

Supporting Information

Catalytic Asymmetric Passerini Type Reaction: Chiral Aluminium–Organophosphate—Catalyzed Enantioselective α -Addition of Isocyanides to Aldehydes

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1. General information

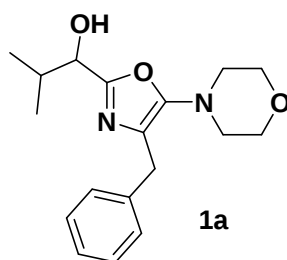
¹H and ¹³C NMR spectra were recorded on a 300 spectrometer at ambient temperature. Melting points are uncorrected. All chemicals were dried or purified according to standard procedures prior to use. Enantiomeric excess values of all compounds were

obtained from HPLC analyses.

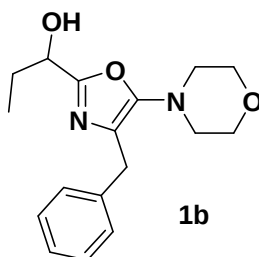
2. General procedure for the experiment

In a flame-dried round-bottom flask equipped with a stir bar were added binol-derived organophosphoric acid (0.025 mmol) and dry toluene (1 mL). The mixture was stirred at room temperature for several minutes, to which the solution of Et₂AlCl (0.0125 mmol) in toluene was added carefully. The mixture was stirred at room temperature until the solution to be clear about 2h. The aldehyde (0.25 mmol, in 0.5mL of toluene) was then introduced and the resulting mixture was stirred at room temperature for 30 min. The reaction mixture was cooled to -40°C and a solution of α-isocyanoacetamide (0.25mmol) in toluene (2.0 mL) was added slowly via a syringe pump (addition time 1.5h). After being stirred at -40 °C for 48 h, the reaction mixture was purified by flash column chromatography (SiO₂, petroleum ether then petroleum ether/EtOAc = 1/1) to give the corresponding oxazole.

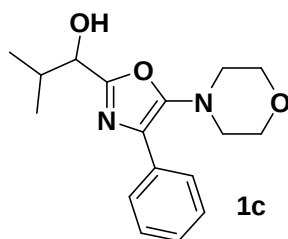
3. Spectroscopic data of all compounds prepared



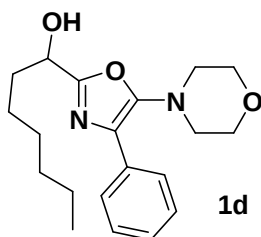
1-(4-benzyl-5-morpholinooxazol-2-yl)-2-methylpropan-1-ol (1a) White solid; $[\alpha]_D^{20} = +15.3$ (c 2.65, CHCl₃); yield: 93%, ee: 87% (ADH, hexane/ⁱPrOH = 9/1, 15 °C, 0.5mL/min). (lit. Wang, S. -X.; Wang, M. -X.; Wang, D. -X.; Zhu, J. *Org. Lett.* **2007**, 9, 3615-3618)



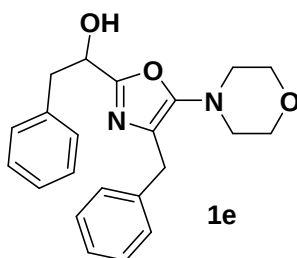
1-(4-benzyl-5-morpholinooxazol-2-yl)propan-1-ol (1b) White solid; $[\alpha]_D^{20} = +5.3$ (c 3, CHCl₃); yield: 80%, ee: 60% (ADH, hexane/ⁱPrOH = 9/1, 15 °C, 0.5mL/min). (lit. Wang, S. -X.; Wang, M. -X.; Wang, D. -X.; Zhu, J. *Org. Lett.* **2007**, 9, 3615-3618)



2-methyl-1-(5-morpholino-4-phenyloxazol-2-yl)propan-1-ol (1c) White solid mp 117-118 °C; $[\alpha]_D^{20} = +5.5$ (c 0.85, CHCl₃); yield: 95%, ee: 81% (ADH, hexane/ⁱPrOH = 9/1, 25 °C 0.5mL/min); IR (KBr) ν 3237, 2966, 2849, 1636, 1381, 1114, cm⁻¹; ¹HNMR (CDCl₃, 300MHz) δ 7.95 (d, J = 8.5Hz, 2H), 7.42-7.37 (m, 2H), 7.29-7.24 (m, 1H), 4.49 (t, J = 5.9Hz, 1H), 3.87-3.84 (m, 4H), 3.11-3.08 (m, 4H), 2.96 (d, J = 6.0Hz, 1H), 2.21-2.15 (m, 1H), 1.00 (d, J = 7.1Hz, 3H), 0.98 (d, J = 7.1Hz, 3H); ¹³CNMR (CDCl₃, 75MHz) δ 159.7, 151.1, 131.6, 128.5, 127.1, 125.9, 123.7, 73.0, 66.9, 50.4, 33.5, 18.4, 17.3 ; MS (ESI) m/z 303 (M+H), 325 (M+Na); Anal. Calcd. for C₁₇H₂₂N₂O₃: C: 67.53, H: 7.33, N: 9.26; Found: C: 67.24, H: 7.33, N: 9.26.

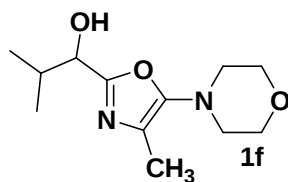


1-(5-morpholino-4-phenyloxazol-2-yl)heptan-1-ol (1d) Colorless oil; $[\alpha]_D^{20} = +8.8$ (c 3.4, CHCl₃); yield: 87%, ee: 68% (ADH, hexane/ⁱPrOH = 9/1, 25 °C, 0.5mL/min); IR (KBr) ν 3409, 2925, 2855, 1633, 1453, 1116, cm⁻¹; ¹HNMR (CDCl₃, 300MHz) δ 7.91 (d, J = 6.5Hz, 2H), 7.41-7.36 (m, 2H), 7.27-7.22 (m, 1H), 4.74-4.68 (m, 1H), 3.83 (t, J = 4.6Hz, 4H), 3.73 (d, J = 5.3Hz, 1H), 3.06 (t, J = 4.7Hz, 4H), 1.94-1.85 (m, 2H), 1.50-1.28 (m, 8H), 0.87 (t, J = 6.4Hz, 3H); ¹³CNMR (CDCl₃, 75MHz) δ 160.3, 151.0, 131.6, 128.5, 127.1, 125.9, 123.6, 67.8, 66.9, 50.3, 35.3, 31.7, 29.0, 25.1, 22.6, 14.1 ; HRMS m/z calculated for C₂₀H₂₈N₂O₃ +H: 345.2172, found 345.2170, C₂₀H₂₈N₂O₃ -HO: 327.2067 found 327.2070.

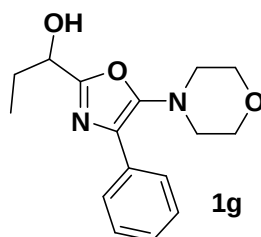


1-(4-benzyl-5-morpholinooxazol-2-yl)-2-phenylethanol (1e) Colorless oil; $[\alpha]_D^{20} = +6.0$ (c 1.1,

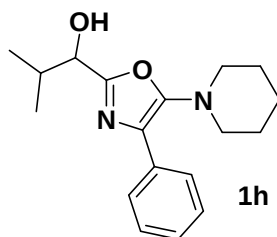
CHCl₃); yield: 78%, ee: 50% (ADH, hexane/ⁱPrOH = 9/1, 15 °C, 0.5mL/min). (lit. Wang, S. -X.; Wang, M. -X.; Wang, D. -X.; Zhu, J. *Org. Lett.* **2007**, 9, 3615-3618)



2-methyl-1-(5-morpholino-4-phenyloxazol-2-yl)propan-1-ol (1f) White solid, mp 66-67 °C; $[\alpha]_D^{20} = +9.7$ (c 0.55, CHCl₃); yield: 57%, ee: 63% (ADH, hexane/ⁱPrOH = 9/1, 25 °C, 0.5mL/min); IR (KBr) ν 3236, 2959, 2860, 1673, 1217, 1050, cm⁻¹; ¹HNMR (CDCl₃, 300MHz) δ 4.36 (br, s, 1H), 3.80-3.77 (m, 5H), 3.03-3.00 (m, 4H), 2.29-2.08 (m, 4H), 0.99 (d, J = 6.6Hz, 3H), 0.91 (d, J = 6.7Hz, 3H); ¹³CNMR (CDCl₃, 75MHz) δ 159.7, 151.3, 121.0, 72.9, 66.9, 50.9, 33.3, 18.4, 17.6, 10.9; MS (ESI) m/z 241 (M+H), 263 (M+Na); Anal. Calcd. for C₁₂H₂₀N₂O₃: C: 59.98, H: 8.39, N: 11.66; Found: C: 59.83, H: 8.43, N: 11.60.

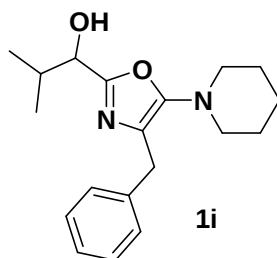


1-(5-morpholino-4-phenyloxazol-2-yl)propan-1-ol (1g) White solid, mp 99-100 °C; $[\alpha]_D^{20} = +10.0$ (c 1.0, CHCl₃); yield: 90%, ee: 57% (ADH, hexane/ⁱPrOH = 9/1, 25 °C, 0.5mL/min); IR (KBr) ν 3284, 2967, 2845, 1635, 1264, 1109, cm⁻¹; ¹HNMR (CDCl₃, 300MHz) δ 7.91 (d, J = 5.9Hz, 2H), 7.38-7.25 (m, 3H), 4.66 (br, s, 1H), 3.83 (br, s, 4H), 3.65 (br, s, 1H), 3.07 (br, s, 4H), 1.94 (br, s, 2H), 1.00 (br, s, 3H); ¹³CNMR (CDCl₃, 75MHz) δ 160.1, 151.0, 131.6, 128.5, 127.1, 125.9, 123.6, 69.0, 66.9, 50.3, 28.5, 9.5; MS (ESI) m/z 289 (M+H), 311 (M+Na); Anal. Calcd. for C₁₆H₂₀N₂O₃: C: 66.65, H: 6.99, N: 9.72; Found: C: 66.45, H: 7.18, N: 9.50.

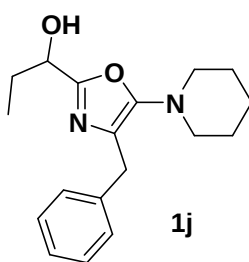


2-methyl-1-(5-morpholino-4-phenyloxazol-2-yl)propan-1-ol (1h) White solid, mp 107-108 °C; $[\alpha]_D^{20} = +13.3$ (c 0.7, CHCl₃); yield: 83%, ee: 80% (ADH, hexane/ⁱPrOH = 9/1, 25 °C, 0.5mL/min);

IR (KBr) ν 3248, 2946, 2838, 1628, 1385, 1037, cm^{-1} ; ^1H NMR (CDCl_3 , 300MHz) δ 7.95-7.93 (m, 2H), 7.41-7.36 (m, 2H), 7.25-7.21 (m, 1H), 4.47(t, J = 5.8Hz, 1H), 3.07-3.02 (m, 5H), 2.22-2.13 (m, 1H), 1.75-1.69 (m, 4H), 1.63-1.56 (m, 2H), 0.99(d, J = 6.9Hz, 3H), 0.97 (d, J = 7.0Hz, 3H); ^{13}C NMR (CDCl_3 , 75MHz) δ 158.4, 151.9, 131.3, 127.6, 125.9, 125.0, 121.7, 72.2, 50.7, 32.7, 25.1, 23.1, 17.6, 16.6 ; MS (ESI) m/z 301 (M+H), 323 (M+Na); Anal. Calcd. for $\text{C}_{18}\text{H}_{24}\text{N}_2\text{O}_2$: C: 71.97, H: 8.05, N: 9.33; Found: C: 71.82, H: 8.10, N: 9.37.

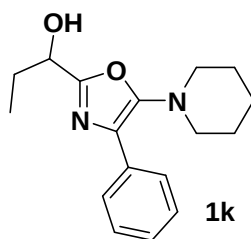


1-(4-benzyl-5-(piperidin-1-yl)oxazol-2-yl)-2-methylpropan-1-ol (1i) White solid, mp 107-108 $^{\circ}\text{C}$; $[\alpha]_{\text{D}}^{20}$ = +14.2 (c 0.7, CHCl_3); yield: 82%, ee: 87% (ADH, hexane/ i PrOH = 9/1, 15 $^{\circ}\text{C}$, 0.5mL/min); IR (KBr) ν 3209, 2937, 1664, 1461, 1235, 1067, cm^{-1} ; ^1H NMR (CDCl_3 , 300MHz) δ 7.25-7.17 (m, 5H), 4.35-4.31 (m, 1H), 3.78 (s, 2H), 3.45 (br, s, 1H), 2.92 (br, s, 4H), 2.13-2.04 (m, 1H), 1.60-1.53 (m, 6H), 0.94 (d, J = 6.6Hz, 3H), 0.89 (d, J = 6.7Hz, 3H); ^{13}C NMR (CDCl_3 , 75MHz) δ 159.6, 153.5, 139.8, 128.5, 128.3, 126.0, 123.3, 72.9, 52.2, 33.4, 31.7, 25.9, 23.9, 18.4, 17.5; MS (ESI) m/z 315 (M+H), 337 (M+Na), 353 (M+K) ; Anal. Calcd. for $\text{C}_{19}\text{H}_{26}\text{N}_2\text{O}_2$: C: 72.58, H: 8.33, N: 8.91; Found: C: 72.58, H: 8.44 N: 8.95.

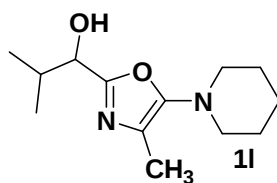


1-(4-benzyl-5-(piperidin-1-yl)oxazol-2-yl)propan-1-ol (1j) White solid, mp 77-78 $^{\circ}\text{C}$; $[\alpha]_{\text{D}}^{20}$ = +1.5 (c 0.9, CHCl_3); yield: 75%, ee: 54% (ADH, hexane/ i PrOH = 9/1, 15 $^{\circ}\text{C}$, 0.5mL/min); IR (KBr) ν 3207, 2935, 2849, 1657, 1446, 1233, 1104, cm^{-1} ; ^1H NMR (CDCl_3 , 300MHz) δ 7.28-7.14 (m, 5H), 4.51 (br, s, 1H), 3.78 (s, 2H), 2.95-2.91 (m, 4H), 1.91-1.75 (m, 2H), 1.64-1.49 (m, 6H), 0.93 (t, J = 7.4Hz 3H); ^{13}C NMR (CDCl_3 , 75MHz) δ 160.0, 153.4, 139.7, 128.5, 128.3, 126.0, 123.4, 68.9, 52.2, 31.7, 28.4, 25.9, 23.9, 9.5; MS (ESI) m/z 301 (M+H), 323 (M+Na), 339 (M+K);

Anal. Calcd. for C₁₈H₂₄N₂O₂: C: 71.97, H: 8.05, N: 9.33; Found: C: 71.84, H: 8.03 N: 9.16.

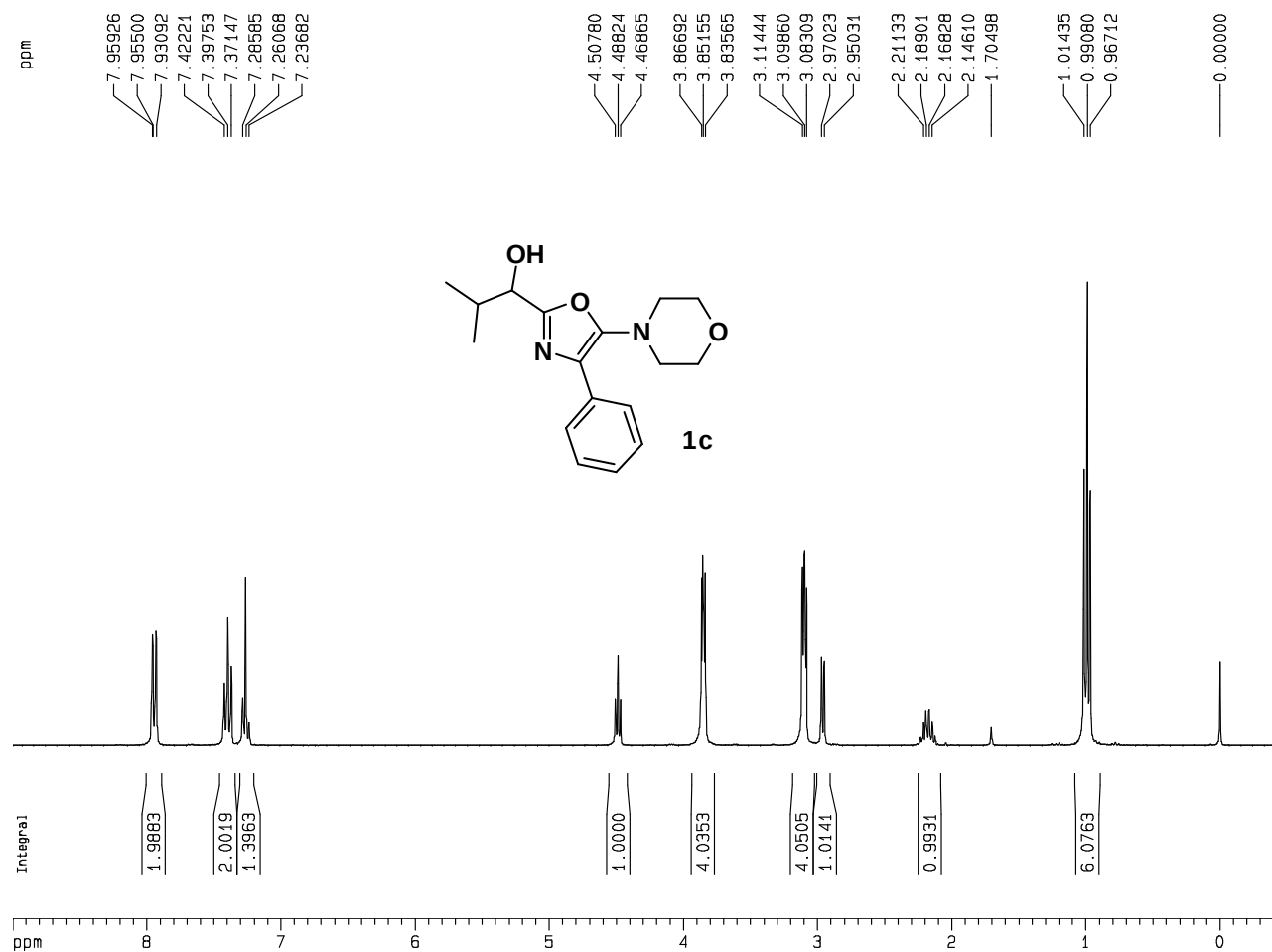


1-(4-phenyl-5-(piperidin-1-yl)oxazol-2-yl)propan-1-ol (1k) White solid, mp 89-90 °C; [α]_D²⁰ = +11.1 (c 1.2, CHCl₃); yield: 88%, ee: 58% (ADH, hexane/*i*PrOH = 9/1, 25 °C, 0.5mL/min); IR (KBr) ν 3299, 2958, 2828, 1619, 1401, 1197, cm⁻¹; ¹HNMR (CDCl₃, 300MHz) δ 7.91 (br, s, 2H), 7.38-7.23 (m, 3H), 4.65 (br, s, 1H), 3.32 (s, 1H), 3.03 (br, s, 4H), 1.93-1.60 (m, 8H), 1.00 (br, s, 3H); ¹³CNMR (CDCl₃, 75MHz) δ 159.5, 152.6, 132.1, 128.3, 126.6, 125.8, 122.4, 69.1, 51.4, 28.6, 25.9, 23.9, 9.4; MS (ESI) *m/z* 287 (M+H), 309 (M+Na); Anal. Calcd. for C₁₇H₂₂N₂O₂: C: 71.30, H: 7.74, N: 9.78; Found: C: 71.23, H: 7.96, N: 9.56.



2-methyl-1-(5-morpholino-4-phenyloxazol-2-yl)propan-1-ol (1l) Colorless oil, [α]_D²⁰ = +8.5 (c 1.65, CHCl₃); yield: 77%, ee: 57% (ADH, hexane/*i*PrOH = 9/1, 25 °C, 0.5mL/min); IR (KBr) ν 3272, 2937, 1664, 1220, 1038, cm⁻¹; ¹HNMR (CDCl₃, 300MHz) δ 4.33 (d, *J* = 6.4Hz, 1H), 3.92 (br, s, 1H), 2.98-2.94 (m, 4H), 2.17-2.08 (m, 1H), 2.05 (s, 3H), 1.68-1.61 (m, 4H), 1.57-1.53 (m, 2H), 0.99 (d, *J* = 6.7Hz, 3H), 0.92 (d, *J* = 6.8Hz, 3H); ¹³CNMR (CDCl₃, 75MHz) δ 159.1, 152.7, 119.6, 72.9, 52.0, 33.3, 25.9, 23.9, 18.4, 17.7, 11.0; MS (ESI) *m/z* 239 (M+H), 261 (M+Na), 277 (M+K); Anal. Calcd. for C₁₃H₂₂N₂O₂: C: 65.51, H: 9.30, N: 11.75; Found: C: 65.31, H: 9.29, N: 11.46.

4. Copies of ¹H and ¹³C NMR spectra of all new compounds



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EXPNO 1
PROCNO 1

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FIDRES 0.137219 Hz
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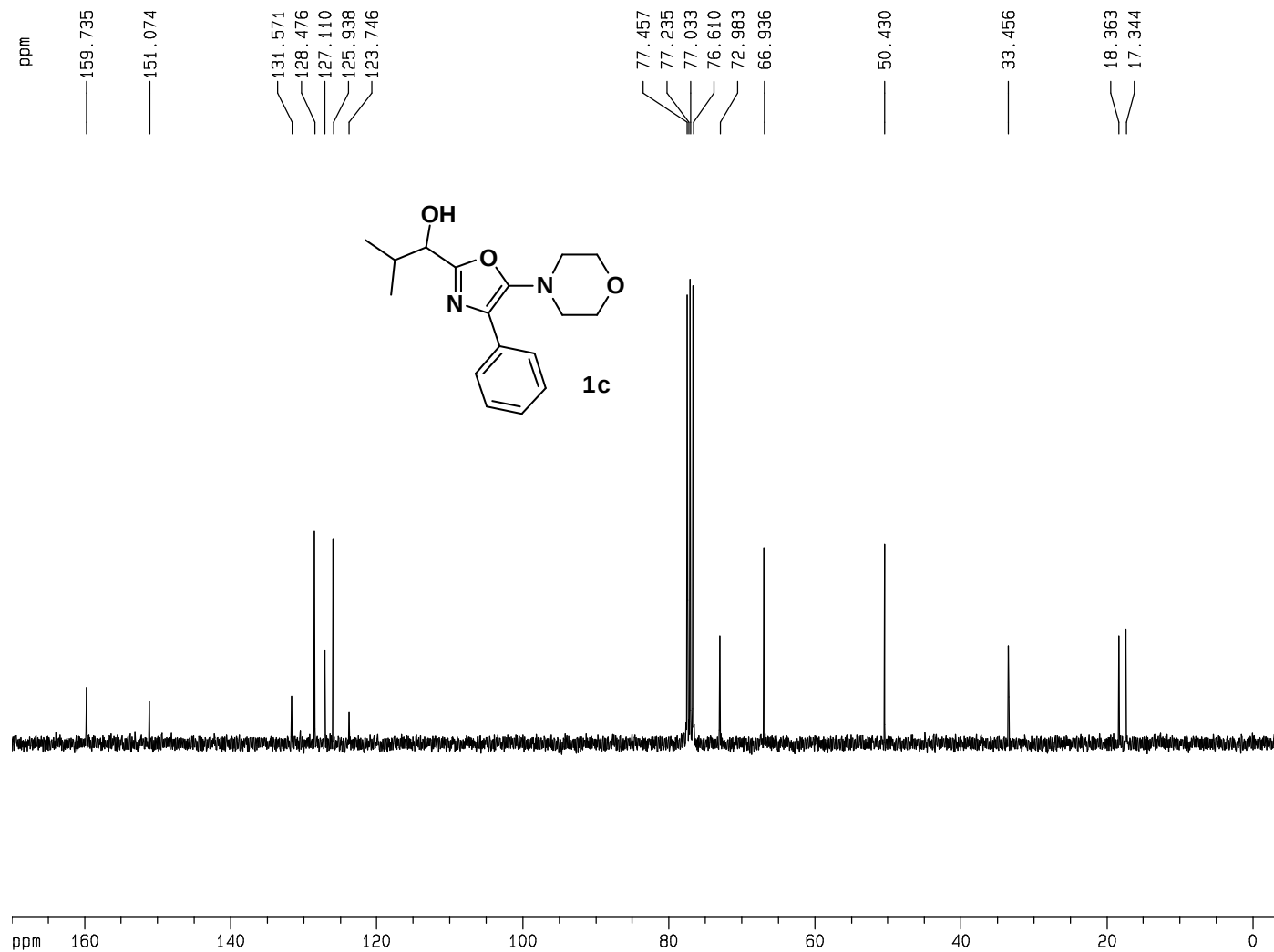
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1D NMR plot parameters

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PROCNO 1

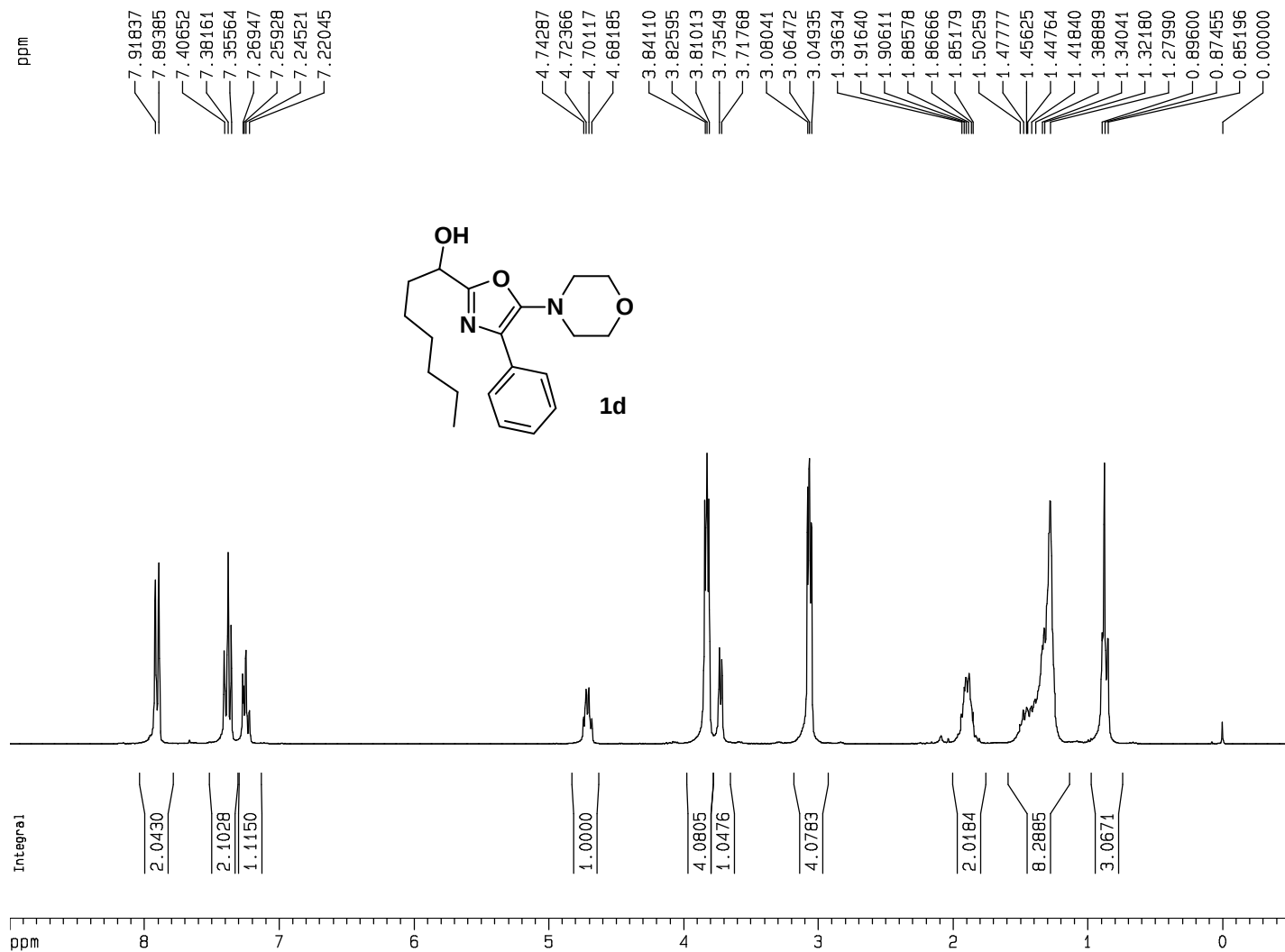
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1D NMR plot parameters
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CY 8.00 cm
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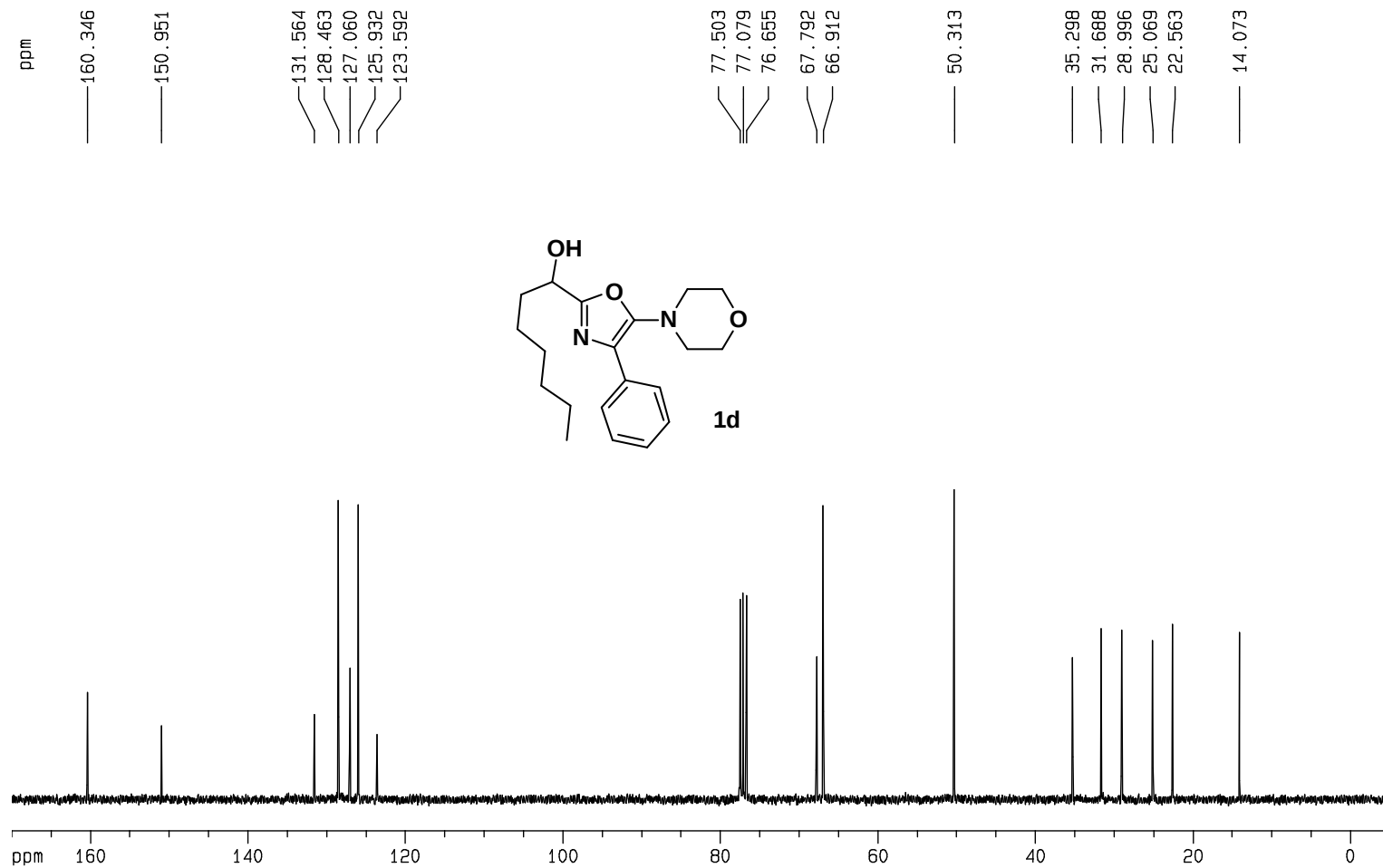
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1D NMR plot parameters
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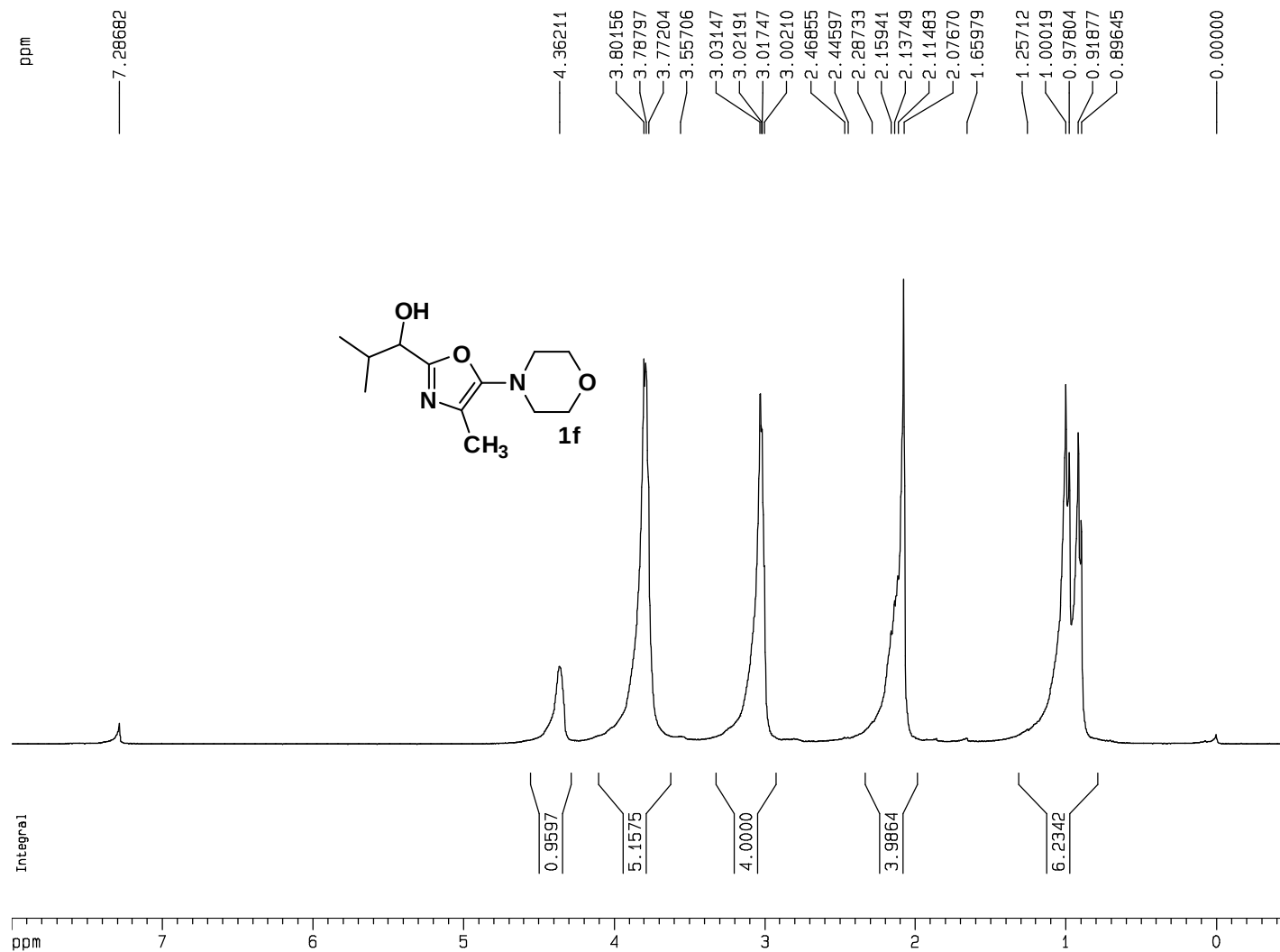
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1D NMR plot parameters
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PROCNO        1

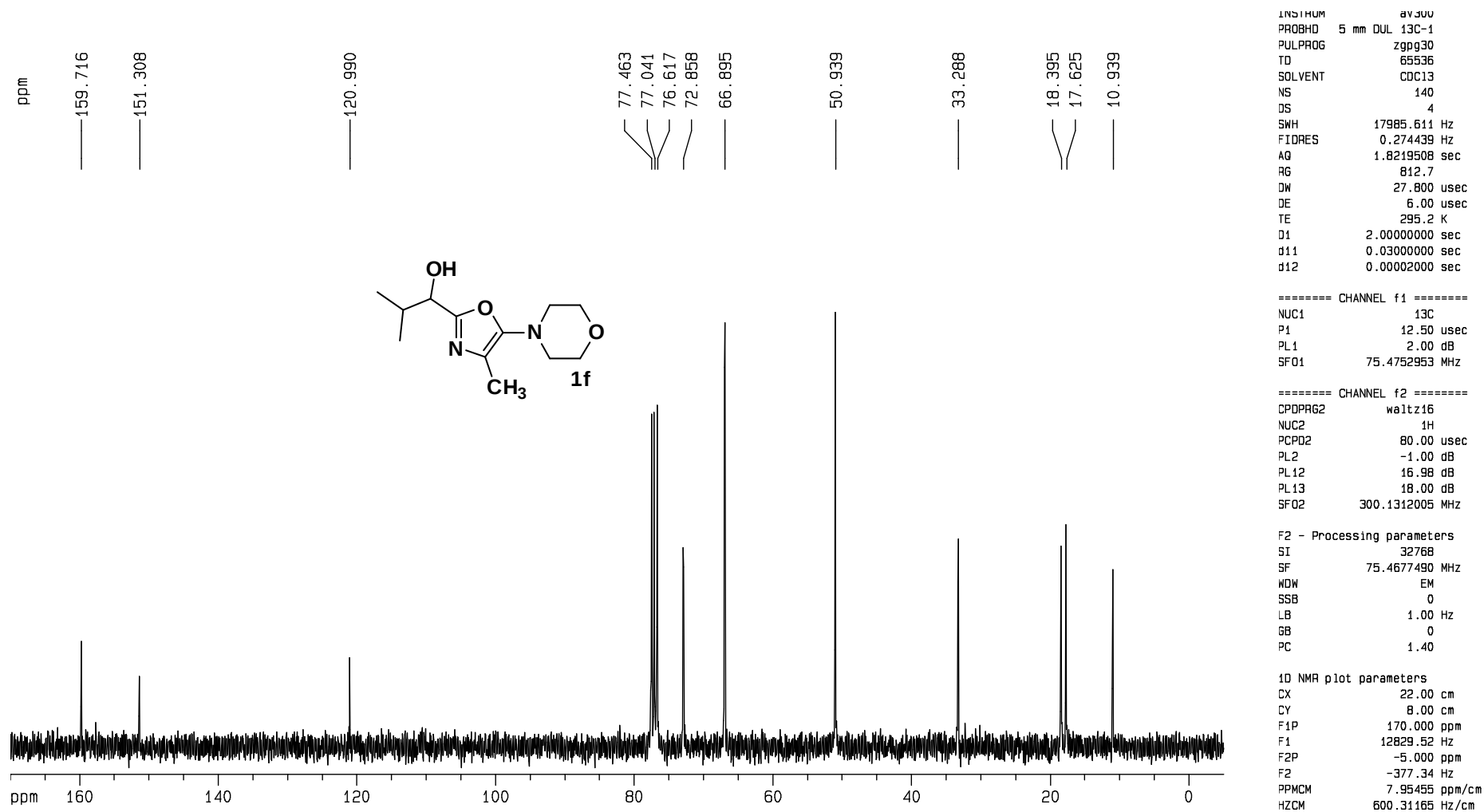
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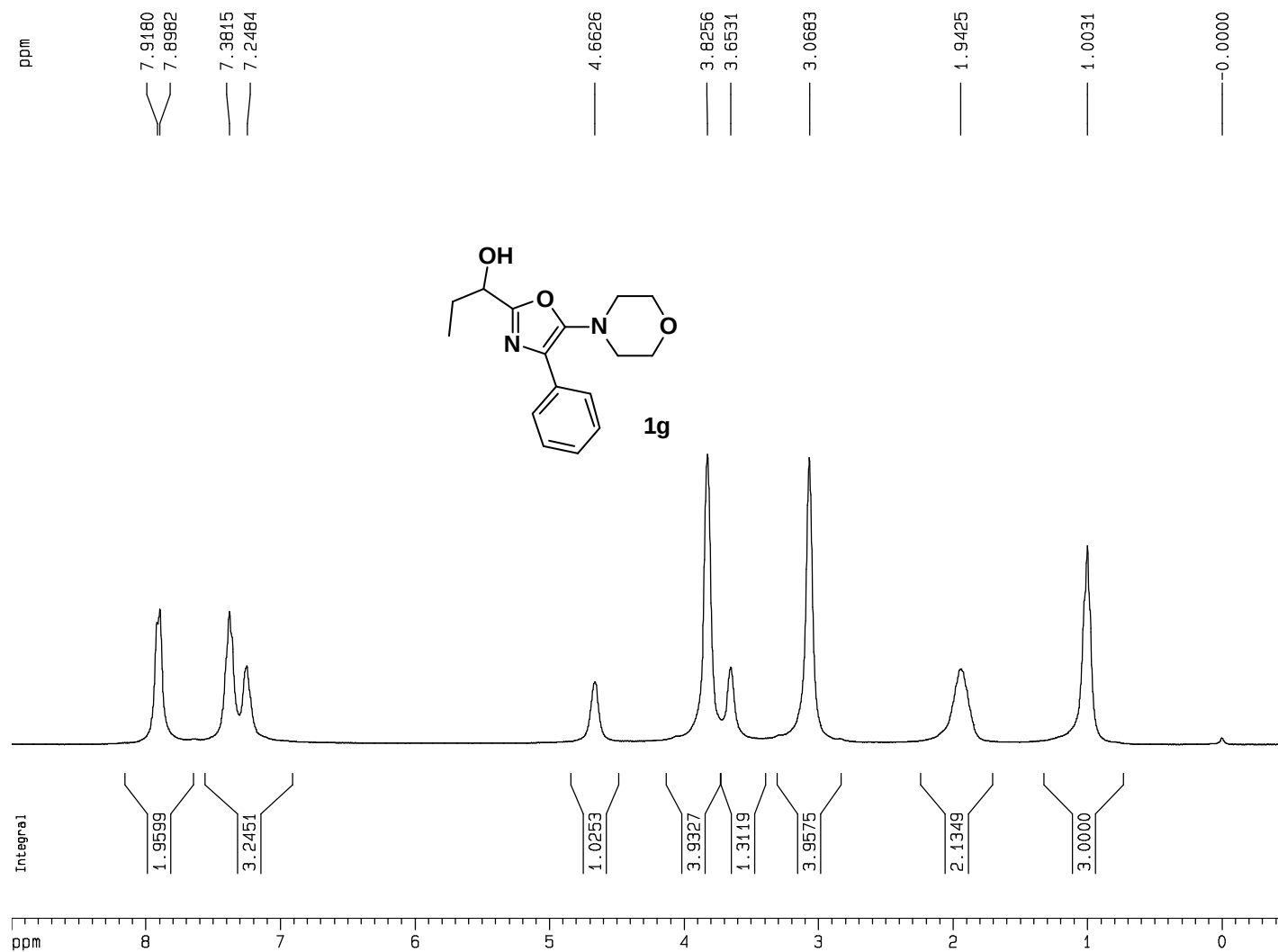
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WDW           EM
SSB           0
LB            0.35 Hz
GB            0
PC            1.00

===== 1D NMR plot parameters =====
CX            22.00 cm
CY            8.00 cm
F1P           8.000 ppm
F1            2401.04 Hz
F2P           -0.500 ppm
F2            -150.06 Hz
PMCM          0.38636 ppm/cm
HZCM          115.95932 Hz/cm

```





NAME yt-p2q
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20080229
Time 19.40
INSTRUM av300
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
VS 9
JS 0
SWH 8992.806 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 80.6
DW 55.600 usec
DE 6.00 usec
TE 673.2 K
D1 5.00000000 sec

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

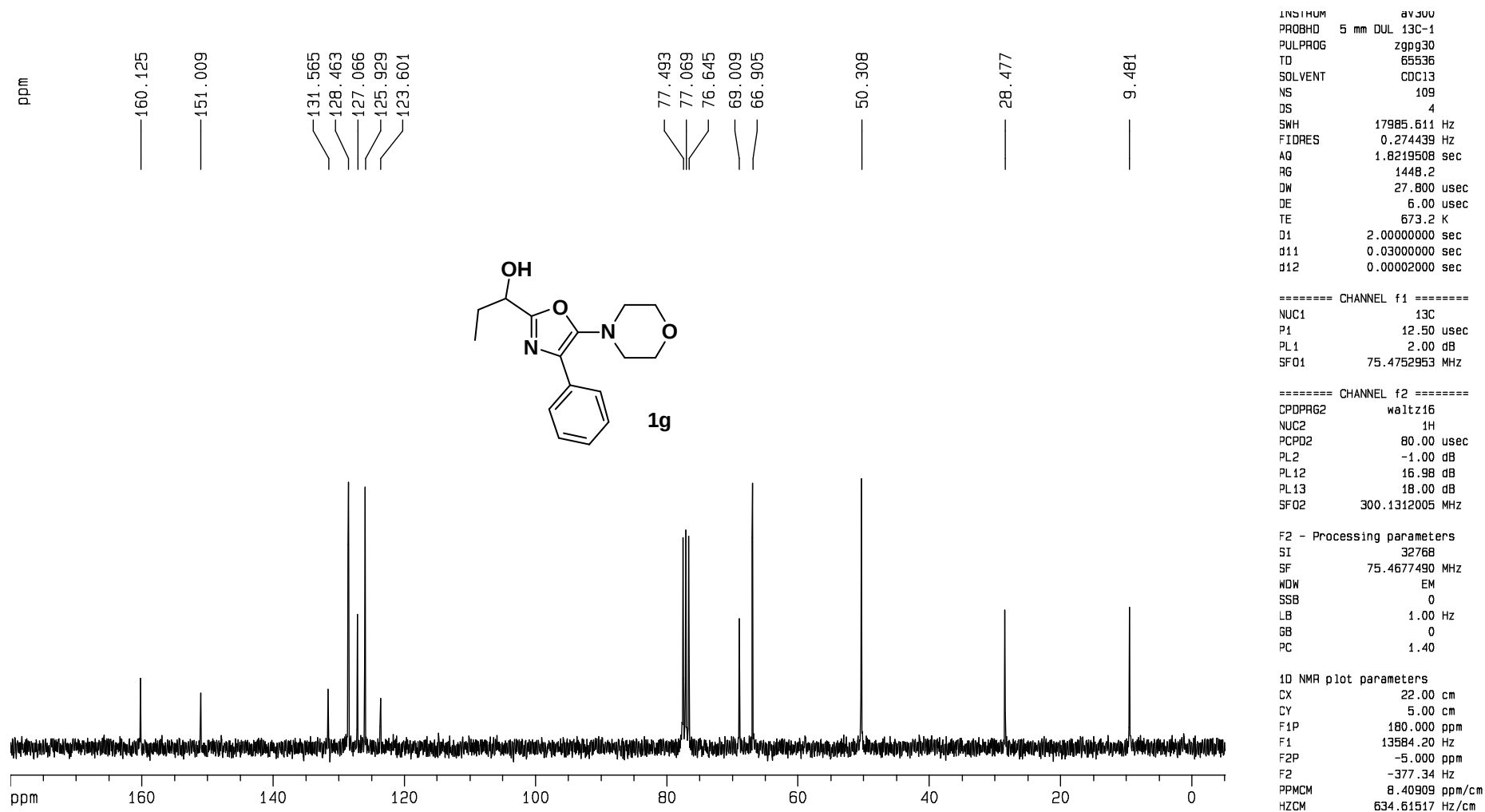
VUC1 1H
P1 10.10 usec
PL1 -1.00 dB
SF01 300.1318534 MHz

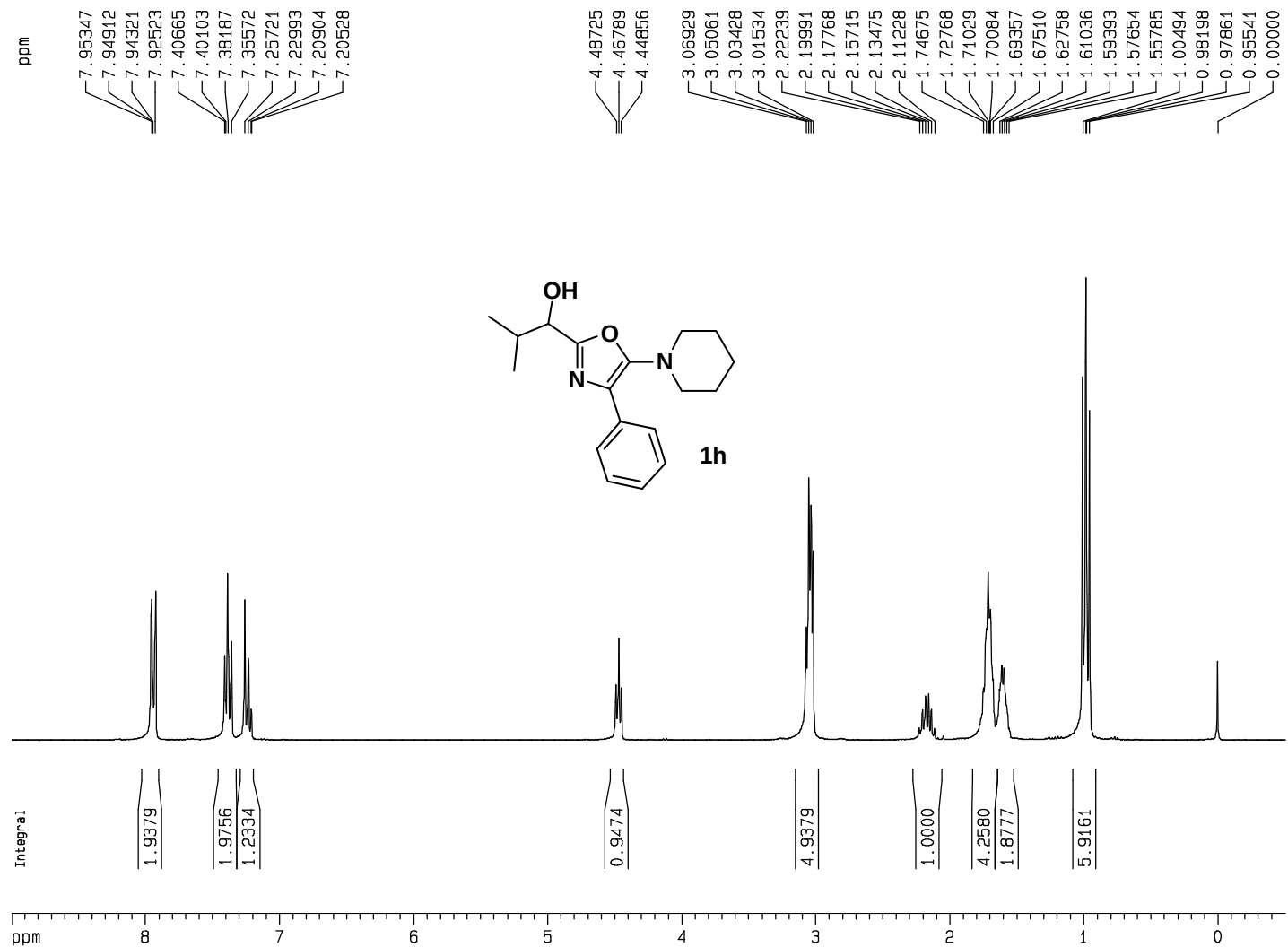
F2 - Processing parameters

SI 32768
SF 300.1300042 MHz
WDW EM
SSB 0
LB 0.35 Hz
GB 0
PC 1.00

1D NMR plot parameters

CX 22.00 cm
CY 5.00 cm
F1P 9.000 ppm
F1 2701.17 Hz
F2P -0.500 ppm
F2 -150.07 Hz
PMCM 0.43182 ppm/cm
IZCM 129.60159 Hz/cm





```

NAME          yt-p2n
EXPNO         1
PROCNO        1

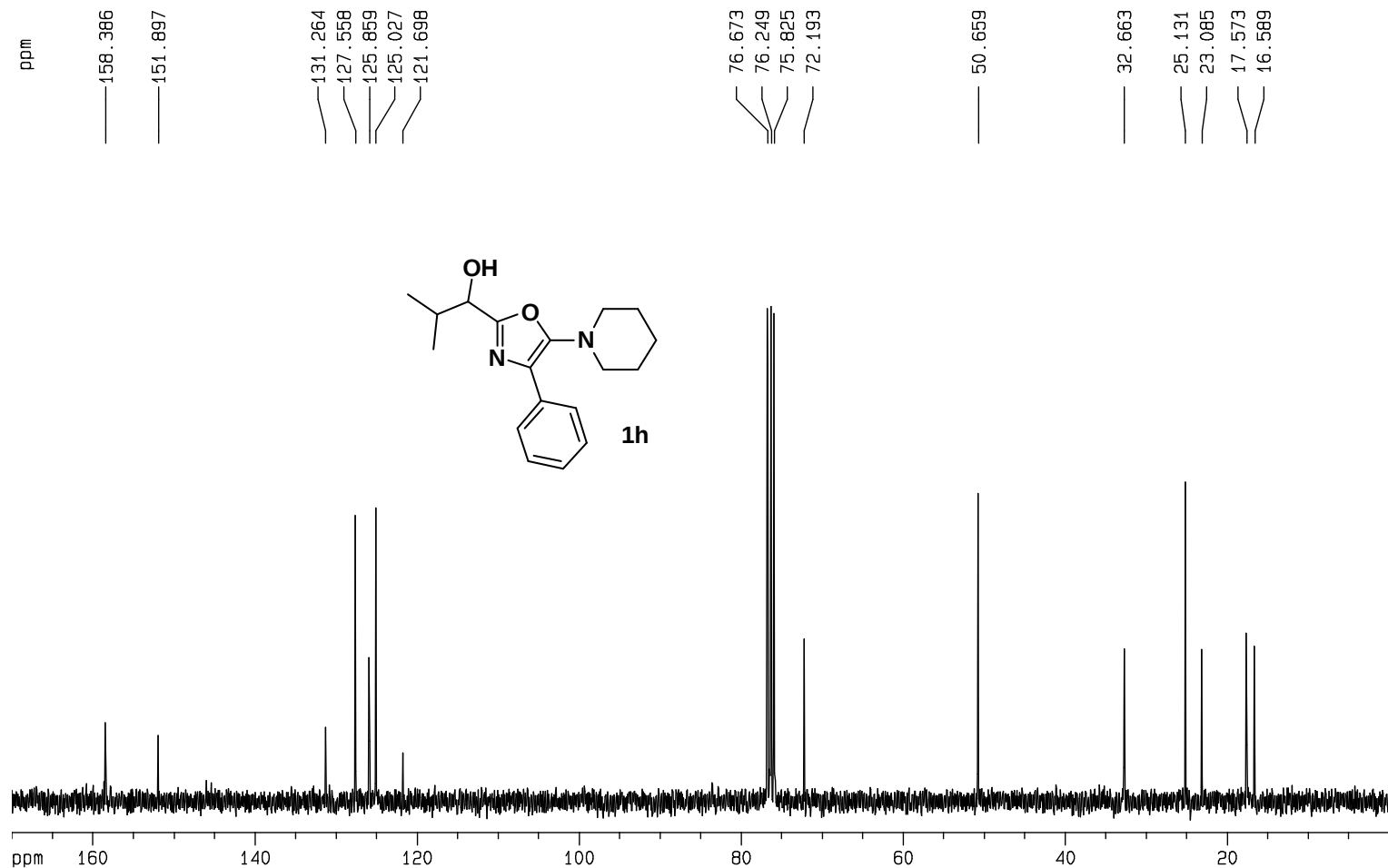
===== Acquisition Parameters =====
Date_         20080213
Time          15.00
INSTRUM       av300
PROBHD        5 mm DUL 13C-1
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
VS            6
DS            0
SWH           8992.806 Hz
FIDRES        0.137219 Hz
AQ           3.6438515 sec
RG            203.2
DW           55.600 usec
DE            6.00 usec
TE            295.0 K
D1           5.00000000 sec

===== CHANNEL f1 =====
NUC1           1H
P1            10.10 usec
PL1           -1.00 dB
SFO1          300.1318534 MHz

===== Processing parameters =====
SI            32768
SF           300.1300063 MHz
WDW           EM
SSB           0
LB            0.35 Hz
GB            0
PC            1.00

===== 1D NMR plot parameters =====
CX            22.00 cm
CY            8.00 cm
F1P           9.000 ppm
F1            2701.17 Hz
F2P          -0.500 ppm
F2           -150.07 Hz
PMCM          0.43182 ppm/cm
HZCM          129.60159 Hz/cm

```



```

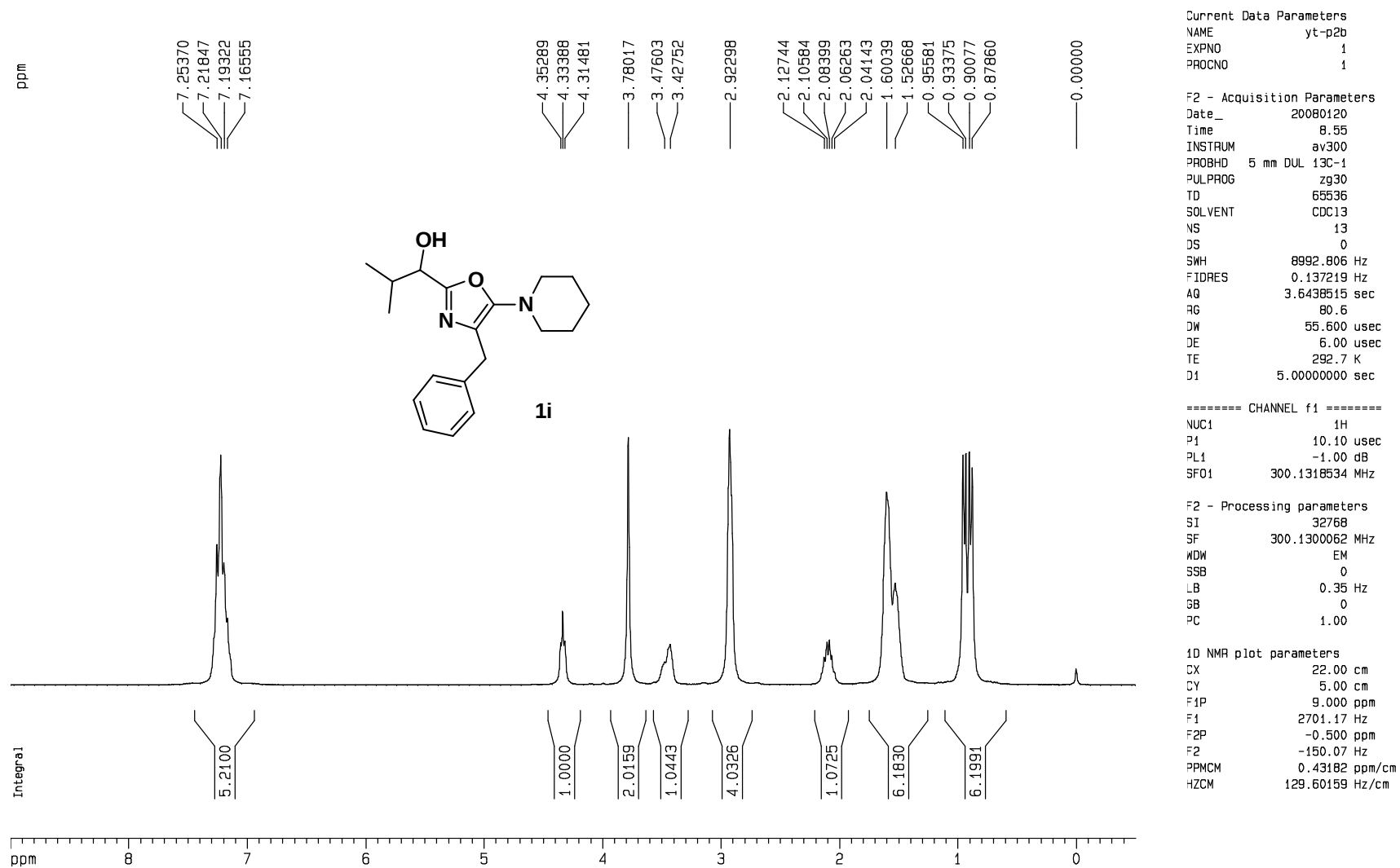
===== CHANNEL f1 =====
NUC1      13C
P1        12.50 usec
PL1       -2.00 dB
SFO1      75.4752953 MHz

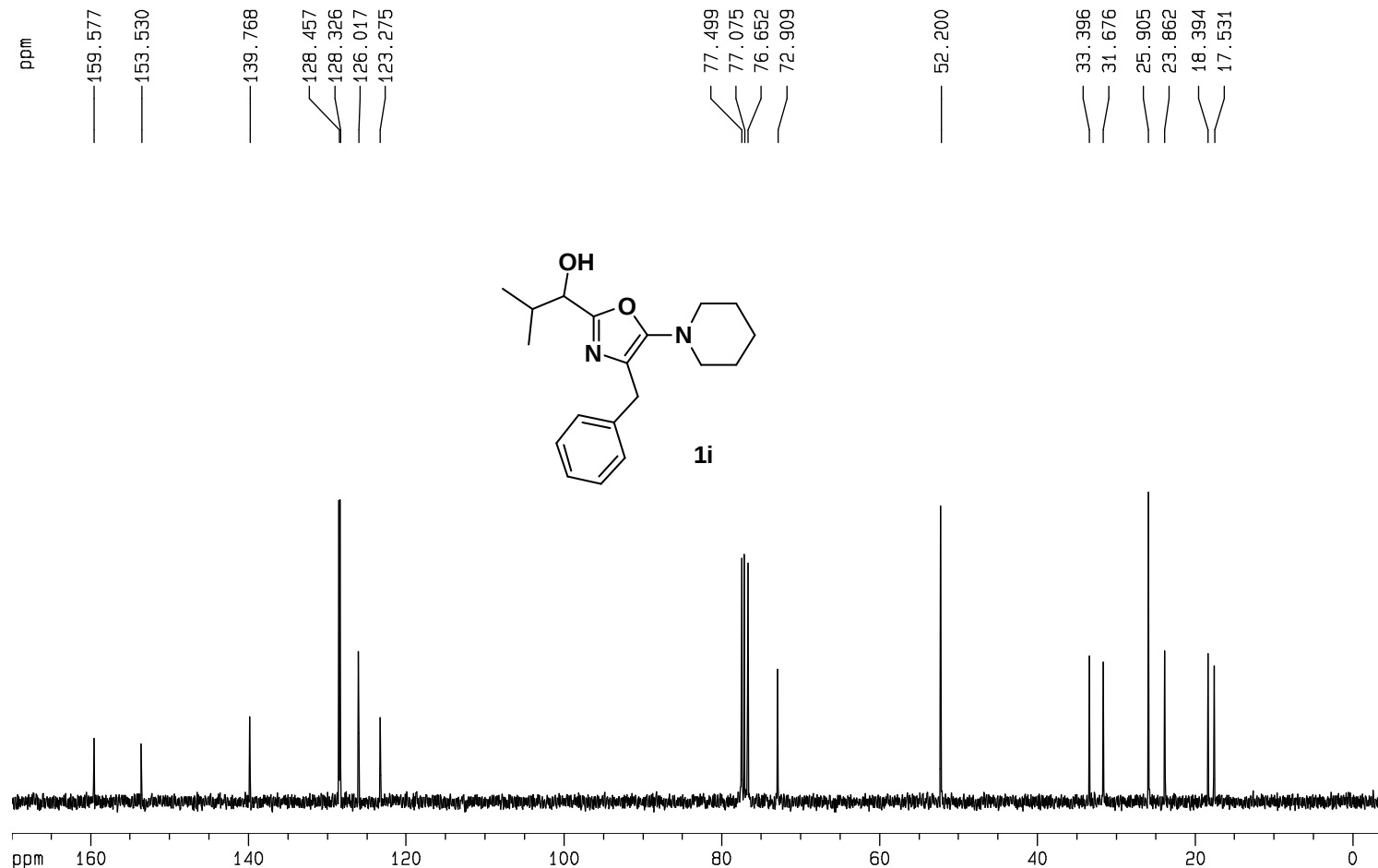
===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2       1H
PCPD2      80.00 usec
PL2       -1.00 dB
PL12      16.98 dB
PL13      18.00 dB
SFO2      300.1312005 MHz

F2 - Processing parameters
SI         32768
SF         75.4678085 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40

1D NMR plot parameters
CX         22.00 cm
CY         8.00 cm
F1P        170.000 ppm
F1         12829.53 Hz
F2P        -0.500 ppm
F2         -37.73 Hz
PPMCM      7.75000 ppm/cm
HZCM       584.87555 Hz/cm

```





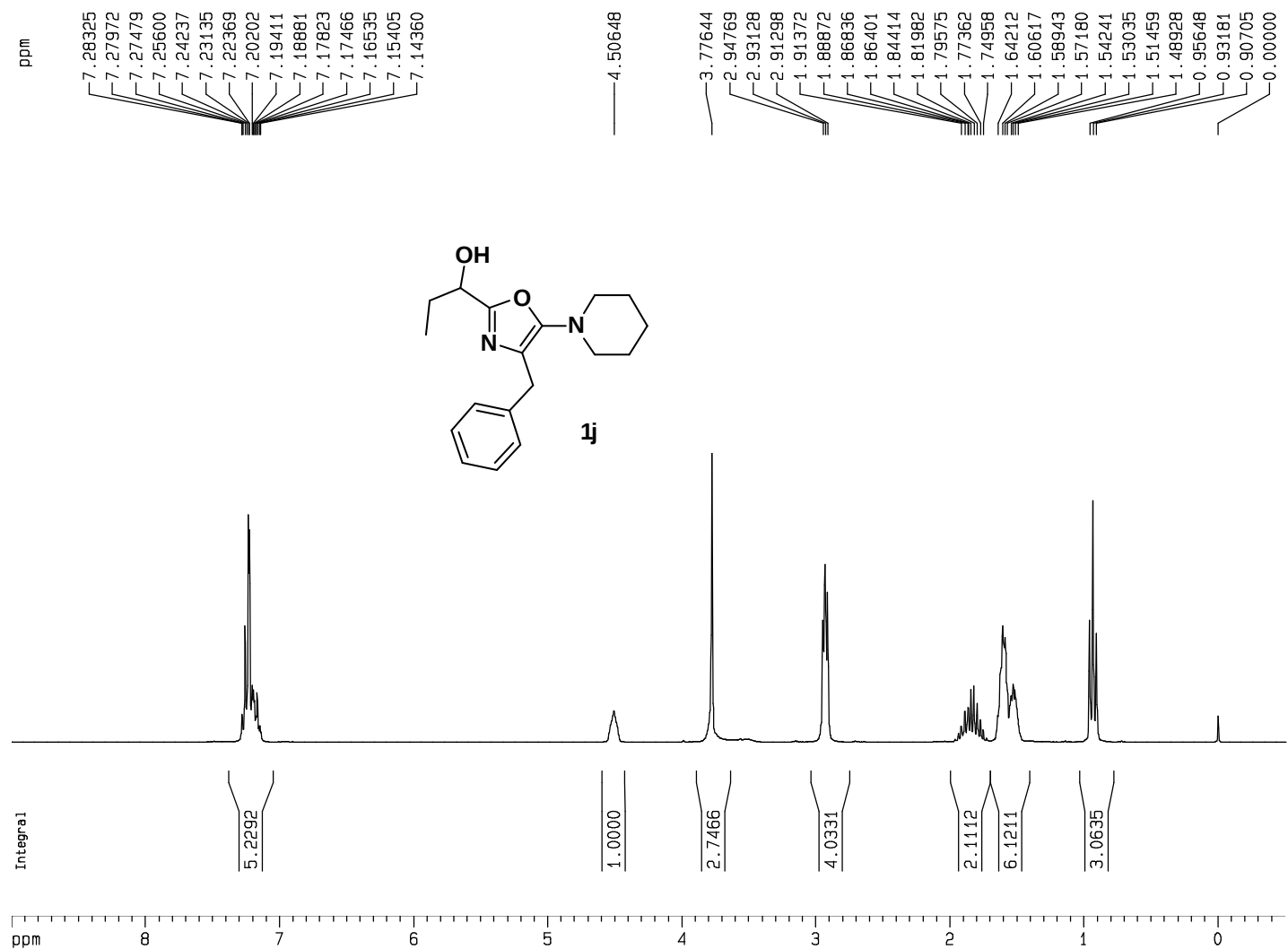
Time 8.57
INSTRUM av300
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 102
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 456.1
DW 27.800 usec
DE 6.00 usec
TE 292.8 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 12.50 usec
PL1 2.00 dB
SF01 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 16.98 dB
PL13 18.00 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

1D NMR plot parameters
CX 22.00 cm
CY 5.00 cm
F1P 170.000 ppm
F1 12829.52 Hz
F2P -5.000 ppm
F2 -377.34 Hz
PPMCM 7.95455 ppm/cm
HZCM 600.31165 Hz/cm



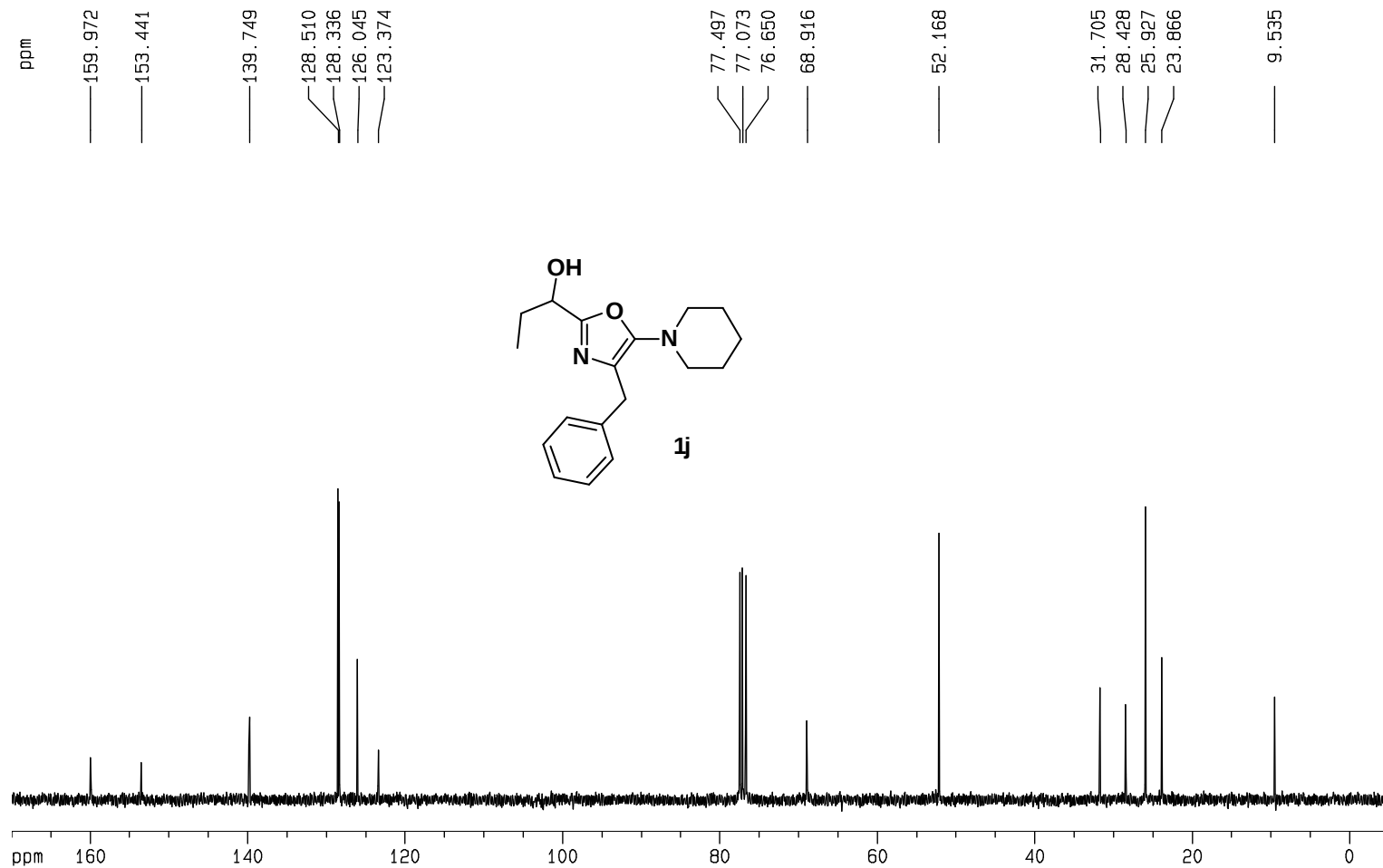
NAME yt-p2f
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20080120
Time 9.23
INSTRUM av300
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 14
DS 0
SWH 8992.806 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 101.6
DW 55.600 usec
DE 6.00 usec
TE 292.1 K
D1 5.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.10 usec
PL1 -1.00 dB
SF01 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300067 MHz
WDW EM
SSB 0
LB 0.35 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 22.00 cm
CY 5.00 cm
F1P 9.000 ppm
F1 2701.17 Hz
F2P -0.500 ppm
F2 -150.07 Hz
PPMCM 0.43182 ppm/cm
HZCM 129.60159 Hz/cm



```

===== CHANNEL f1 =====
PULPROG      zgpg30
TD            65536
SOLVENT       CDCl3
NS            83
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            292.2 K
D1            2.00000000 sec
d11           0.03000000 sec
d12           0.00002000 sec

```

```

===== CHANNEL f2 =====
NUC1          13C
P1            12.50 usec
PL1           2.00 dB
SF01          75.4752953 MHz

```

```

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           -1.00 dB
PL12          16.98 dB
PL13          18.00 dB
SF02          300.1312005 MHz

```

```

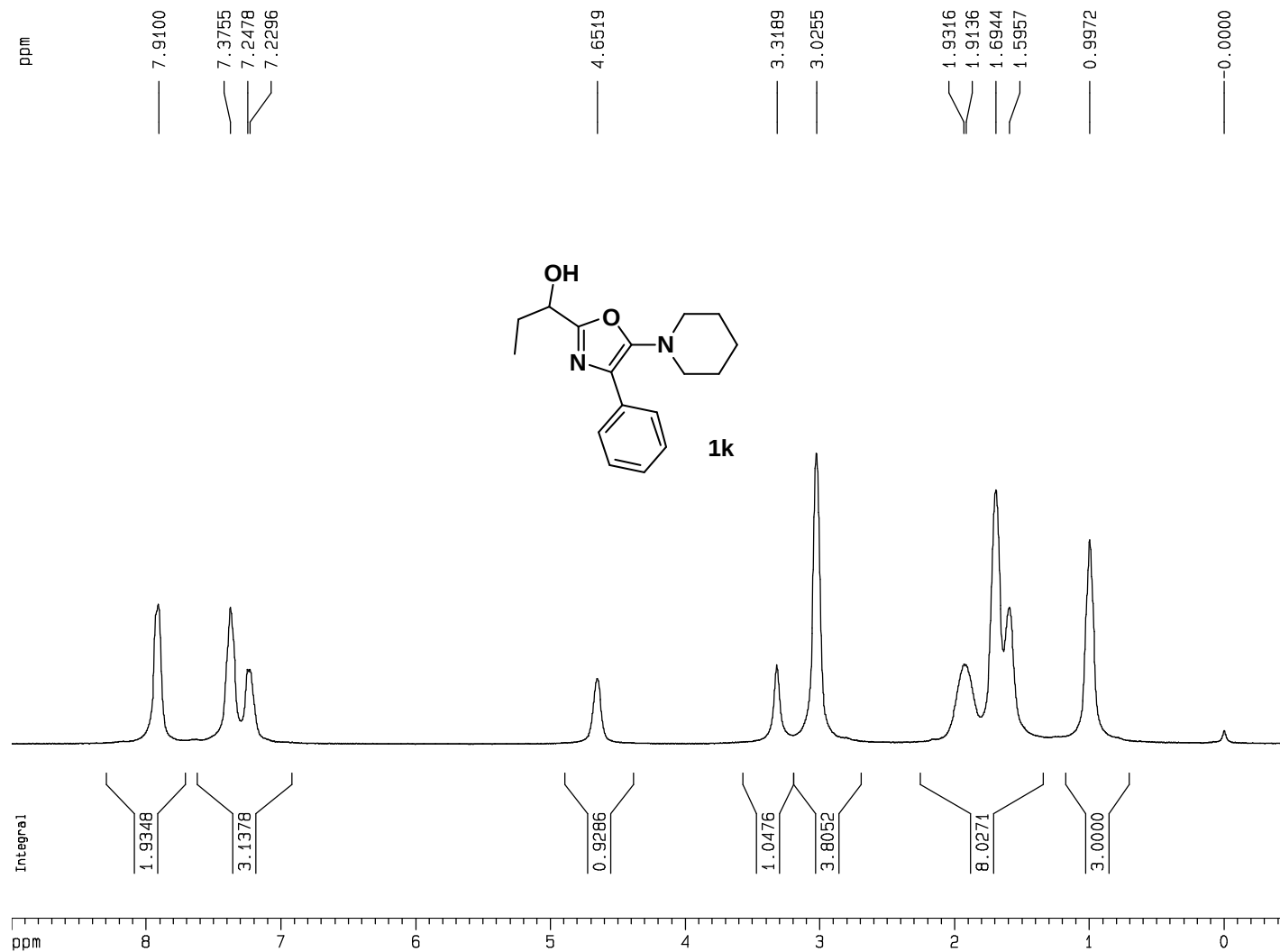
F2 - Processing parameters
SI            32768
SF            75.4677490 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40

```

```

1D NMR plot parameters
CX            22.00 cm
CY            5.00 cm
F1P           170.000 ppm
F1            12829.52 Hz
F2P           -5.000 ppm
F2            -377.34 Hz
PPMCM         7.95455 ppm/cm
HZCM          600.31165 Hz/cm

```



```

NAME          yt-p2r
EXPNO         1
PROCNO        1

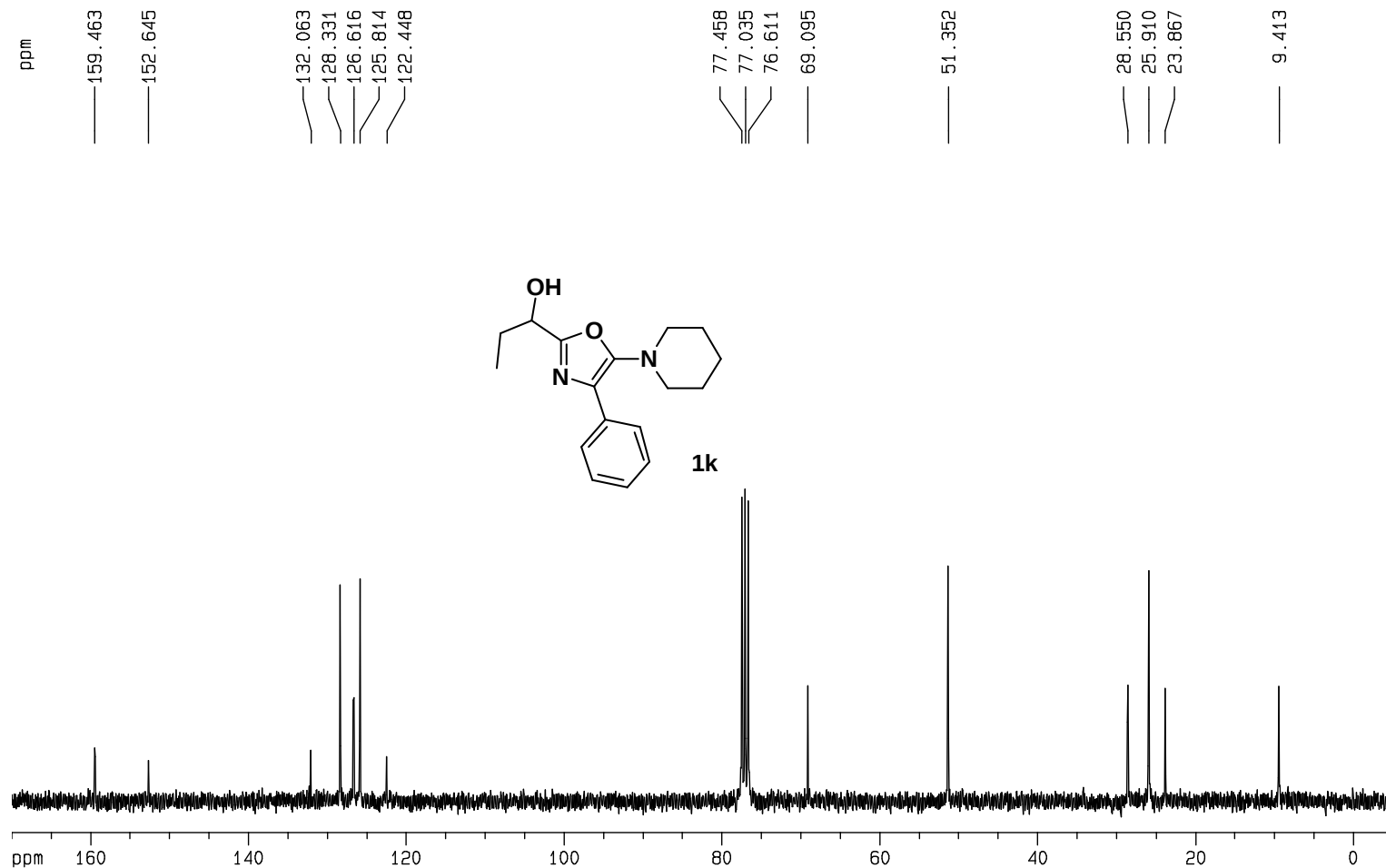
F2 - Acquisition Parameters
Date_         20080229
Time          19.54
INSTRUM       av300
PROBHD        5 mm DUL 13C-1
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
VS            10
DS            0
SWH           8992.806 Hz
FIDRES        0.137219 Hz
AQ            3.6438515 sec
RG            161.3
DW            55.600 usec
DE            6.00 usec
TE            673.2 K
D1            5.00000000 sec

===== CHANNEL f1 =====
NUC1          1H
P1            10.10 usec
PL1           -1.00 dB
SF01          300.1318534 MHz

F2 - Processing parameters
SI            32768
SF            300.1300053 MHz
WDW           EM
SSB           0
GB            0.35 Hz
CB            0
PC            1.00

1D NMR plot parameters
CX            22.00 cm
CY            5.00 cm
F1P           9.000 ppm
F1            2701.17 Hz
F2P           -0.500 ppm
F2            -150.07 Hz
PMCM          0.43182 ppm/cm
HZCM          129.60159 Hz/cm

```



```

===== CHANNEL f1 =====
PULPROG      zgpg30
TD            65536
SOLVENT      CDCl3
NS            216
DS            4
SWH           17985.611 Hz
FIDRES        0.274439 Hz
AQ            1.8219508 sec
RG            1824.6
DW            27.800 usec
DE            6.00 usec
TE            673.2 K
D1            2.0000000 sec
d11           0.03000000 sec
d12           0.00002000 sec

```

```

===== CHANNEL f2 =====
NUC1          13C
P1            12.50 usec
PL1           2.00 dB
SFO1          75.4752953 MHz

```

```

===== CHANNEL f2 =====
CPDPRG2      waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           -1.00 dB
PL12          16.98 dB
PL13          18.00 dB
SFO2          300.1312005 MHz

```

```

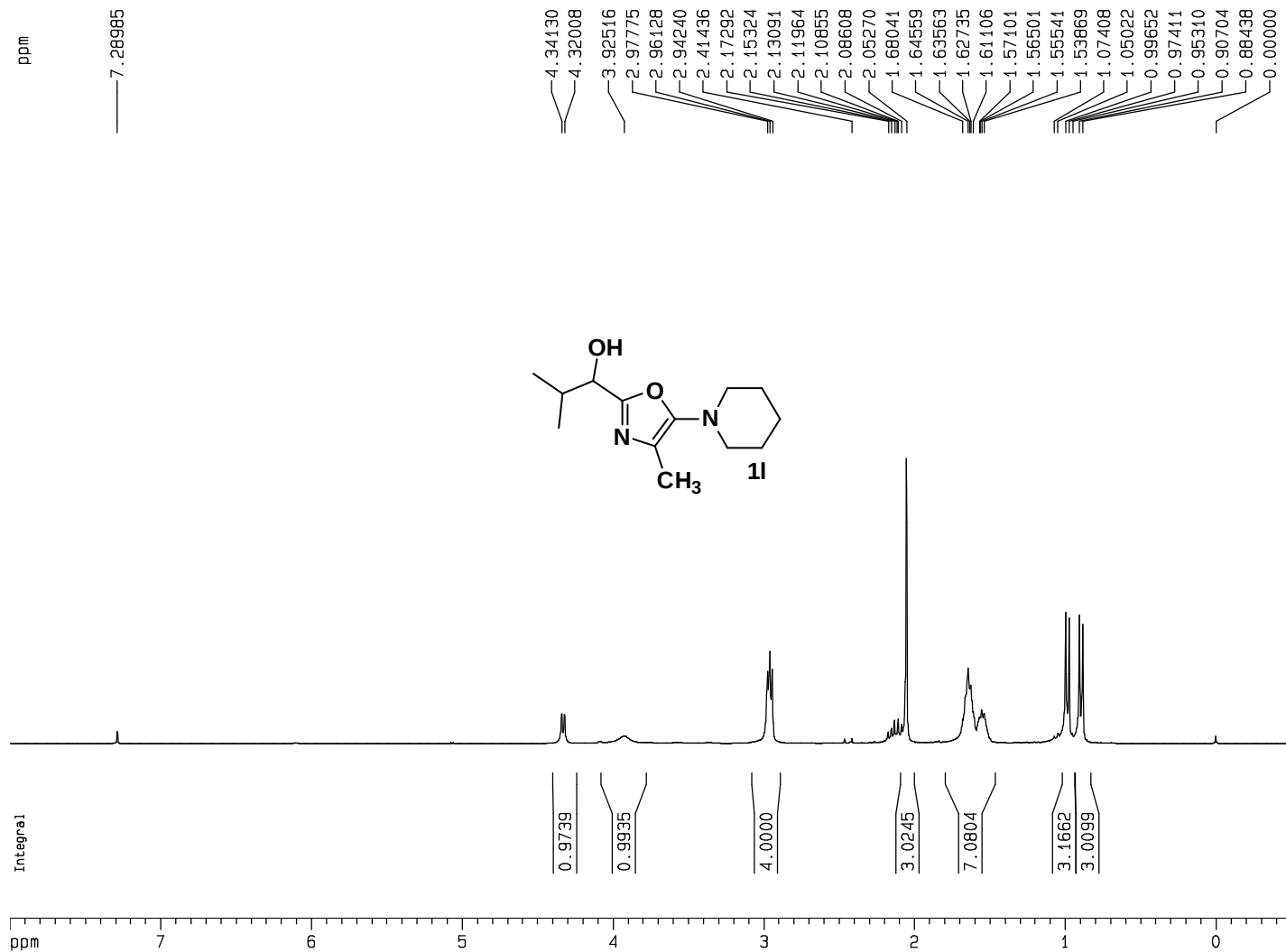
F2 - Processing parameters
SI            32768
SF            75.4677490 MHz
WDW           EM
SSB            0
LB            1.00 Hz
GB            0
PC            1.40

```

```

1D NMR plot parameters
CX            22.00 cm
CY            5.00 cm
F1P           170.000 ppm
F1            12829.52 Hz
F2P           -5.000 ppm
F2            -377.34 Hz
PPMCM         7.95455 ppm/cm
HZCM          600.31165 Hz/cm

```



```

=====
NAME          yt-p2p
EXPNO         1
PROCNO        1

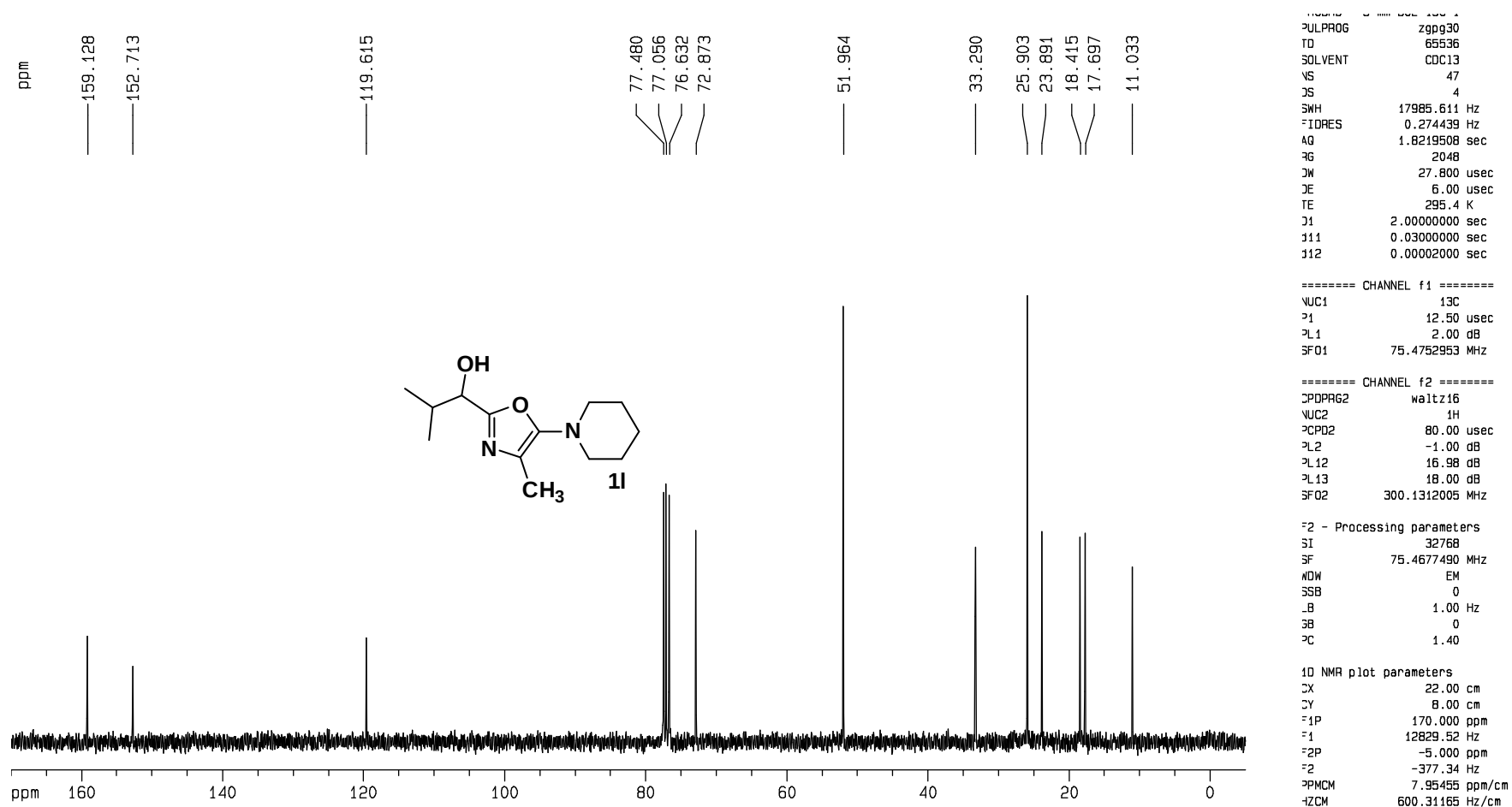
F2 - Acquisition Parameters
Date_         20080213
Time          16.39
INSTRUM       av300
PROBHD        5 mm DUL 13C-1
PULPROG       zg30
TD            65536
SOLVENT       CDC13
VS            13
JS            0
SWH           8992.806 Hz
FIDRES        0.137219 Hz
AQ            3.6438515 sec
RG            64
DW            55.600 usec
DE            6.00 usec
TE            295.2 K
D1            5.00000000 sec

===== CHANNEL f1 =====
NUC1           1H
P1            10.10 usec
PL1           -1.00 dB
SF01          300.1318534 MHz

F2 - Processing parameters
SI            32768
SF           300.1299962 MHz
WDW           EM
SSB           0
GB            0.35 Hz
SB            0
GC            1.00

1D NMR plot parameters
CX            22.00 cm
CY            5.00 cm
F1P           8.000 ppm
F1            2401.04 Hz
F2P           -0.500 ppm
F2            -150.06 Hz
PMCM          0.38636 ppm/cm
HZCM          115.95932 Hz/cm

```

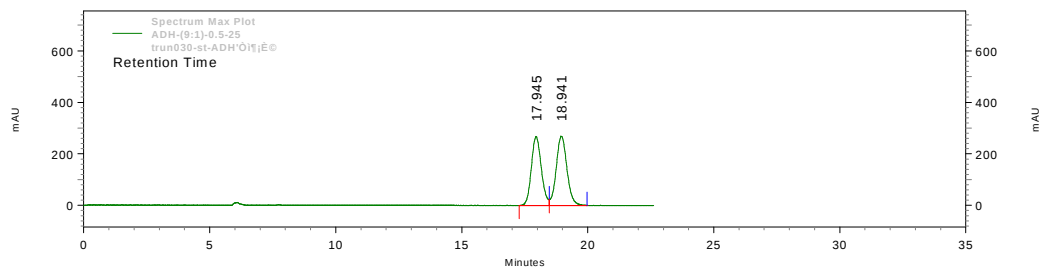


5. Chiral HPLC trace of 1a-1l

Compound	Column chiralcel	Mobile Phase	ML/min	T(°C)	t ₁ (min)	t ₂ (min)
1a	ADH	Hex:IPA 9:1	0.5	15	19.5	20.7
1b	ADH	Hex:IPA 9:1	0.5	15	20.1	21.1
1c	ADH	Hex:IPA 9:1	0.5	25	17.3	24.6
1d	ADH	Hex:IPA 9:1	0.5	15	16.3	18.0
1e	ADH	Hex:IPA 9:1	0.5	15	32.6	34.3
1f	ADH	Hex:IPA 9:1	0.5	25	16.0	17.8
1g	ADH	Hex:IPA 9:1	0.5	25	17.7	21.1
1h	ADH	Hex:IPA 9:1	0.5	25	12.2	15.7
1i	ADH	Hex:IPA 9:1	0.5	15	13.0	14.0
1j	ADH	Hex:IPA 9:1	0.5	15	25.9	27.6
1k	ADH	Hex:IPA 9:1	0.5	25	12.0	14.4
1l	ADH	Hex:IPA 9:1	0.5	15	10.7	12.2

1a

ADH 9:1(正己烷:异丙醇) 15°C

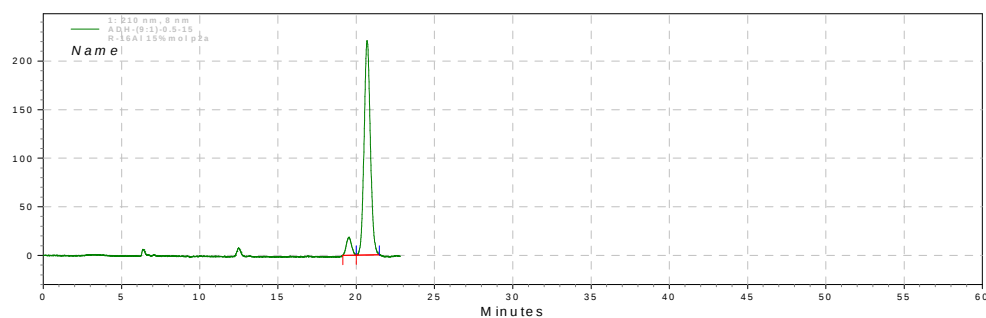


1: 212 nm, 8 nm

Pk #	Retention Time	Area	Area %
1	17.945	17603316	48.607
2	18.948	18612260	51.393
Totals		36215576	100.000

Sample ID : ADH-(9:1)-0.5-15
 User Name : System
 Filename : E:\yuetao\R-16Al 15%mol p2a
 Method Name: C:\CLASS-VP\Methods\Multi_pac.met
 Sequence Name : C:\CLASS-VP\Sequence\Multi_pac.seq
 Run Time : 2008-1-27 17:17:09

Data Graph



Run Report

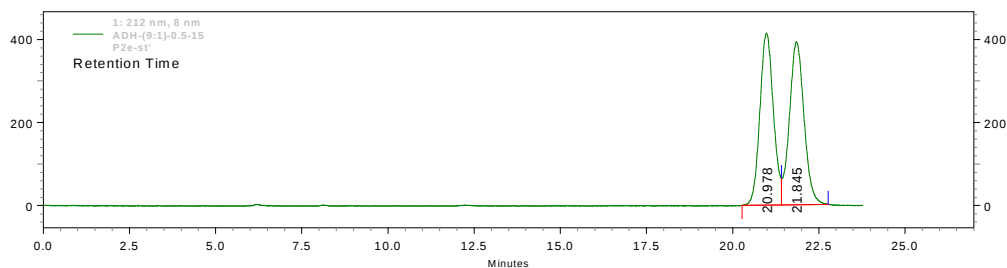
1: 212 nm, 8 nm

Pk #	Retention Time	Area	Area %
1	19.529	428621	6.54
2	20.685	6129439	93.46

1b

Totals

100.000

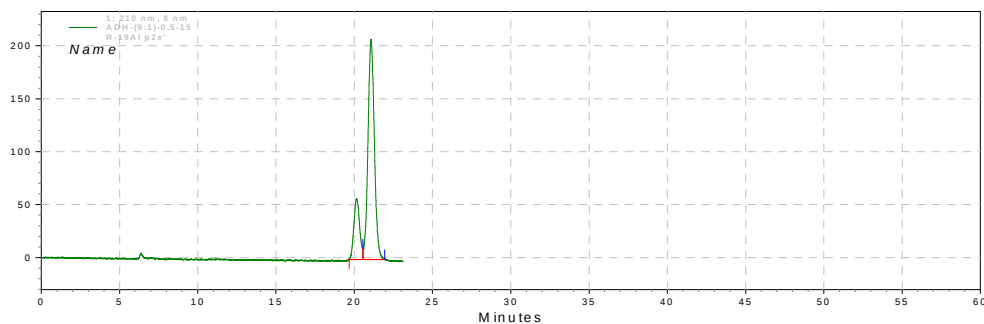


1: 212 nm, 8 nm

Pk #	Retention Time	Area	Area %
1	20.978	11314043	49.454
2	21.845	11563826	50.546
Totals		22877868	100.000

Sample ID : ADH-(9:1)-0.5-15
User Name : System
Filename : E:\yuetao\AI\R-19Al p2e'
Method Name: C:\CLASS-VP\Methods\Multi_pac.met
Sequence Name : C:\CLASS-VP\Sequence\Multi_pac.seq
Run Time : 2008-2-2 20:01:52

Data Graph



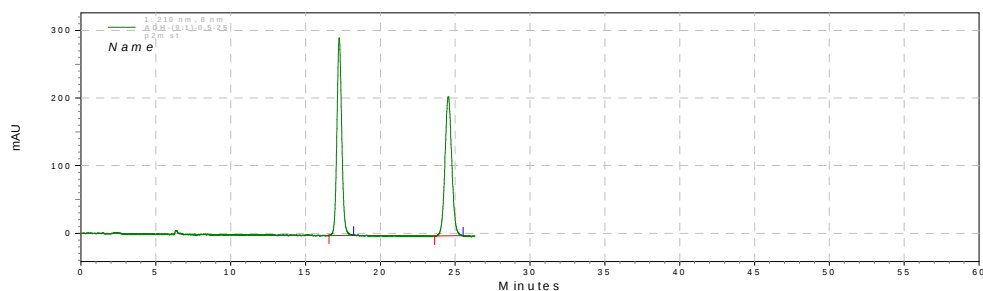
Run Report

1: 212 nm, 8 nm

Pk #	Retention Time	Area	Area Percent
1	20.141	1474530	20.06
2	21.065	5875719	79.94
Totals		7350249	100.00

1c

Sample ID : ADH-(9:1)-0.5-25
 User Name : System
 Filename : E:\yuetao\p2m st
 Method Name: C:\CLASS-VP\Methods\Multi_pac.met
 Sequence Name : {Sequence Name}
 Run Time : 2008-2-4 17:37:17

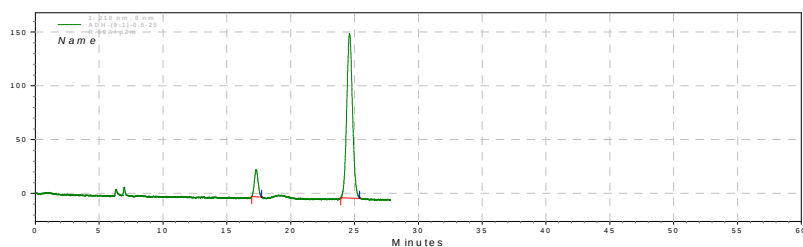


1: 212 nm, 8 nm

Pk #	Retention Time	Area	Area Percent
1	17.247	6534895	50.06
2	24.528	6520008	49.94
Totals		13054902	100.00

Sample ID : ADH-(9:1)-0.5-25
 User Name : System
 Filename : E:\yuetao\AI\R-19Al p2m
 Method Name: C:\CLASS-VP\Methods\Multi_pac.met
 Sequence Name : C:\CLASS-VP\Sequence\Multi_pac.seq
 Run Time : 2008-2-14 17:41:11

Data Graph



Run Report

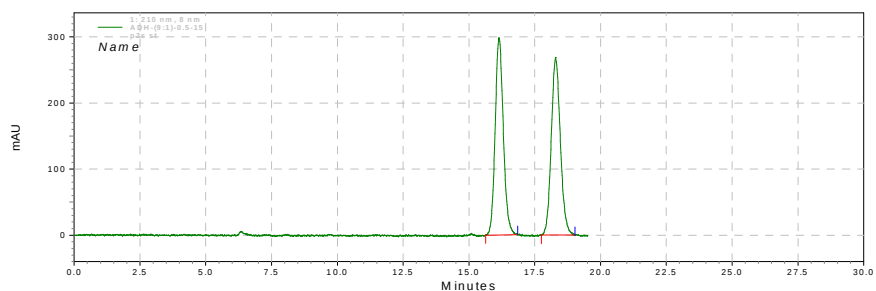
1: 212 nm, 8 nm

Pk #	Retention Time	Area	Area Percent
1	17.296	514076	9.72
2	24.605	4775268	90.28

Totals 5289344 100.00

1d

Sample ID : ADH-(9:1)-0.5-15
 User Name : System
 Filename : E:\yuetao\Al\p2s st
 Method Name: C:\CLASS-VP\Methods\Multi_pac.met
 Sequence Name : {Sequence Name}
 Run Time : 2008-2-20 22:44:26

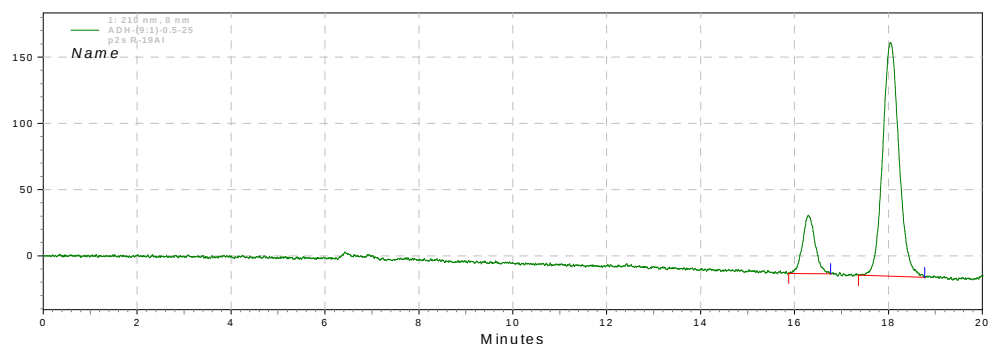


1: 212 nm, 8 nm

Pk #	Retention Time	Area	Area Percent
1	16.137	6446598	50.01
2	18.287	6444665	49.99
Totals		12891262	100.00

Sample ID : ADH-(9:1)-0.5-25
 User Name : System
 Filename : E:\yuetao\Al\p2s R-19Al
 Method Name: C:\CLASS-VP\Methods\Multi_pac.met
 Sequence Name : C:\CLASS-VP\Sequence\Multi_pac.seq
 Run Time : 2008-4-4 15:53:41

Data Graph



Run Report

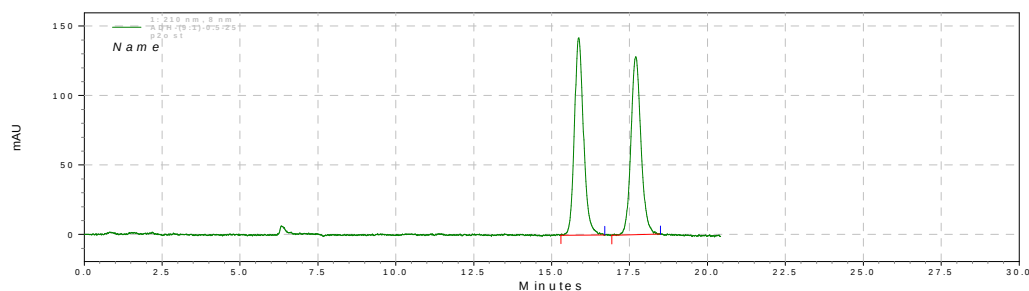
1: 212 nm, 8 nm

Pk #	Retention Time	Area	Area Percent
1	16.288	814695	16.14
2	18.039	4234365	83.86

Totals 5049060 100.00

1f

Sample ID : ADH-(9:1)-0.5-25
 User Name : System
 Filename : E:\yuetao\p2o st
 Method Name: C:\CLASS-VP\Methods\Multi_pac.met
 Sequence Name : {Sequence Name}
 Run Time : 2008-2-4 18:36:28

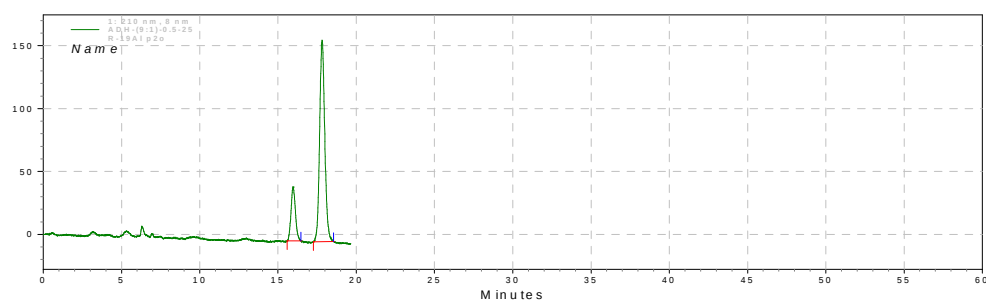


1: 212 nm, 8 nm

Pk #	Retention Time	Area	Height	Area Percent
1	15.861	2901027	141651	50.20
2	17.692	2877993	127522	49.80
Totals		5779020	269173	100.00

Sample ID : ADH-(9:1)-0.5-25
 User Name : System
 Filename : E:\yuetao\AI\R-19Al p2o
 Method Name: C:\CLASS-VP\Methods\Multi_pac.met
 Sequence Name : C:\CLASS-VP\Sequence\Multi_pac.seq
 Run Time : 2008-2-14 17:20:10

Data Graph



Run Report

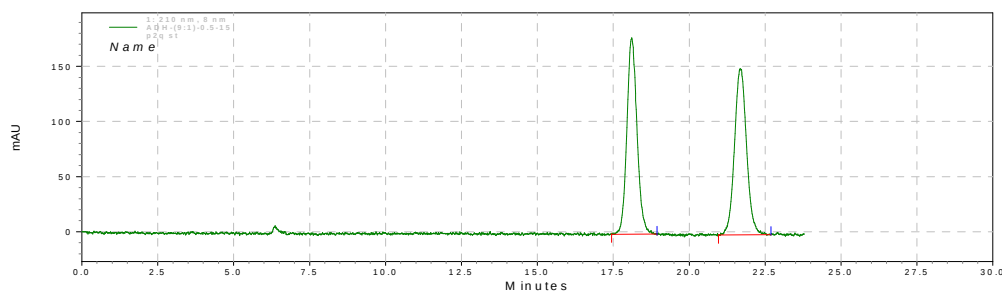
1: 212 nm, 8 nm

Pk #	Retention Time	Area	Area Percent
1	15.960	841093	18.64
2	17.809	3671329	81.36

Totals 4512422 100.00

1g

Sample ID : ADH-(9:1)-0.5-15
 User Name : System
 Filename : E:\yuetao\Al\p2q st
 Method Name: C:\CLASS-VP\Methods\Multi_pac.met
 Sequence Name : {Sequence Name}
 Run Time : 2008-2-20 21:19:51

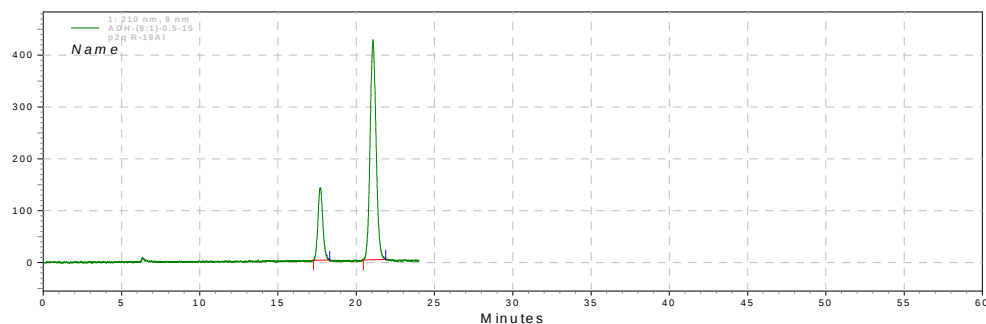


1: 212 nm, 8 nm

Pk #	Retention Time	Area	Area Percent
1	18.102	4099789	49.83
2	21.685	4128362	50.17
Totals		8228151	100.00

Sample ID : ADH-(9:1)-0.5-15
 User Name : System
 Filename : E:\yuetao\Al\p2q R-19Al
 Method Name: C:\CLASS-VP\Methods\Multi_pac.met
 Sequence Name : C:\CLASS-VP\Sequence\Multi_pac.seq
 Run Time : 2008-2-20 21:44:38

Data Graph



Run Report

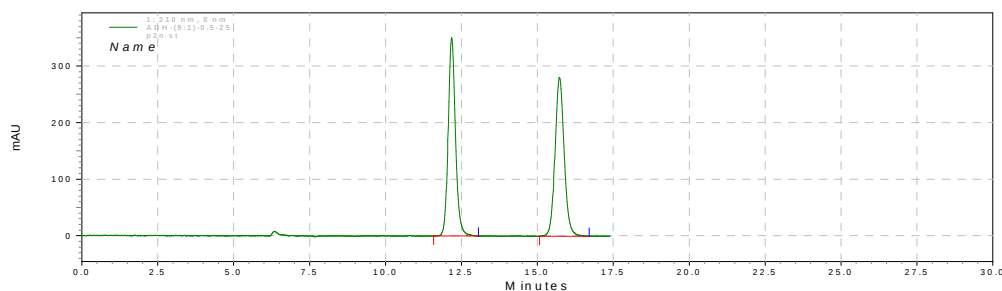
1: 212 nm, 8 nm

Pk #	Retention Time	Area	Area Percent
1	17.687	3058401	21.43
2	21.063	11215208	78.57

Totals 14273609 100.00

1h

Sample ID : ADH-(9:1)-0.5-25
 User Name : System
 Filename : E:\yuetao\p2n st
 Method Name: C:\CLASS-VP\Methods\Multi_pac.met
 Sequence Name : {Sequence Name}
 Run Time : 2008-2-4 18:04:07

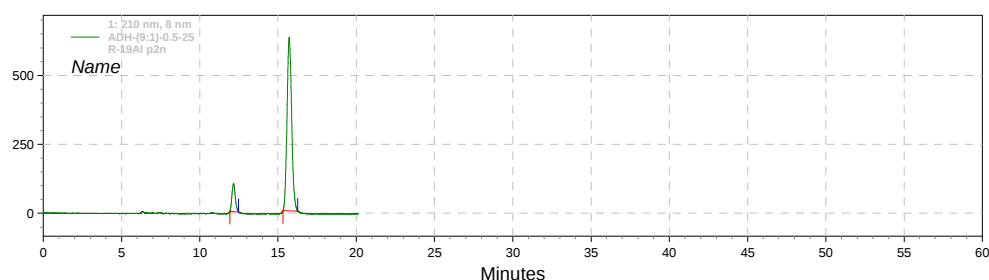


1: 212 nm, 8 nm

Pk #	Retention Time	Area	Area Percent
1	12.170	5850977	49.80
2	15.719	5899024	50.20
Totals		11750000	100.00

Sample ID : ADH-(9:1)-0.5-25
 User Name : System
 Filename : E:\yuetao\AI\R-19Al p2n
 Method Name: C:\CLASS-VP\Methods\Multi_pac.met
 Sequence Name : C:\CLASS-VP\Sequence\Multi_pac.seq
 Run Time : 2008-2-14 18:10:28

Data Graph



Run Report

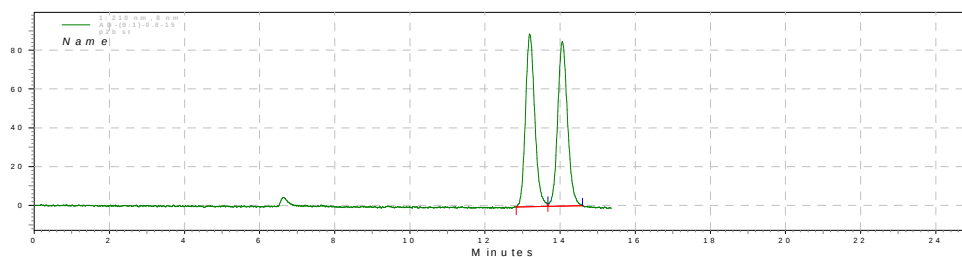
1: 212 nm, 8 nm

Pk #	Retention Time	Area	Area Percent
1	12.151	1484797	10.25
2	15.711	13002692	89.75

Totals 14487489 100.00

1i

Sample ID : AD-(9:1)-0.8-15
 User Name : System
 Filename : E:\yuetao\p2b st
 Method Name: C:\CLASS-VP\Methods\Multi_pac.met
 Sequence Name : C:\CLASS-VP\Sequence\Multi_pac.seq
 Run Time : 2007-12-7 15:34:24

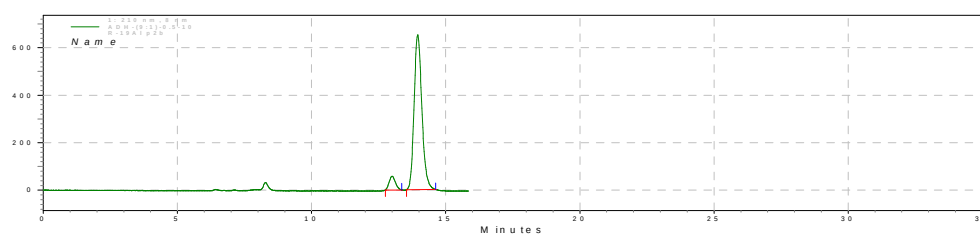


1: 212 nm, 8 nm

Pk #	Retention Time	Area	Area Percent
1	13.184	1525903	49.62
2	14.054	1549566	50.38
Totals		3075469	100.00

Sample ID : ADH-(9:1)-0.5-10
 User Name : System
 Filename : E:\yuetao\AI\R-19Al p2b
 Method Name: C:\CLASS-VP\Methods\Multi_pac.met
 Sequence Name : C:\CLASS-VP\Sequence\Multi_pac.seq
 Run Time : 2008-1-18 19:52:46

Data Graph



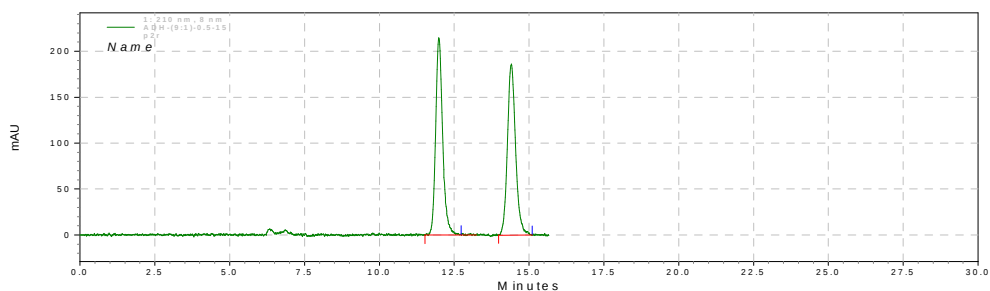
Run Report

1: 212 nm, 8 nm

Pk #	Retention Time	Area	Area Percent
1	12.990	934143	6.61
2	13.949	13200573	93.39
Totals		14134716	100.00

1k

Sample ID : ADH-(9:1)-0.5-15
User Name : System
Filename : E:\yuetao\Al\p2r
Method Name: C:\CLASS-VP\Methods\Multi_pac.met
Sequence Name : {Sequence Name}
Run Time : 2008-2-20 22:10:14

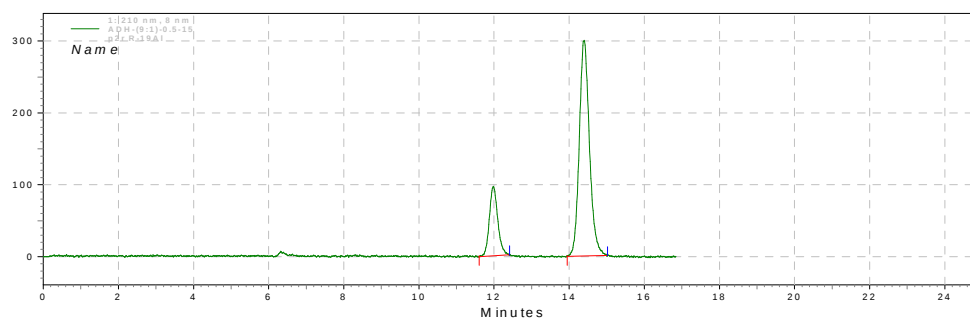


1: 210 nm, 8 nm

Pk #	Retention Time	Area	Area Percent
1	11.979	3501652	49.90
2	14.402	3516378	50.10
Totals		7018030	100.00

Sample ID : ADH-(9:1)-0.5-15
User Name : System
Filename : E:\yuetao\Al\p2r R-19Al
Method Name: C:\CLASS-VP\Methods\Multi_pac.met
Sequence Name : C:\CLASS-VP\Sequence\Multi_pac.seq
Run Time : 2008-2-20 22:26:37

Data Graph



Run Report

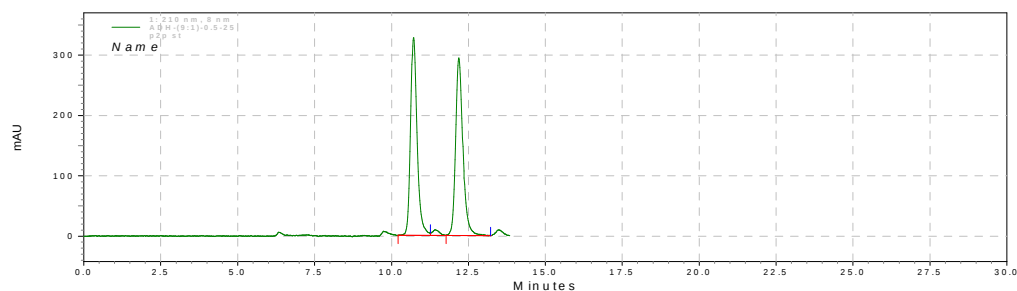
1: 212 nm, 8 nm

Pk #	Retention Time	Area	Area Percent
1	11.976	1504406	21.07
2	14.392	5636628	78.93

Totals 7141034 100.00

11

Sample ID : ADH-(9:1)-0.5-25
 User Name : System
 Filename : E:\yuetao\p2p st
 Method Name: C:\CLASS-VP\Methods\Multi_pac.met
 Sequence Name : {Sequence Name}
 Run Time : 2008-2-4 18:22:03

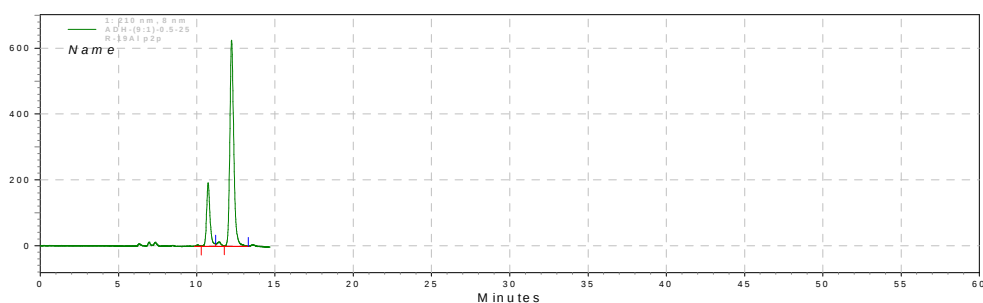


1: 212 nm, 8 nm

Pk #	Retention Time	Area	Height	Area Percent
1	10.709	4848769	325844	49.83
2	12.185	4881624	291962	50.17
Totals		9730394	617806	100.00

Sample ID : ADH-(9:1)-0.5-25
 User Name : System
 Filename : E:\yuetao\Al\R-19Al p2p
 Method Name: C:\CLASS-VP\Methods\Multi_pac.met
 Sequence Name : C:\CLASS-VP\Sequence\Multi_pac.seq
 Run Time : 2008-2-14 17:04:27

Data Graph



Run Report

1: 212 nm, 8 nm

Pk #	Retention Time	Area	Area Percent
1	10.721	2953844	21.35
2	12.219	10882760	78.65
Totals		13836605	100.00

