_	20110318
Time	5.13
INSTRUM	spect
PROBHD	5 mm QNP 1H/13
PULPROG	zgfhigqn
TD	131072
SOLVENT	CDCl3
NS	16
DS	4
SWH	75187.969 Hz
FIDRES	0.573639 Hz
AQ	0.8716788 sec
RG	9195.2
DW	6.650 usec
DE	6.00 usec
TE	295.2 K
D1	1.00000000 sec
d11	0.03000000 sec
d12	0.00002000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	19F
P1	18.00 usec
PL1	-6.00 dB
SFO1	376.4608844 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-3.00 dB
PL12	16.37 dB
SFO2	400.1316005 MHz
SI	65536
SF	376.4985340 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



2,8-difluoro-5H-dibenzo[b,f]azepine
quick.proton CDCl3 (F:\Av400TopSpin) rc 17



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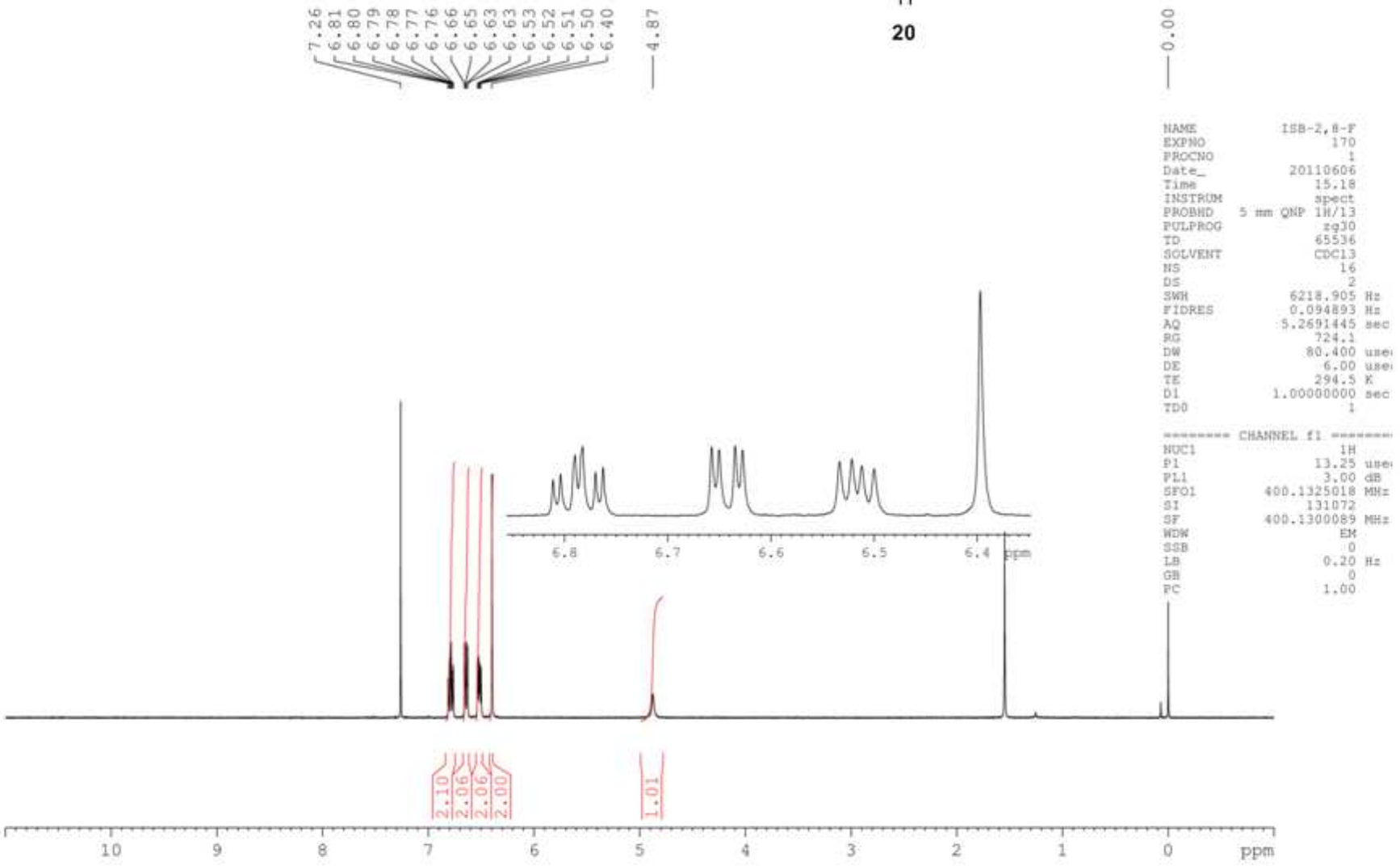
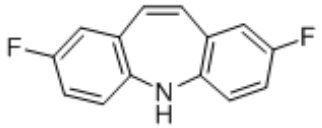
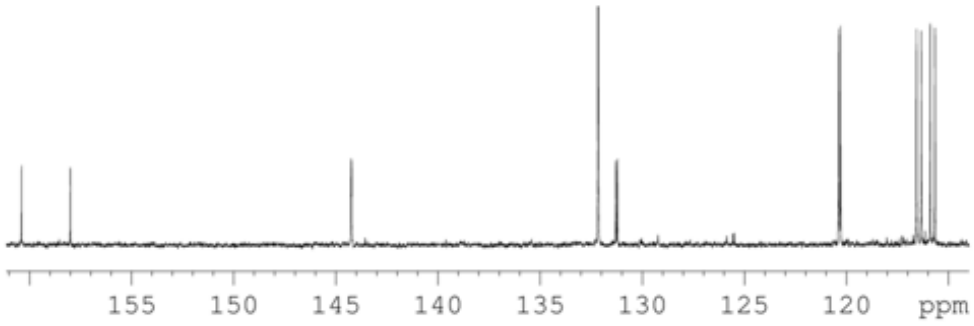


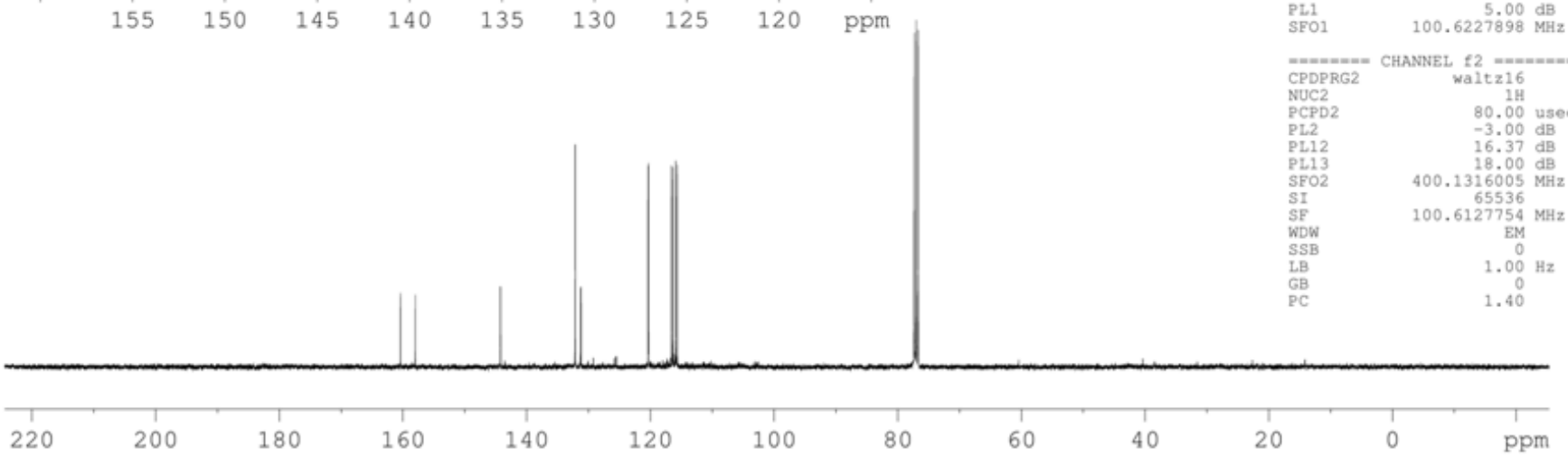
2,8-difluoro-5H-dibenzo[b,f]azepine
carbon.liv CDCl3 {F:\Av400TopSpin} rc 6



20

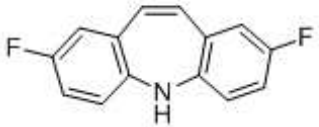
160.389
157.996
144.244
144.220
132.159
132.140
131.281
131.205
120.368
120.287
116.563
116.335
115.885
115.661
77.318
77.000
76.683





NAME	ISB-2,8-F
EXPNO	62
PROCNO	1
Date_	20101022
Time	1.57
INSTRUM	spect
PROBHD	5 mm QNP 1H/13
PULPROG	zgpg30
TD	32768
SOLVENT	CDCl3
NS	1024
DS	4
SWH	25125.629 Hz
FIDRES	0.766773 Hz
AQ	0.6521332 sec
RG	6502
DW	19.900 use
DE	6.00 use
TE	294.6 K
D1	1.00000000 sec
d11	0.03000000 sec
DELTA	0.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	11.12 use
PL1	5.00 dB
SFO1	100.6227898 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 use
PL2	-3.00 dB
PL12	16.37 dB
PL13	18.00 dB
SFO2	400.1316005 MHz
SI	65536
SF	100.6127754 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

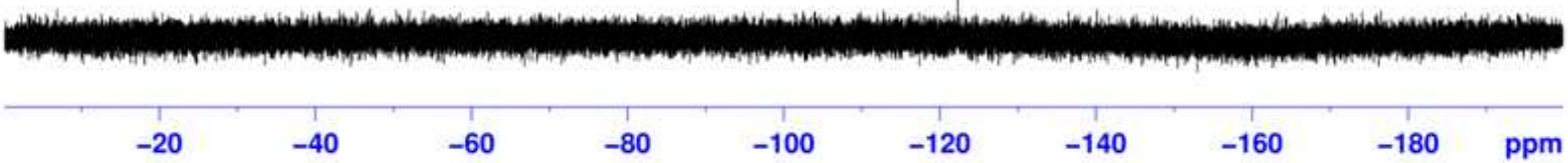
2,8-difluoro-5H-dibenzo[b,f]azepine
F19CPD.liv CDCl3 (F:\Av400TopSpin) rc 17



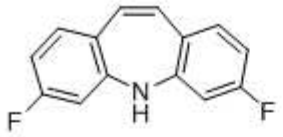
20

-122.31

NAME	ISB-2,8-F
EXPNO	171
PROCNO	1
Date_	20110606
Time	15.20
INSTRUM	spect
PROBHD	5 mm QNP 1H/13
PULPROG	zgfhigqn
TD	131072
SOLVENT	CDCl3
NS	16
DS	4
SWH	75187.969 Hz
FIDRES	0.573639 Hz
AQ	0.8716788 sec
RG	9195.2
DW	6.650 use
DE	6.00 use
TE	294.5 K
D1	1.00000000 sec
d11	0.03000000 sec
d12	0.00002000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	19F
P1	18.00 use
PL1	-6.00 dB
SFO1	376.4608844 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 use
PL2	-3.00 dB
PL12	16.37 dB
SFO2	400.1316005 MHz
SI	65536
SF	376.4985340 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



3,7-difluoro-5H-dibenzo[b,f]azepine
proton.liv CDCl3 (F:\Av400TopSpin) rc 24



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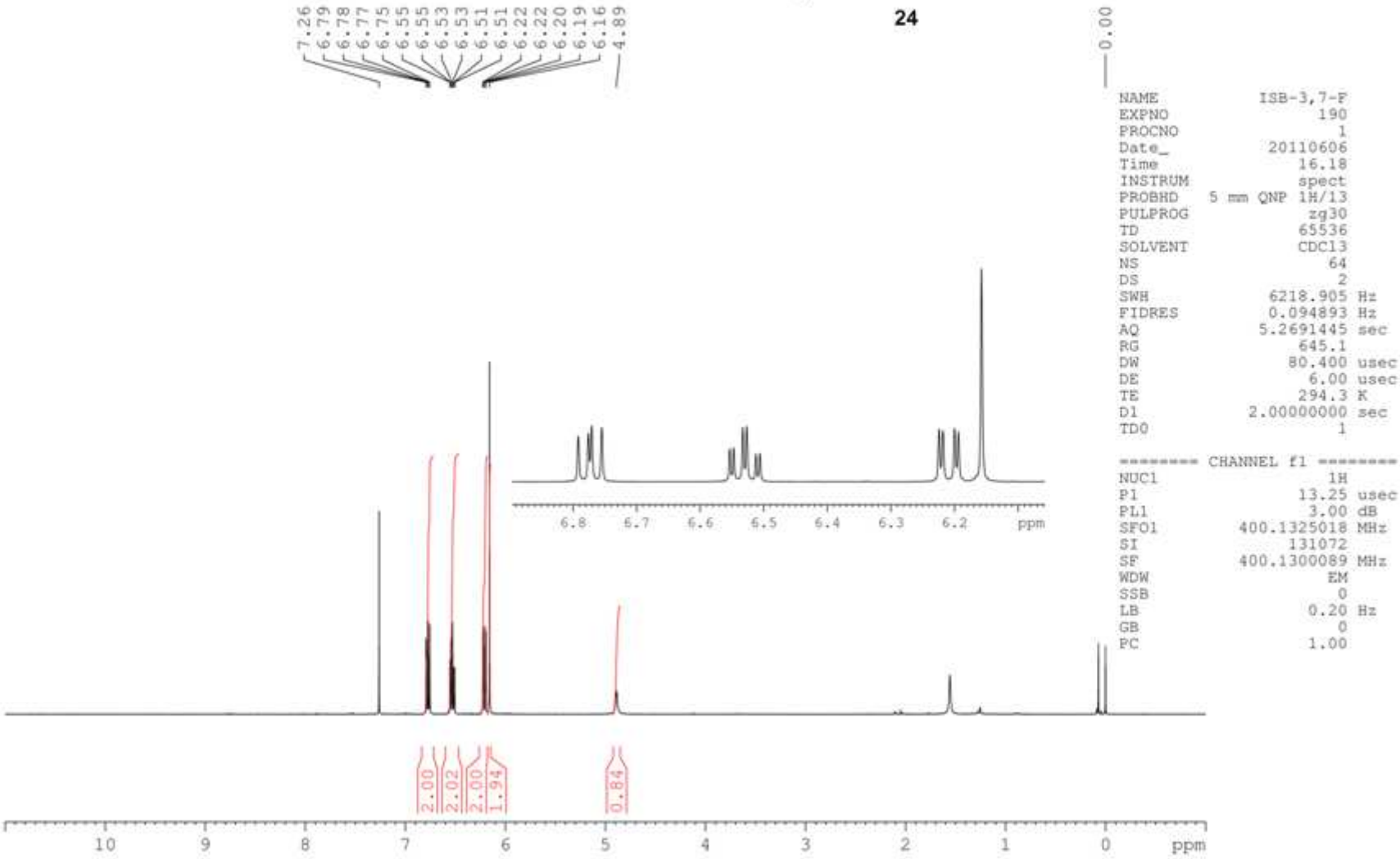
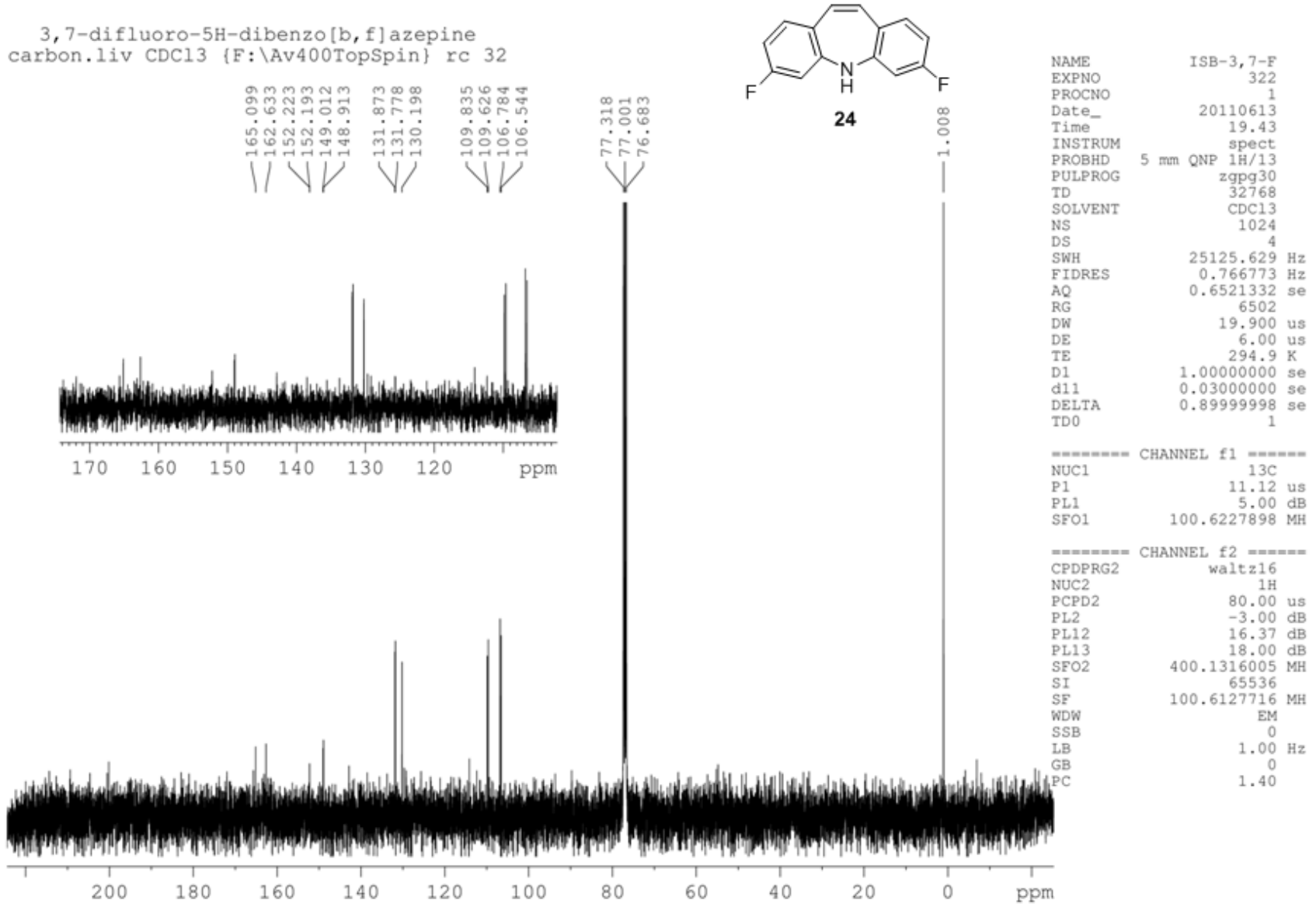
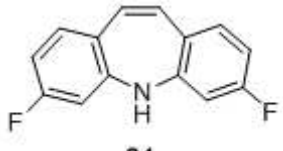


NAME	ISB-3,7-F
EXPNO	190
PROCNO	1
Date_	20110606
Time	16.18
INSTRUM	spect
PROBHD	5 mm QNP 1H/13
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	64
DS	2
SWH	6218.905 Hz
FIDRES	0.094893 Hz
AQ	5.2691445 sec
RG	645.1
DW	80.400 usec
DE	6.00 usec
TE	294.3 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	13.25 usec
PL1	3.00 dB
SFO1	400.1325018 MHz
SI	131072
SF	400.1300089 MHz
WDW	EM
SSB	0
LB	0.20 Hz
GB	0
PC	1.00


3,7-difluoro-5H-dibenzo[b,f]azepine
carbon.liv CDCl3 {F:\Av400TopSpin} rc 32
165.099
162.633
152.223
152.193
149.012
148.913
131.873
131.778
130.198
109.835
109.626
106.784
106.544
77.318
77.001
76.683
1.008
170 160 150 140 130 120 ppm
200 180 160 140 120 100 80 60 40 20 0 ppm
F
N
H
F
24
NAME ISB-3,7-F
EXPNO 322
PROCNO 1
Date_ 20110613
Time 19.43
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1024
DS 4
SWH 25125.629 Hz
FIDRES 0.766773 Hz
AQ 0.6521332 se
RG 6502
DW 19.900 us
DE 6.00 us
TE 294.9 K
D1 1.00000000 se
d11 0.03000000 se
DELTA 0.89999998 se
TD0 1
======== CHANNEL f1 ======
NUC1 13C
P1 11.12 us
PL1 5.00 dB
SFO1 100.6227898 MH
======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 us
PL2 -3.00 dB
PL12 16.37 dB
PL13 18.00 dB
SFO2 400.1316005 MH
SI 65536
SF 100.6127716 MH
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

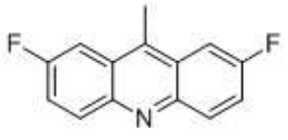
3,7-difluoro-5H-dibenzo[b,f]azepine
F19CPD.liv CDCl3 (F:\Av400TopSpin) rc 24



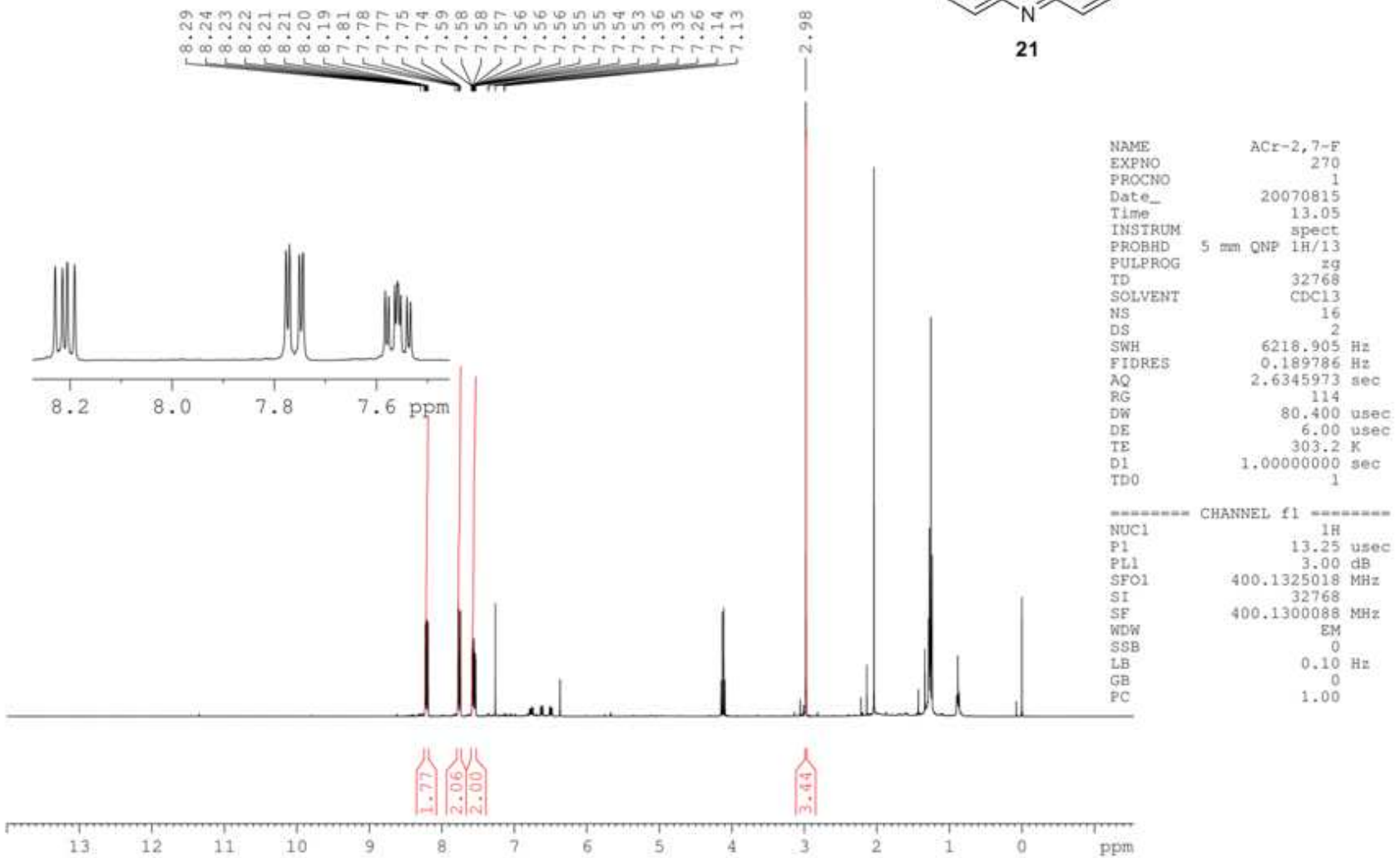
24

NAME	ISB-3,7-F
EXPNO	191
PROCNO	1
Date_	20110606
Time	16.20
INSTRUM	spect
PROBHD	5 mm QNP 1H/13
PULPROG	zgfhigqn
TD	131072
SOLVENT	CDCl3
NS	16
DS	4
SWH	75187.969 Hz
FIDRES	0.573639 Hz
AQ	0.8716788 sec
RG	7298.2
DW	6.650 usec
DE	6.00 usec
TE	294.3 K
D1	1.00000000 sec
d11	0.03000000 sec
d12	0.00002000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	19F
P1	18.00 usec
PL1	-6.00 dB
SFO1	376.4608844 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-3.00 dB
PL12	16.37 dB
SFO2	400.1316005 MHz
SI	65536
SF	376.4985340 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

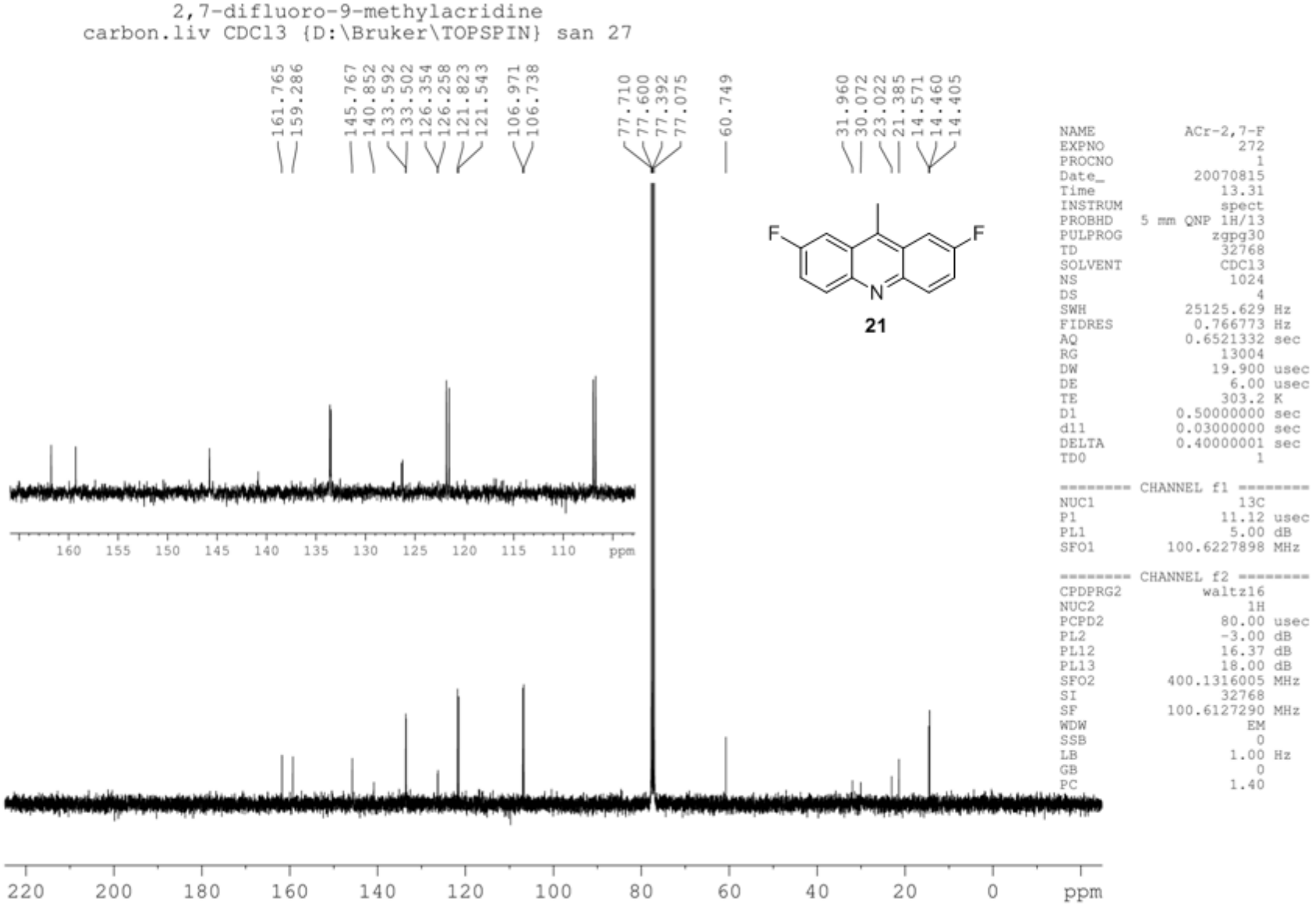
2,7-difluoro-9-methylacridine
proton.liv CDCl3 (D:\Bruker\TOPSPIN) san 27



21



NAME	ACr-2,7-F
EXPNO	270
PROCNO	1
Date_	20070815
Time	13.05
INSTRUM	spect
PROBHD	5 mm QNP 1H/13
PULPROG	zg
TD	32768
SOLVENT	CDCl3
NS	16
DS	2
SWH	6218.905 Hz
FIDRES	0.189786 Hz
AQ	2.6345973 sec
RG	114
DW	80.400 usec
DE	6.00 usec
TE	303.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	13.25 usec
PL1	3.00 dB
SFO1	400.1325018 MHz
SI	32768
SF	400.1300088 MHz
WDW	EM
SSB	0
LB	0.10 Hz
GB	0
PC	1.00


2,7-difluoro-9-methylacridine
carbon.liv CDCl3 {D:\Bruker\TOPSPIN} san 27
161.765
159.286
145.767
140.852
133.592
133.502
126.354
126.258
121.823
121.543
106.971
106.738
77.710
77.600
77.392
77.075
60.749
31.960
30.072
23.022
21.385
14.571
14.460
14.405
F
F
N
21
NAME ACr-2,7-F
EXPNO 272
PROCNO 1
Date_ 20070815
Time 13.31
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1024
DS 4
SWH 25125.629 Hz
FIDRES 0.766773 Hz
AQ 0.6521332 sec
RG 13004
DW 19.900 usec
DE 6.00 usec
TE 303.2 K
D1 0.50000000 sec
d11 0.03000000 sec
DELTA 0.40000001 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 11.12 usec
PL1 5.00 dB
SFO1 100.6227898 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 16.37 dB
PL13 18.00 dB
SFO2 400.1316005 MHz
SI 32768
SF 100.6127290 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
160 155 150 145 140 135 130 125 120 115 110 ppm
220 200 180 160 140 120 100 80 60 40 20 0 ppm

4. References

1. Pretsch, E.; Bühlmann, P.; Affolter, C., *Structure Determination of Organic Compounds: Tables of Spectral Data*. Third Completely Revised and Enlarged English Edition ed.; Springer: Berlin, Heidelberg, New York, HongKong, London, Mailand, Paris, Tokyo, 2000; p 421.
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