

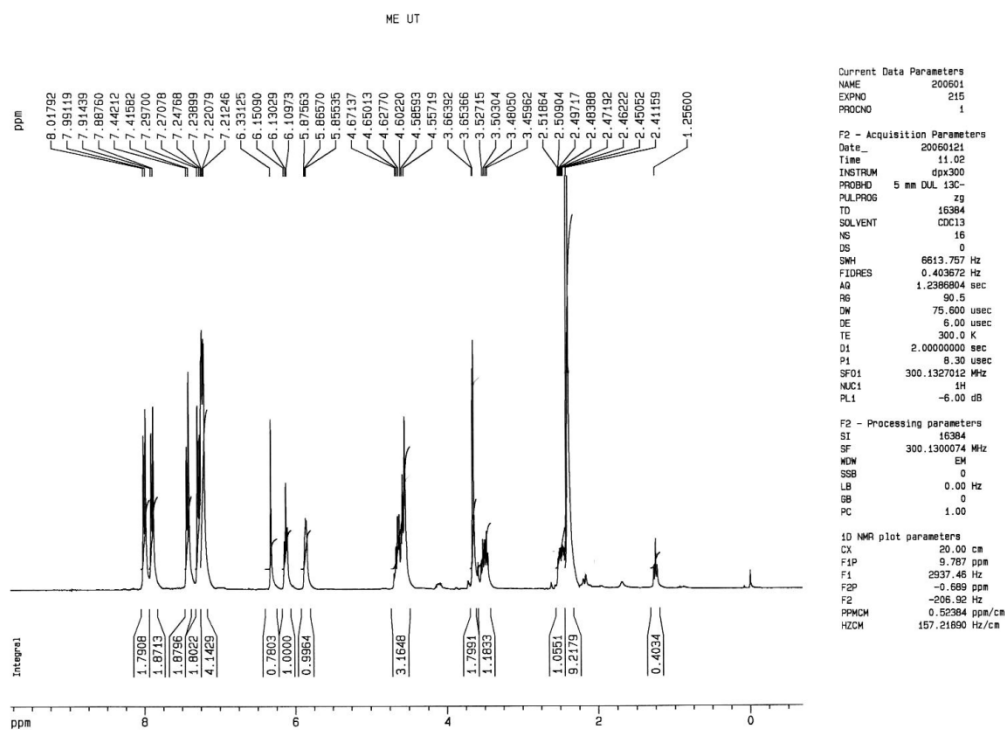
**SUPPORTING INFORMATION OF THE SYNTHETIC, STRUCTURAL AND
ANTICANCER ACTIVITY EVALUATION STUDIES ON NOVEL
PYRAZOLYLNUCLEOSIDES**

EXPERIMENTAL

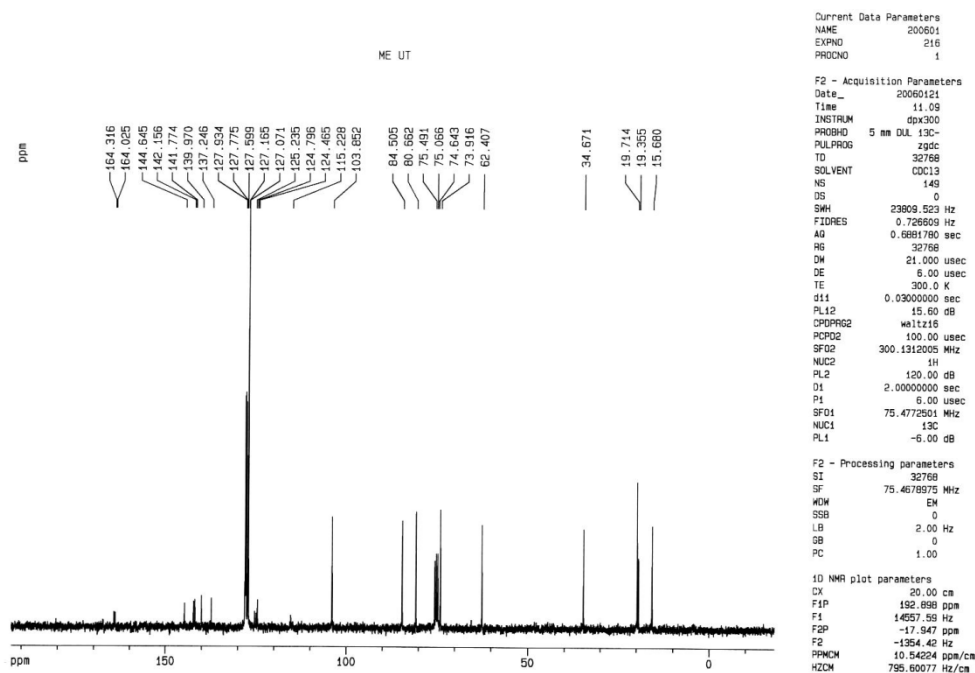
Reactions were conducted under an atmosphere of nitrogen in anhydrous solvents. Column chromatography was carried out using silica gel (100-200 mesh). Melting points were determined using concentrated H₂SO₄ acid bath and are uncorrected. Analytical TLCs were performed on pre-coated Merck silica gel 60F₂₅₄ plates; the spots were detected either using UV light or by charring with 4 % alcoholic sulfuric acid. The IR spectra were recorded on a Perkin-Elmer 2000 FT-IR spectrophotometer. The optical rotations were measured with Bellingham-Stanley AD 220 polarimeter, the concentrations are expressed as g/mL. The ¹H-NMR and ¹³C-NMR spectra were recorded on a Bruker Avance 300 spectrometer at 300 and 75.5 MHz, respectively in CDCl₃, DMSO-d₆ or CD₃CN. All the 2D measurements were performed in acetone-d₆ on a Bruker Avance 400 spectrometer. Chemical shifts are relative to internal TMS. Assignments are based on COSY, NOESY, HMBC (using Bruker's microprogram inv4gslplrnd, which includes low-pass J-filter to suppress one-bond correlations), HSQC and JRES spectra. The chemical shift values are reported as δ ppm relative to TMS used as internal standard and the coupling constants (*J*) are measured in Hz. The ESI-HRMS spectra of all the compounds were recorded on a JEOL JMS-AX505W high-resolution mass spectrometer in positive ion mode using the matrix HEDS (*bis*-hydroxyethylsulphide) doped with sodium acetate. Acetonitrile was used after distillation over freshly ignited potassium carbonate.

2'-Deoxy-1'-(5-cyanomethyl-3-*p*-methylphenyl)pyrazolyl-3',5'-di-*O*-toluoyl- β -D-ribofuranose

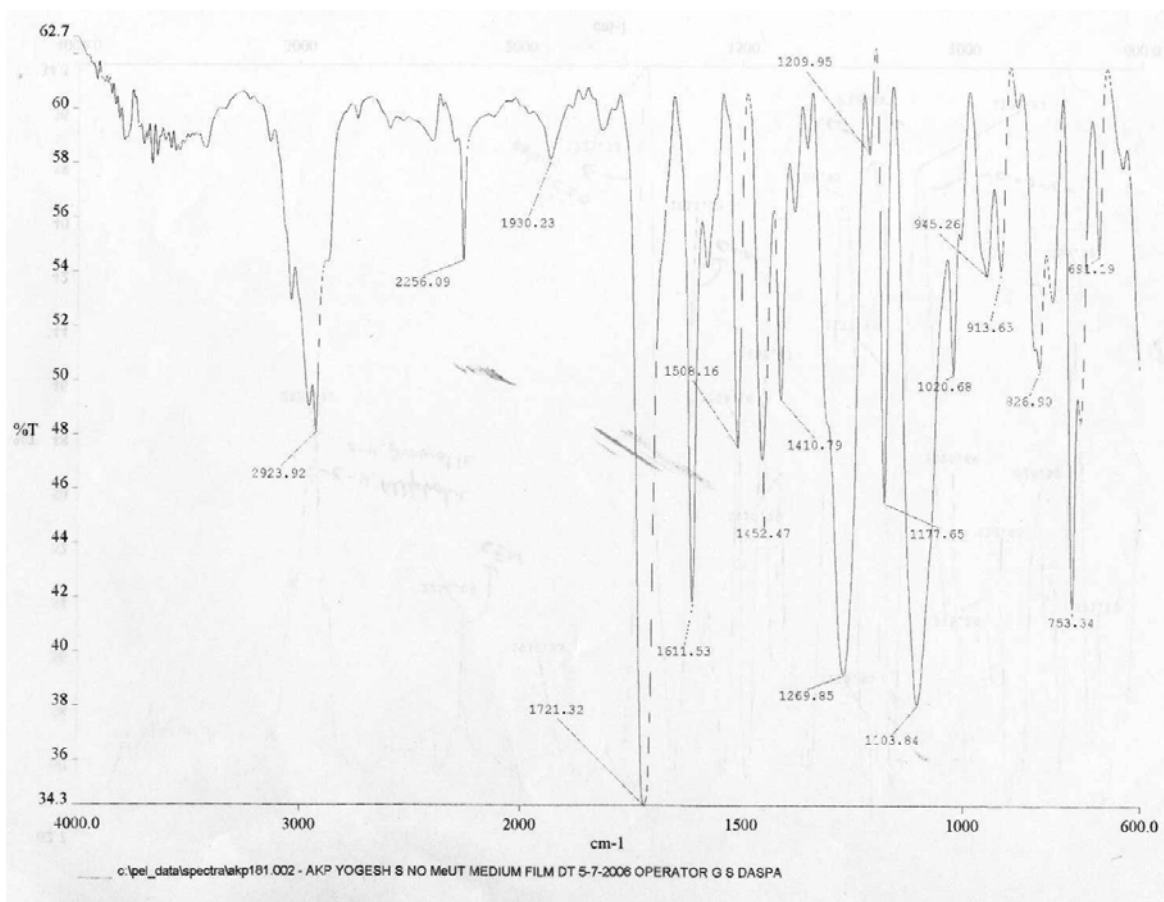
(3a)



^1H NMR spectrum (Bruker, 300MHz, CDCl_3) of compound **3a**

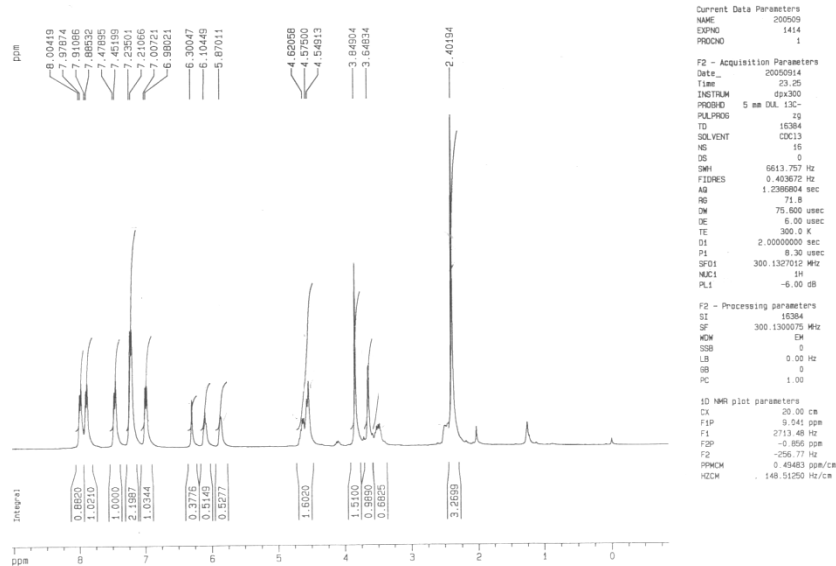


^{13}C NMR spectrum (Bruker, 75.5MHz, CDCl_3) of compound **3a**

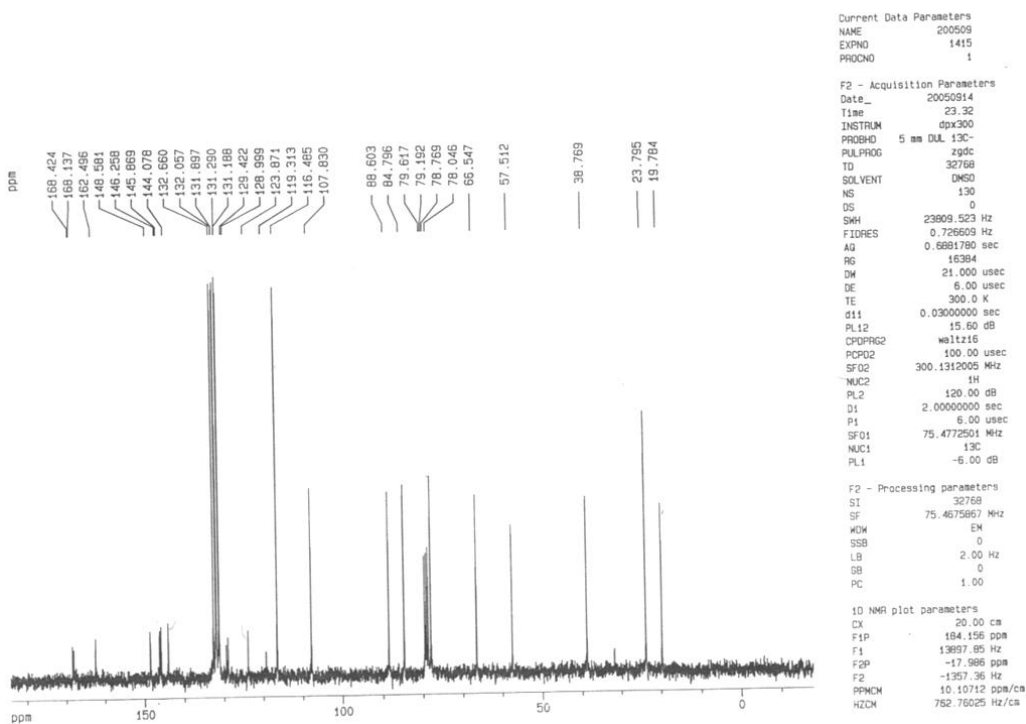


IR spectrum (Perkin-Elmer 2000 FT-IR spectrophotometer) of compound **3a**

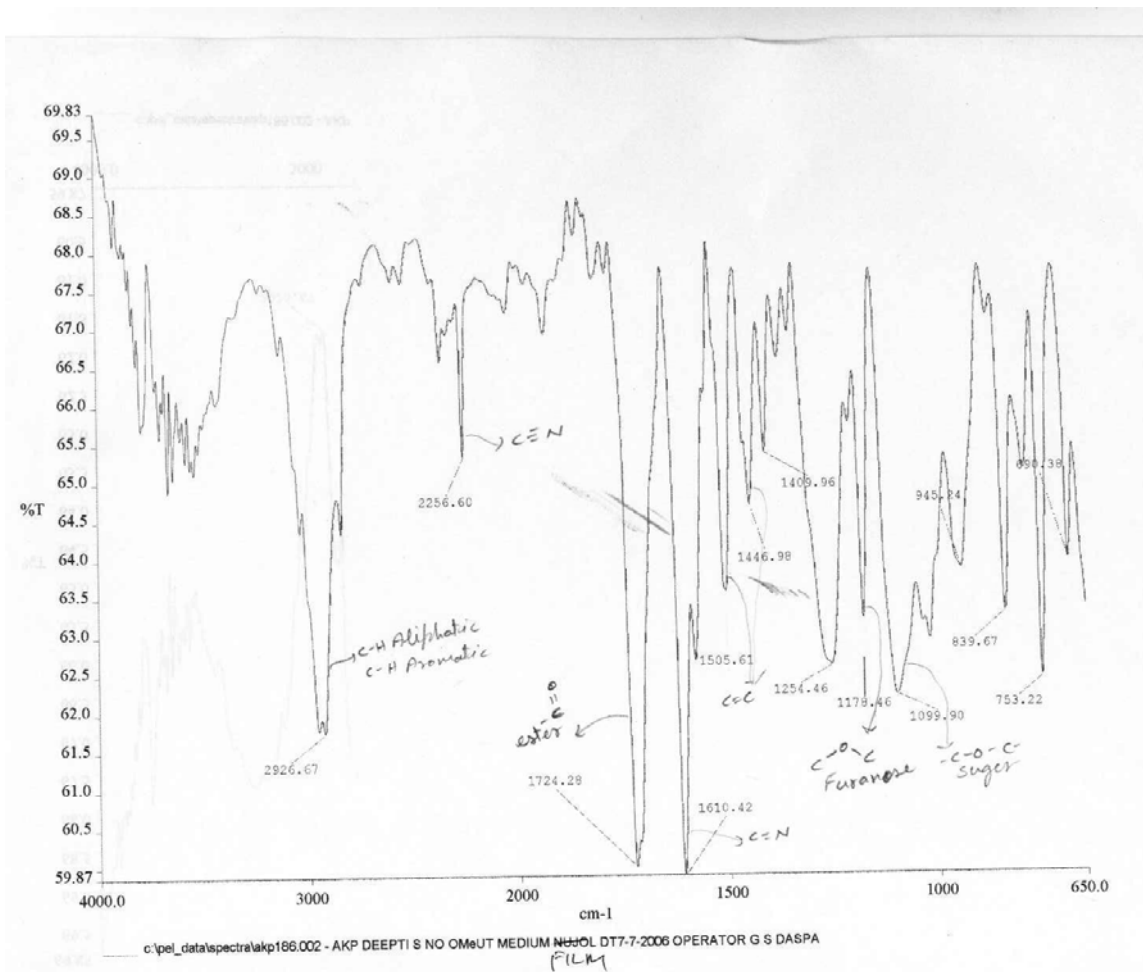
2'-Deoxy-1'-(3-cyanomethyl-5-*p*-methoxyphenyl)pyrazolyl-3',5'-di-*O*-toluoyl- β -D-ribo furanose
(3b).



^1H NMR spectrum (Bruker, 300MHz, CDCl_3) of compound **3b**

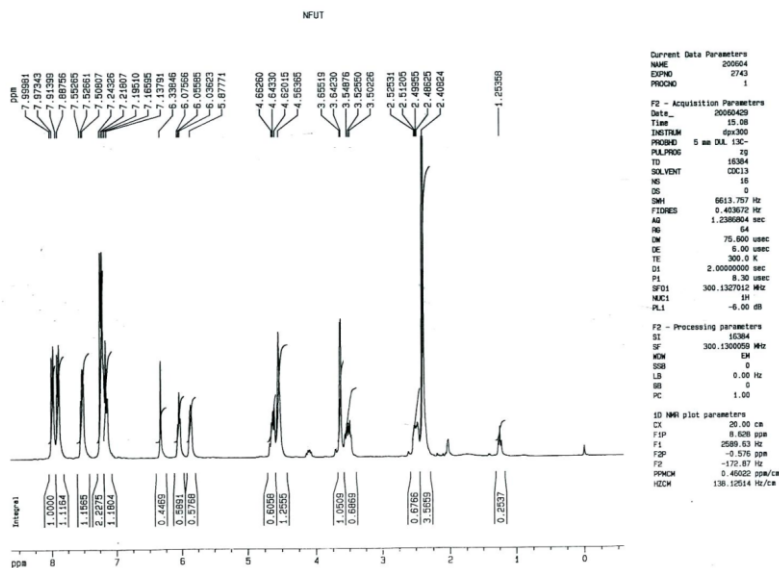


^{13}C NMR spectrum (Bruker, 75.5MHz, CDCl_3) of compound **3b**

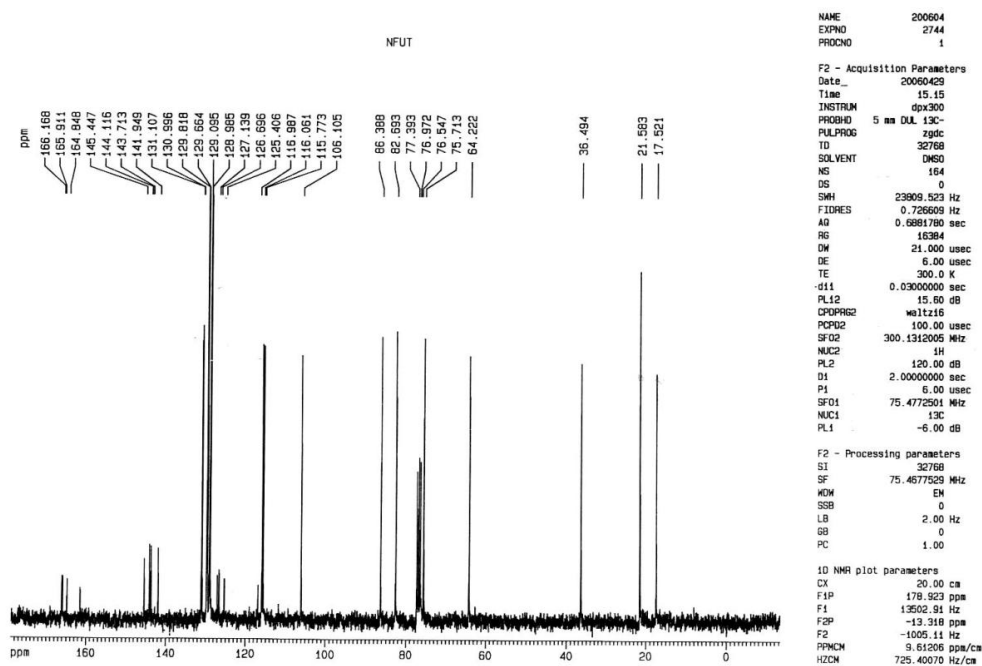


IR spectrum (Perkin-Elmer 2000 FT-IR spectrophotometer) of compound **3b**

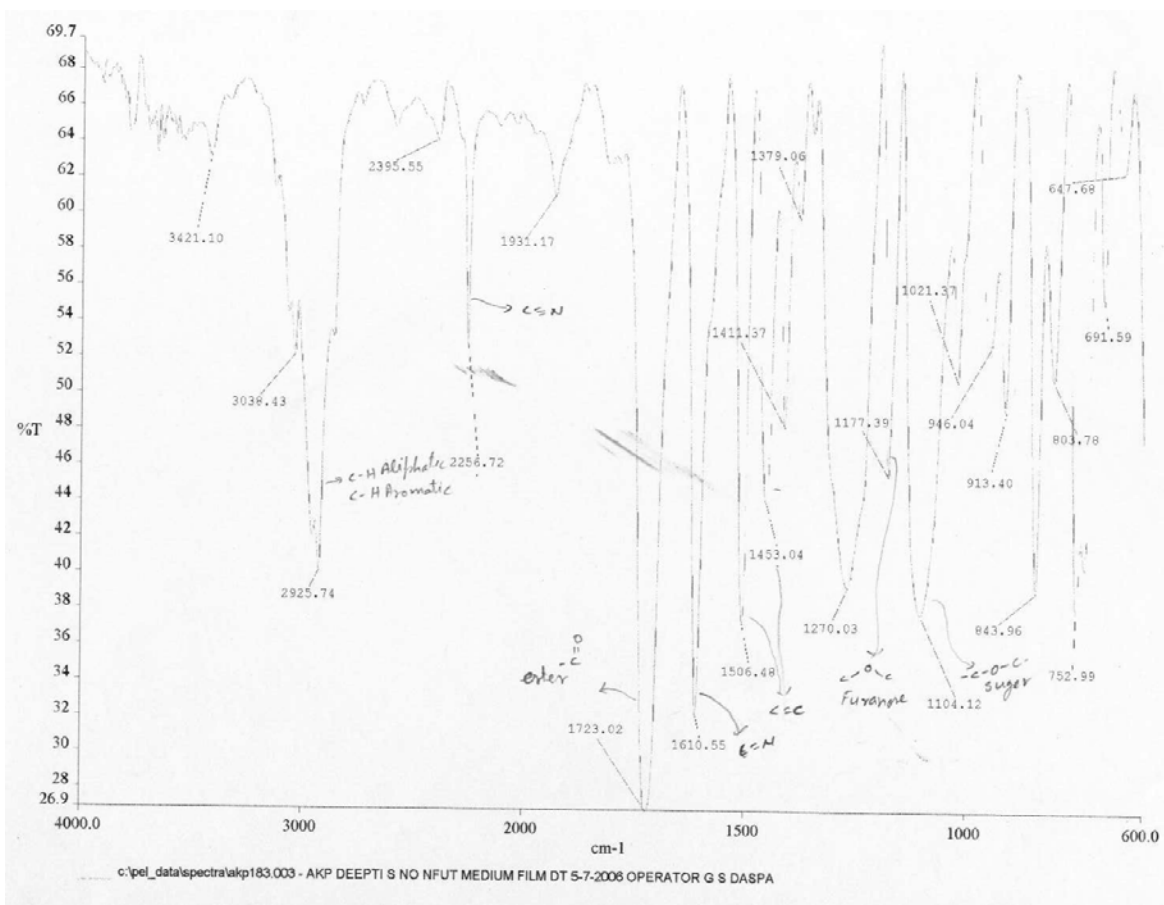
2'-Deoxy-1'-(3-cyanomethyl-5-*p*-fluorophenyl)pyrazolyl-3',5'-di-*O*-toluoyl- β -D-ribofuranose (3c).



¹H NMR spectrum (Bruker, 300MHz, CDCl₃) of compound 3c

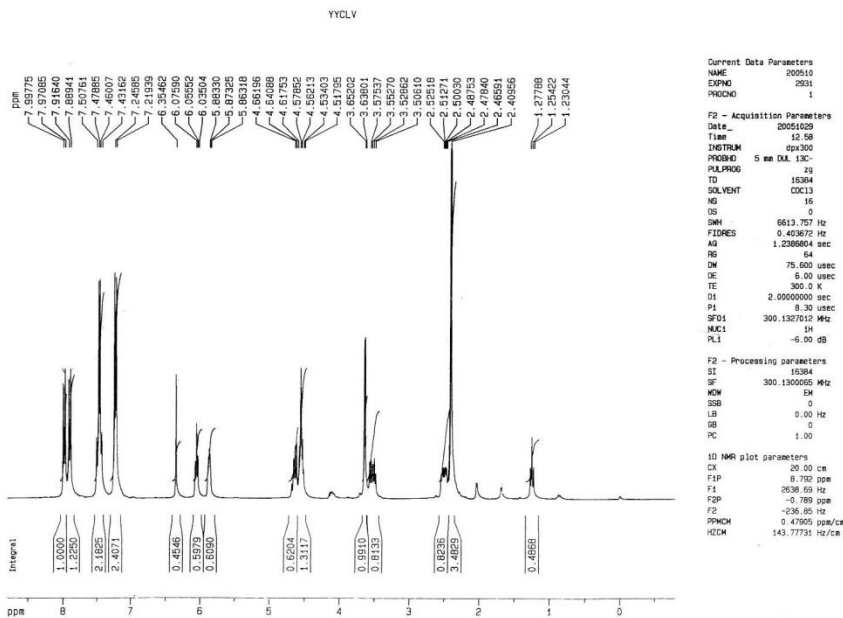


¹³C NMR spectrum (Bruker, 75.5MHz, CDCl₃) of compound 3c

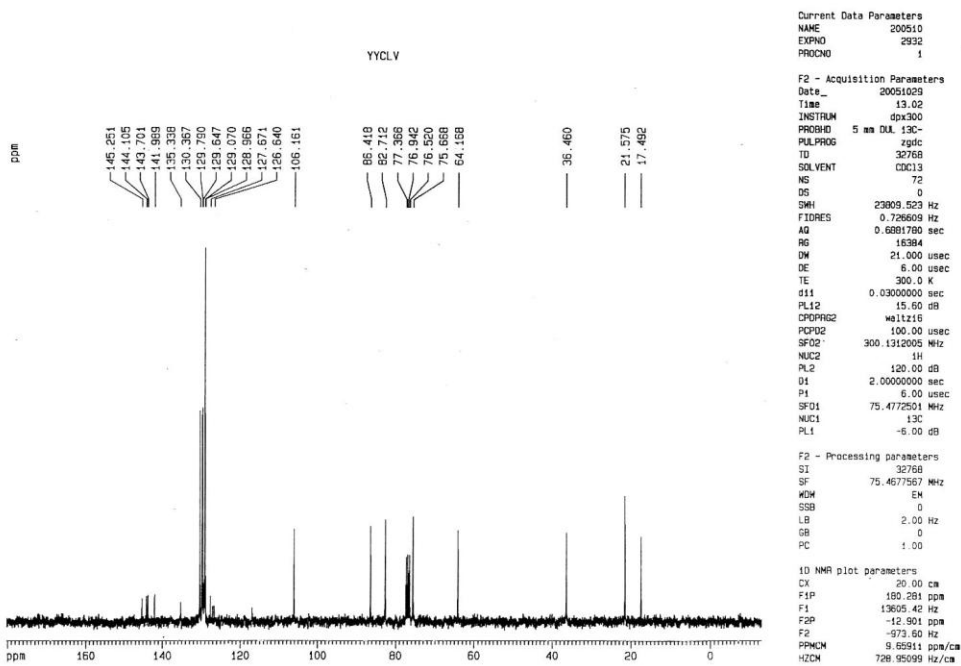


IR spectrum (Perkin-Elmer 2000 FT-IR spectrophotometer) of compound **3c**

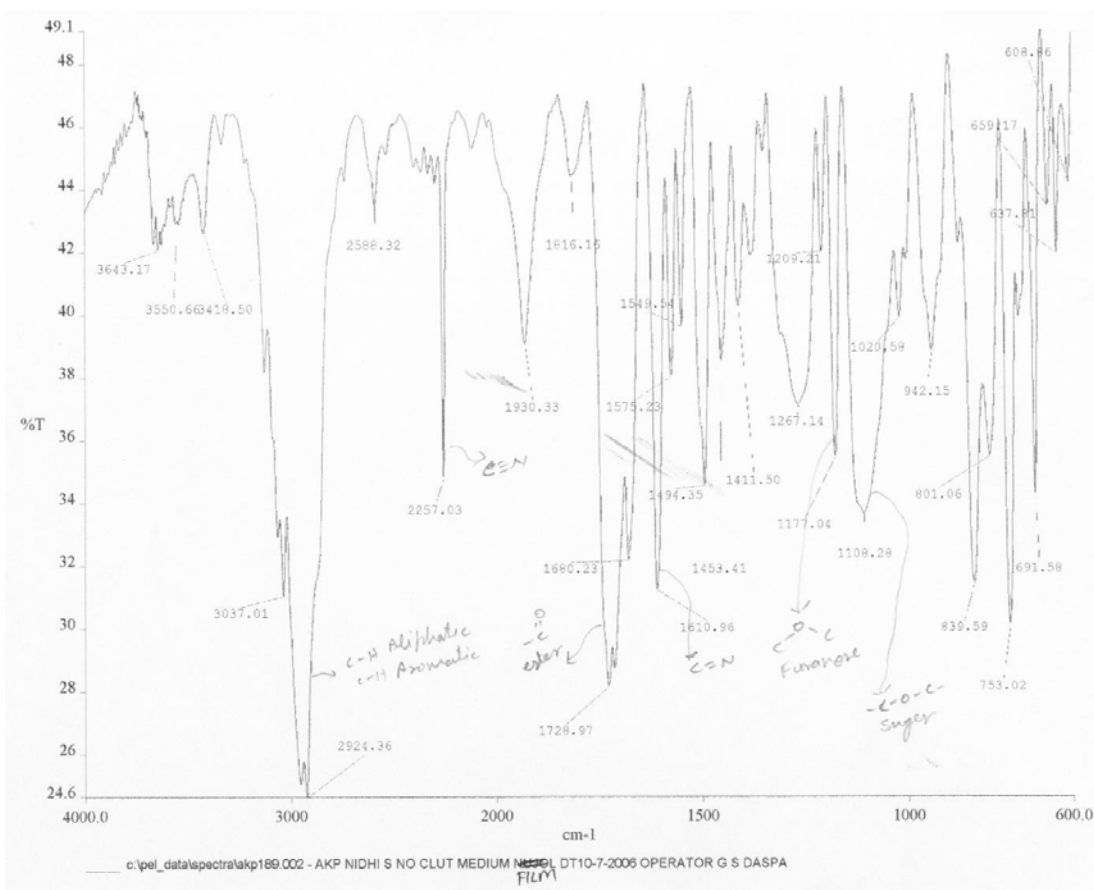
2'-Deoxy-1'-(3-cyanomethyl-5-*p*-chlorophenyl)pyrazolyl-3',5'-di-*O*-toluoyl- β -D-ribofuranose
(3d)



^1H NMR spectrum (Bruker, 300MHz, CDCl_3) of compound 3d

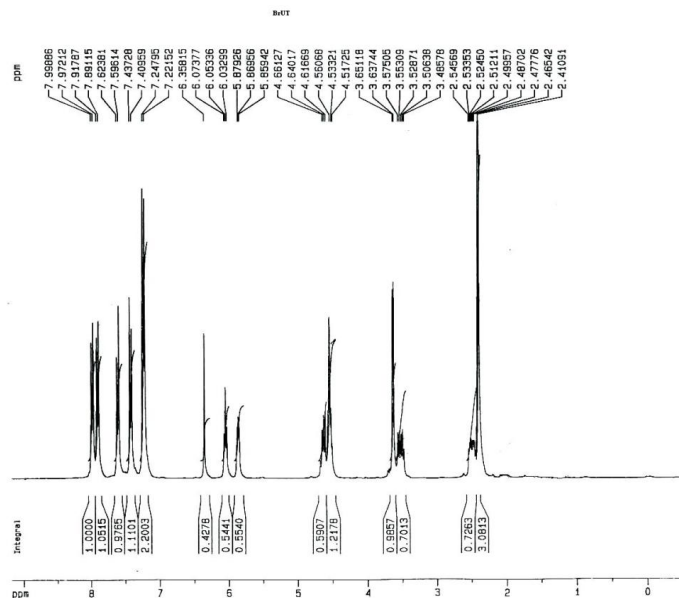


^{13}C NMR spectrum (Bruker, 75.5MHz, CDCl_3) of compound 3d

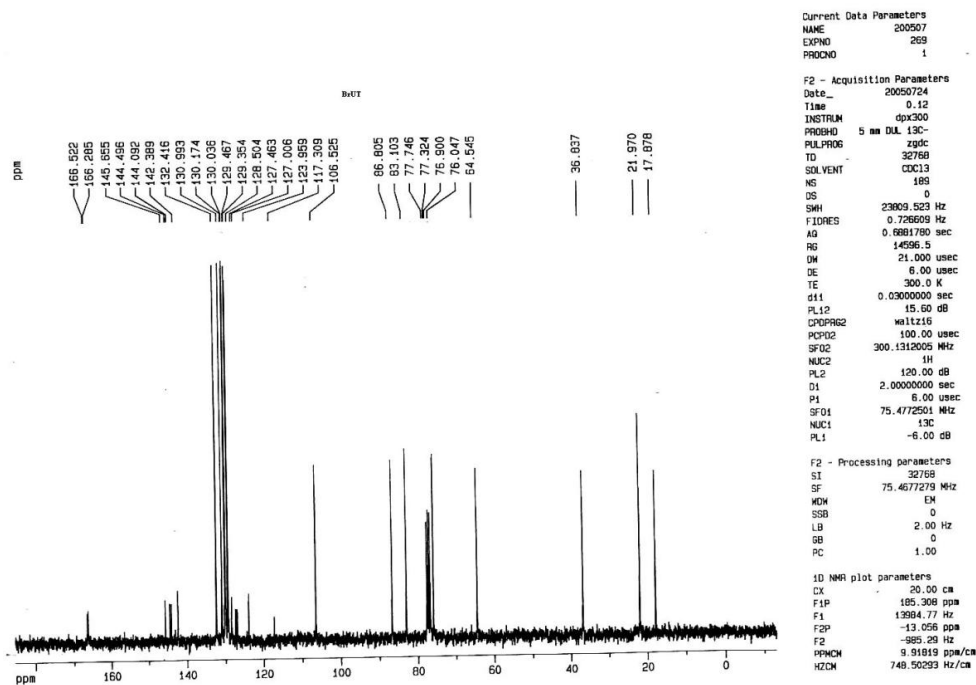


IR spectrum (Perkin-Elmer 2000 FT-IR spectrophotometer) of compound **3d**

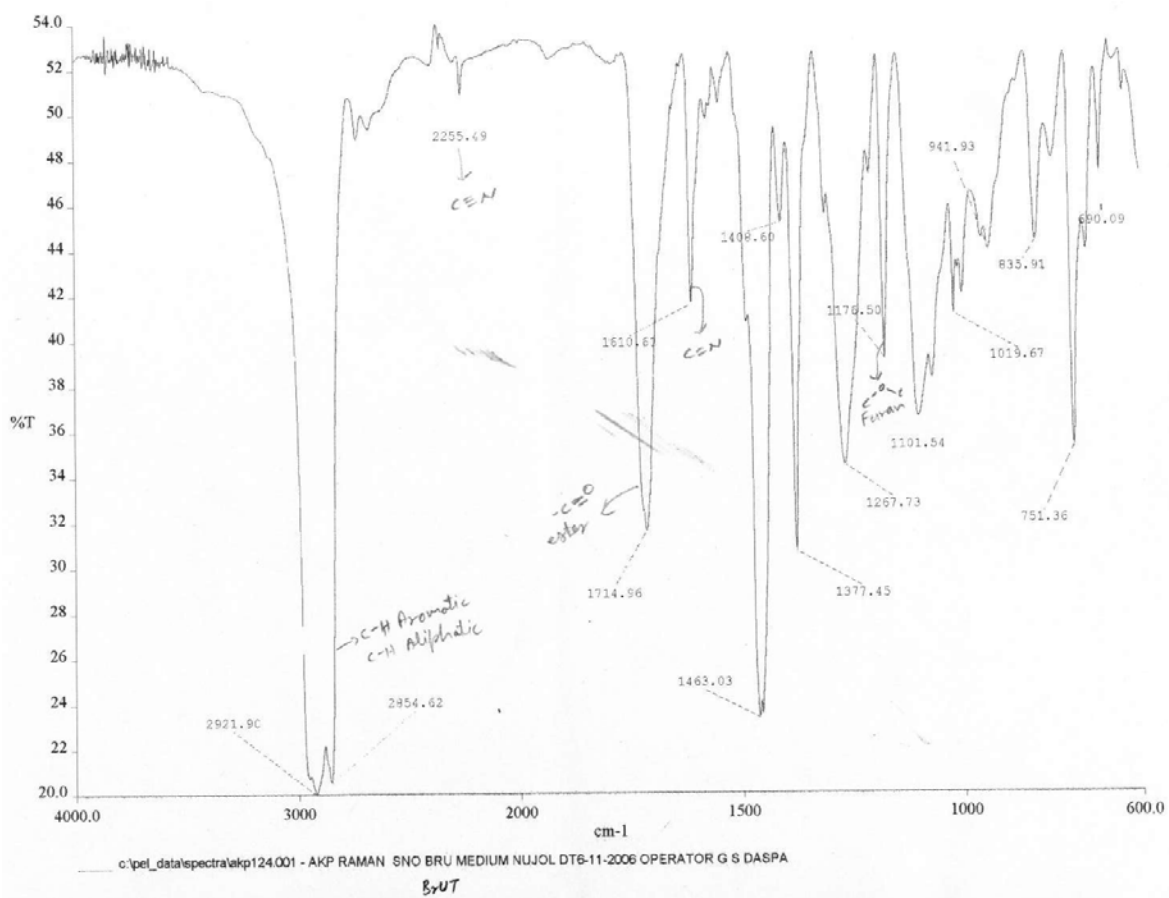
2'-Deoxy-1'-(3-cyanomethyl-5-*p*-bromophenyl)pyrazolyl-3',5'-di-*O*-toluoyl- β -D-ribofuranose (3e)



^1H NMR spectrum (Bruker, 300MHz, CDCl_3) of compound **3e**

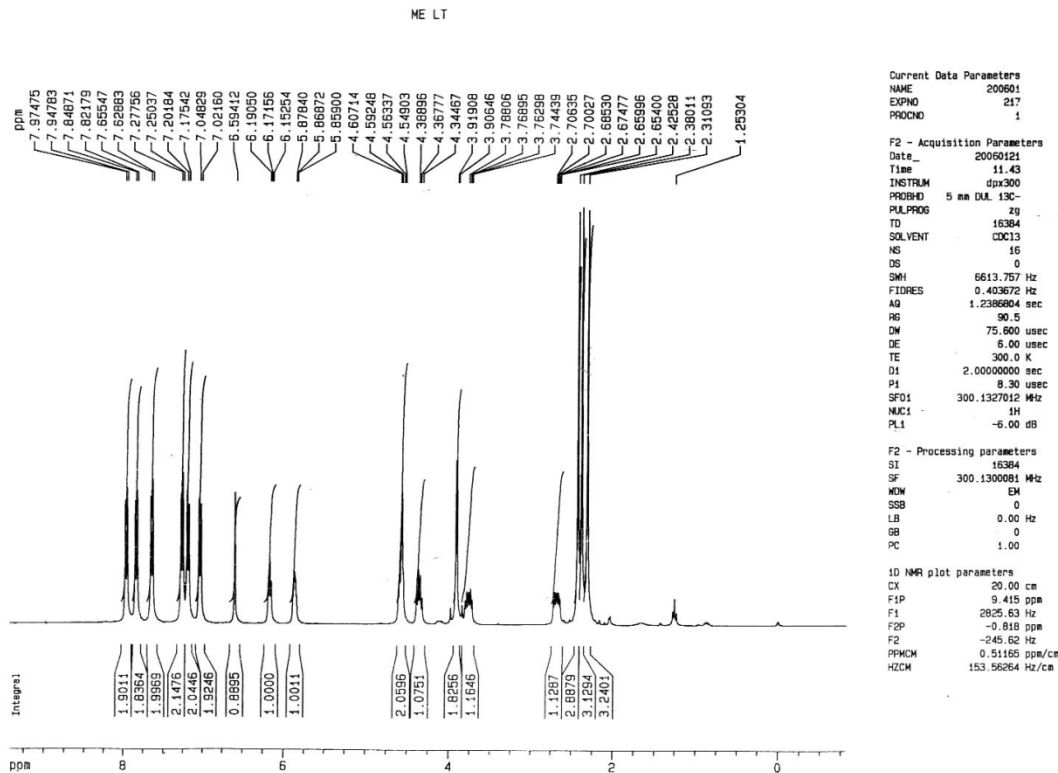


^{13}C NMR spectrum (Bruker, 75.5MHz, CDCl_3) of compound **3e**

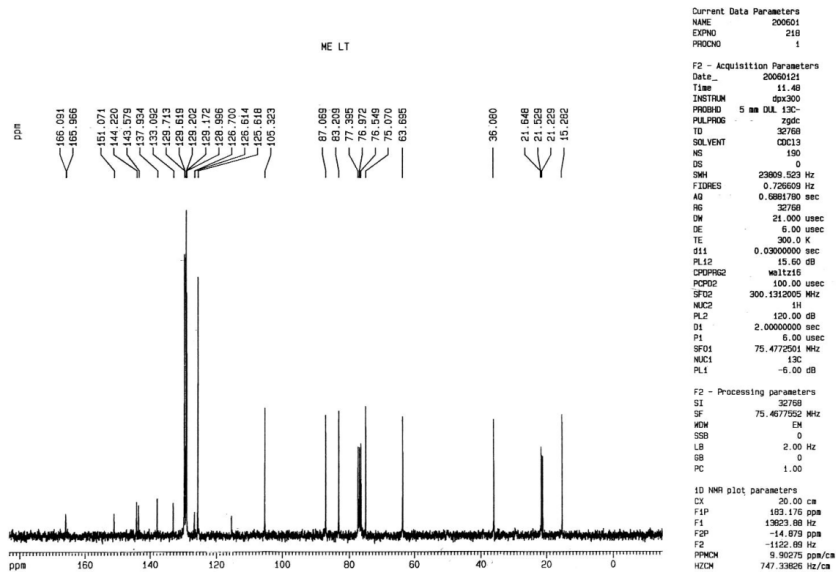


IR spectrum (Perkin-Elmer 2000 FT-IR spectrophotometer) of compound **3e**

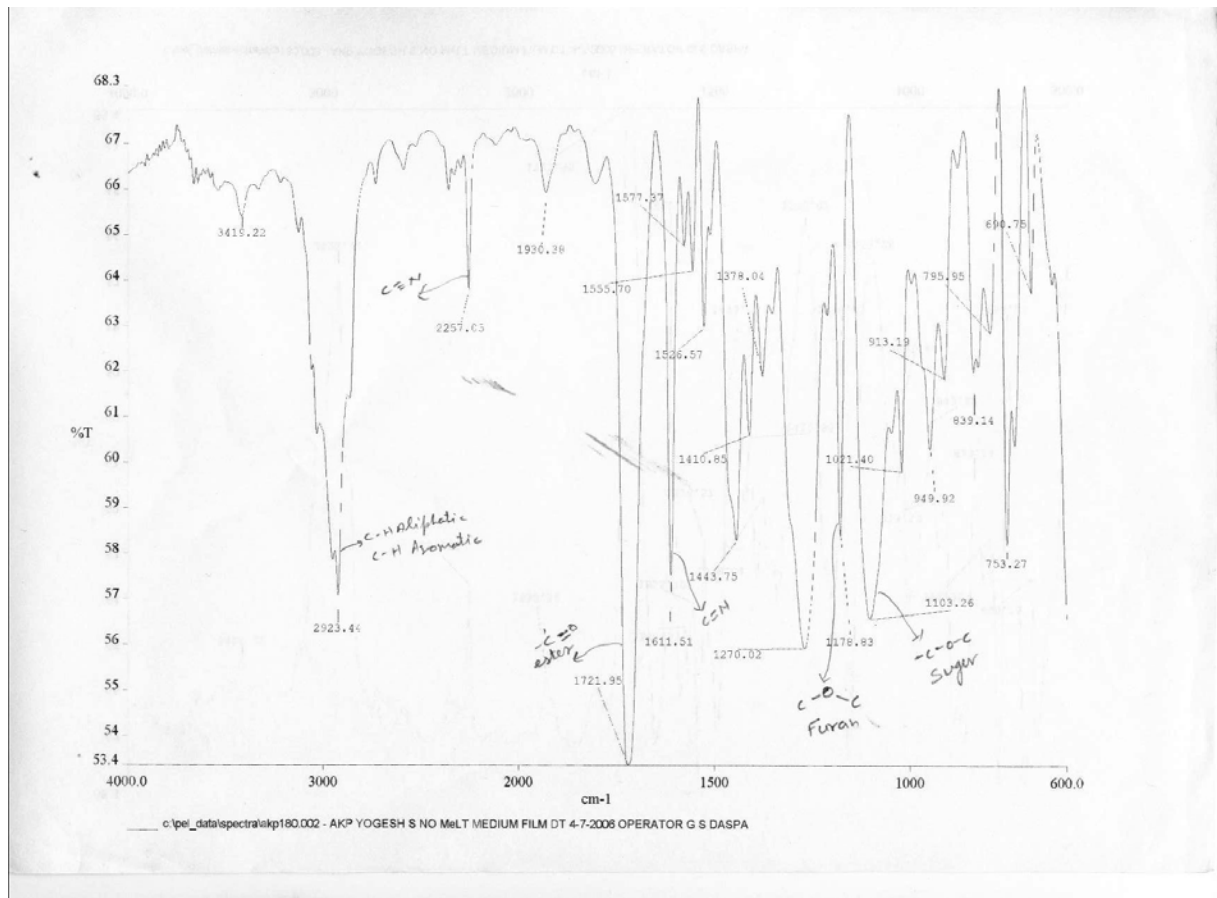
2'-Deoxy-1'-(5-cyanomethyl-3-*p*-methylphenyl)pyrazolyl-3',5'-di-*O*-toluoyl-β-D-ribofuranose (4a)



¹H NMR spectrum (Bruker, 300MHz, CDCl₃) of compound **4a**

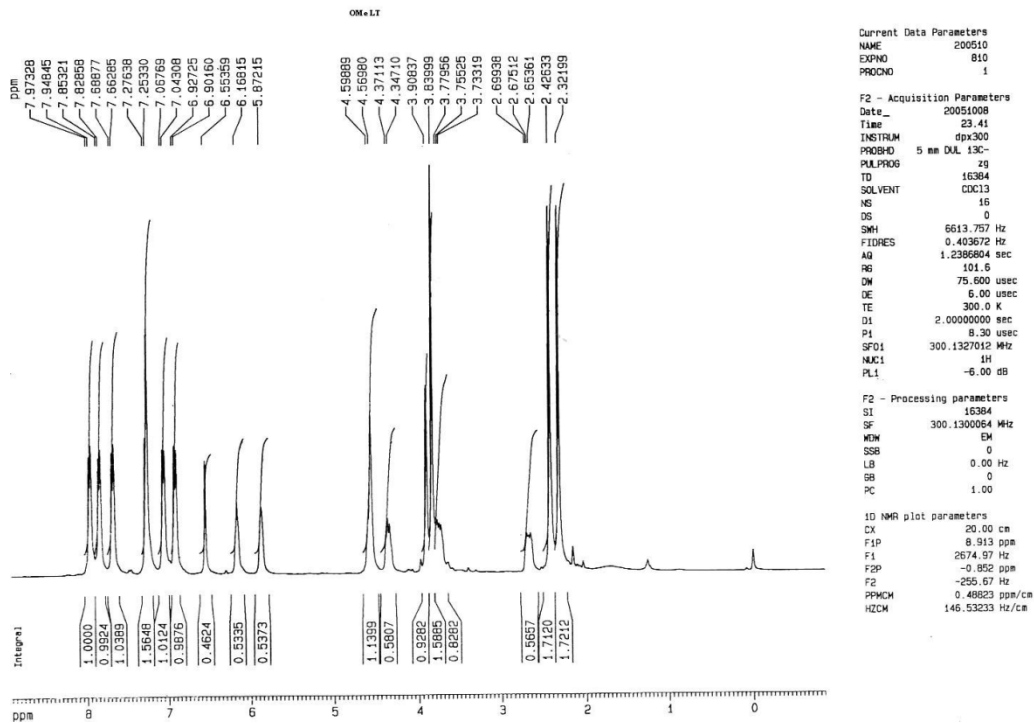


¹³C NMR spectrum (Bruker, 75.5MHz, CDCl₃) of compound **4a**

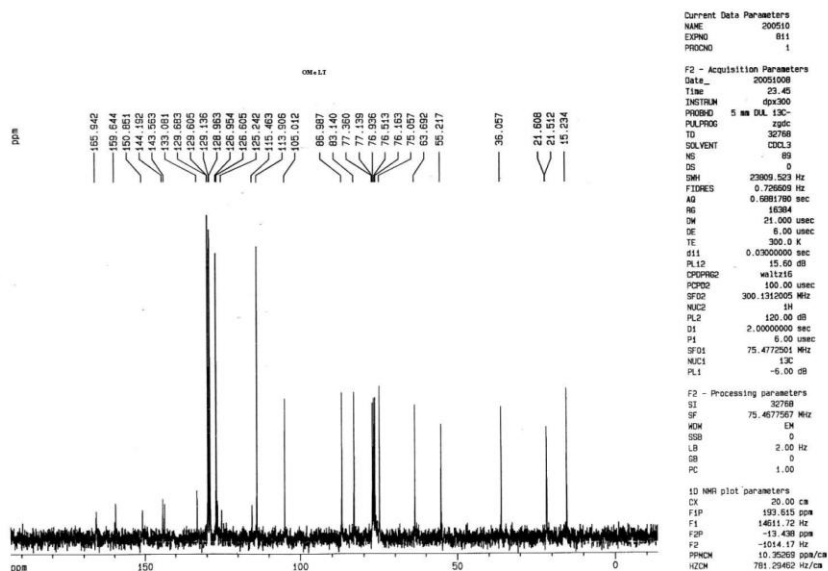


IR spectrum (Perkin-Elmer 2000 FT-IR spectrophotometer) of compound **4a**

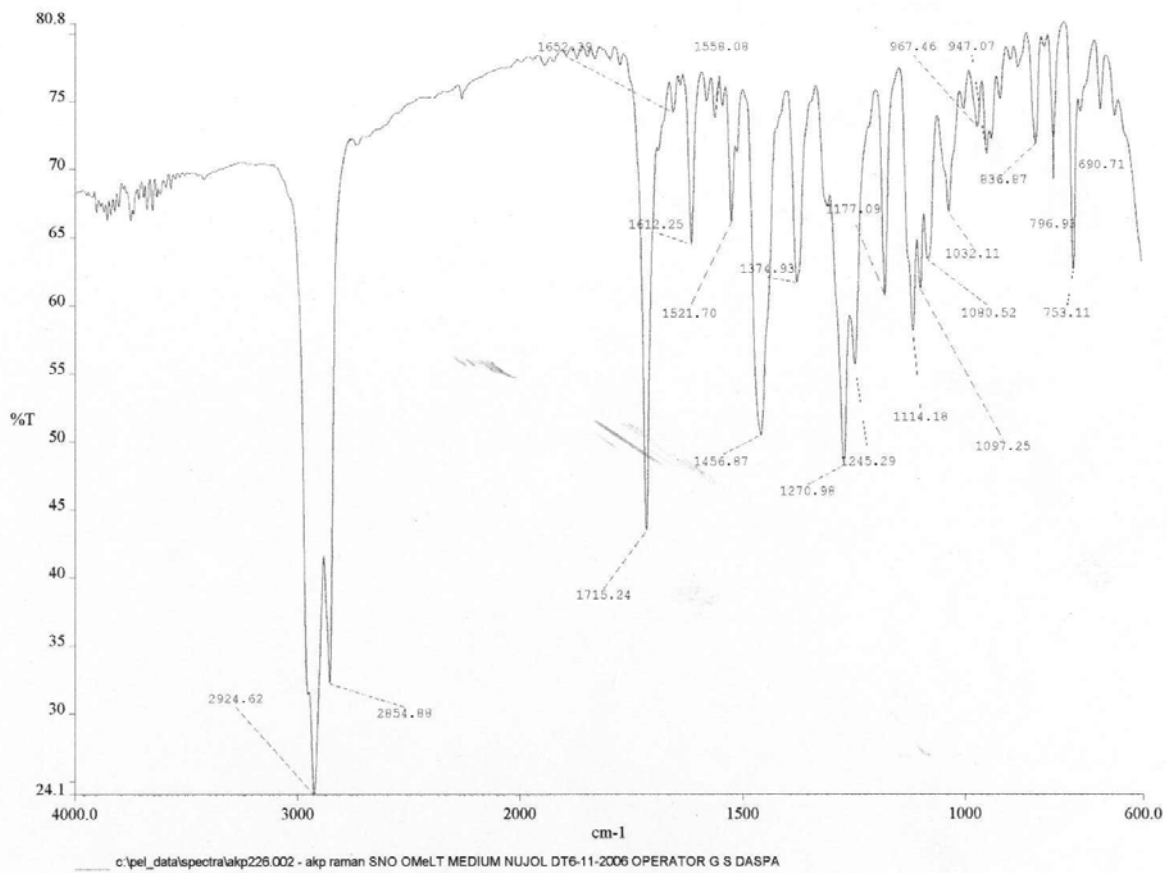
2'-deoxy-1'-(5-cyanomethyl-3-*p*-methoxyphenyl)pyrazolyl-3',5'-di-*O*-toluoyl- β -D-ribofuranose (4b).



¹H NMR spectrum (Bruker, 300MHz, CDCl₃) of compound **4b**

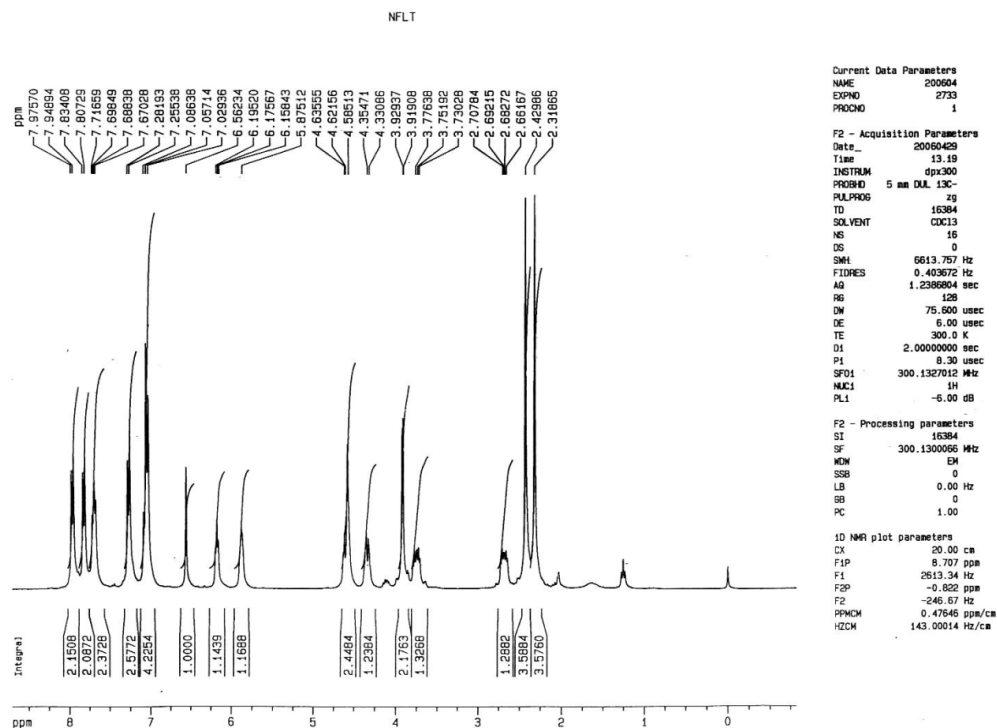


¹³C NMR spectrum (Bruker, 75.5MHz, CDCl₃) of compound **4b**

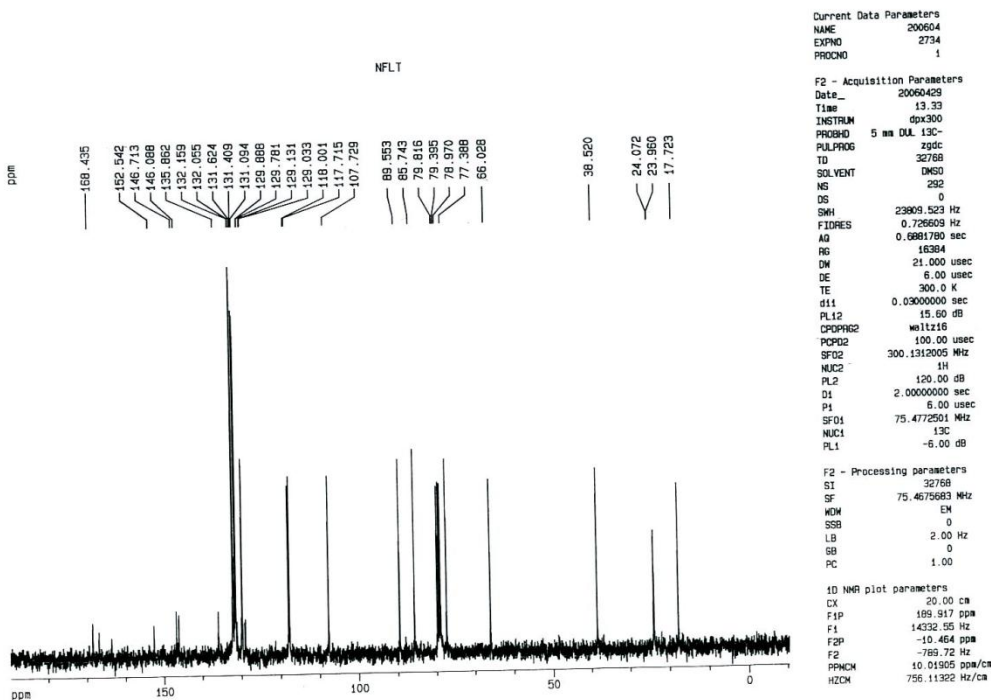


IR spectrum (Perkin-Elmer 2000 FT-IR spectrophotometer) of compound **4b**

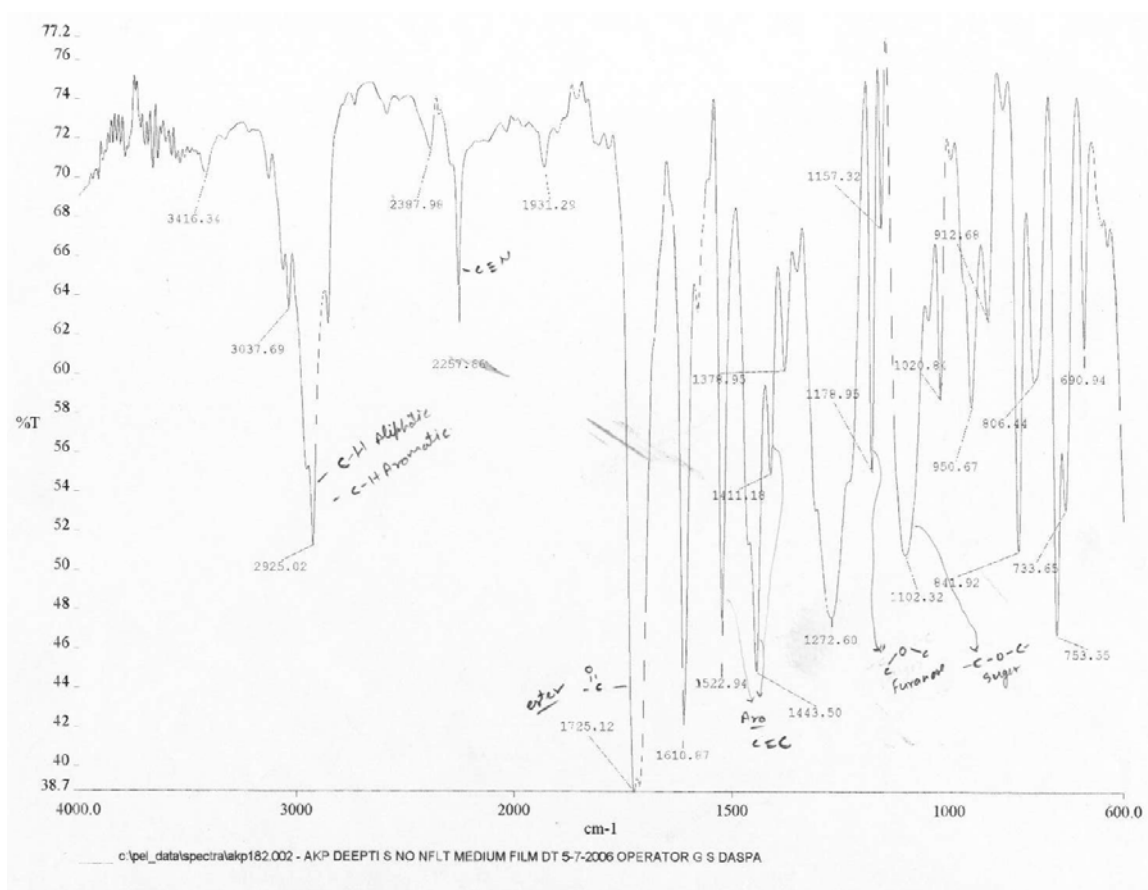
2'-Deoxy-1'-(5-cyanomethyl-3-*p*-fluorophenyl)pyrazolyl-3',5'-di-*O*-toluoyl- β -D-ribofuranose
(4c).



^1H NMR spectrum (Bruker, 300MHz, CDCl_3) of compound 4c

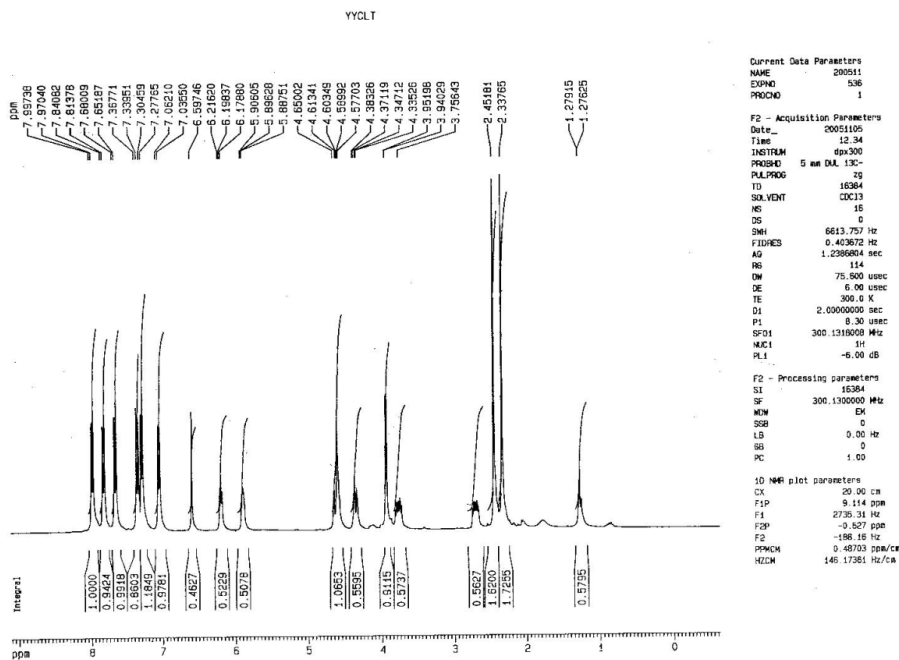


^{13}C NMR spectrum (Bruker, 75.5MHz, CDCl_3) of compound 4c

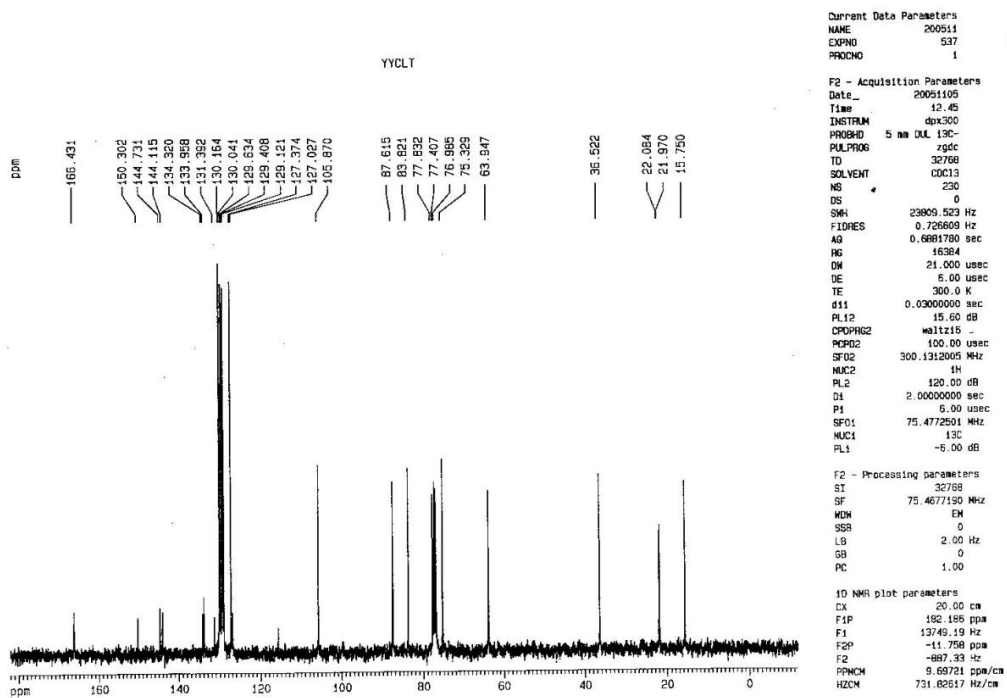


IR spectrum (Perkin-Elmer 2000 FT-IR spectrophotometer) of compound **4c**

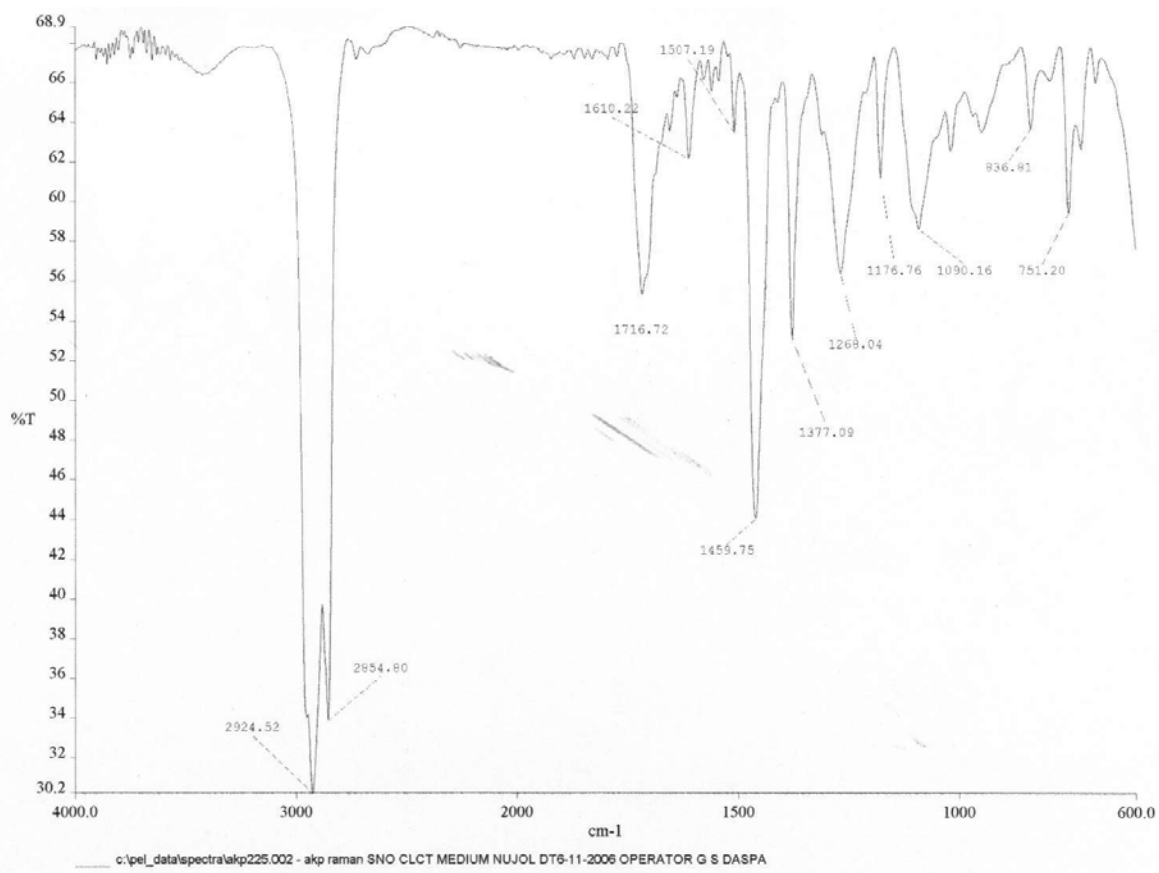
2'-Deoxy-1'-(5-cyanomethyl-3-*p*-chlorophenyl)pyrazolyl-3',5'-di-*O*-toluoyl- β -D-ribofuranose (4d).



¹H NMR spectrum (Bruker, 300MHz, CDCl₃) of compound 4d

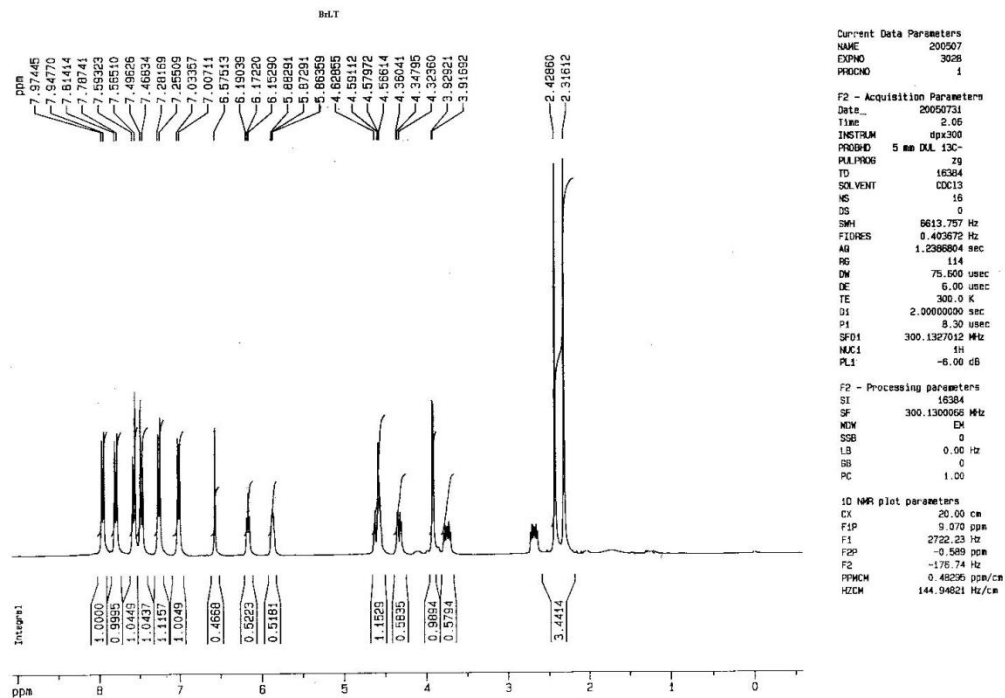


¹³C NMR spectrum (Bruker, 75.5MHz, CDCl₃) of compound 4d

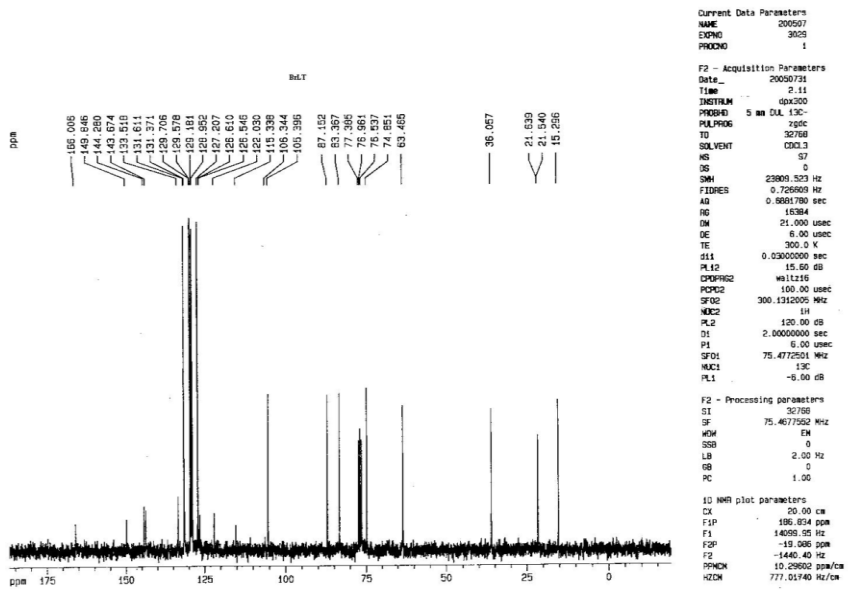


IR spectrum (Perkin-Elmer 2000 FT-IR spectrophotometer) of compound **4d**

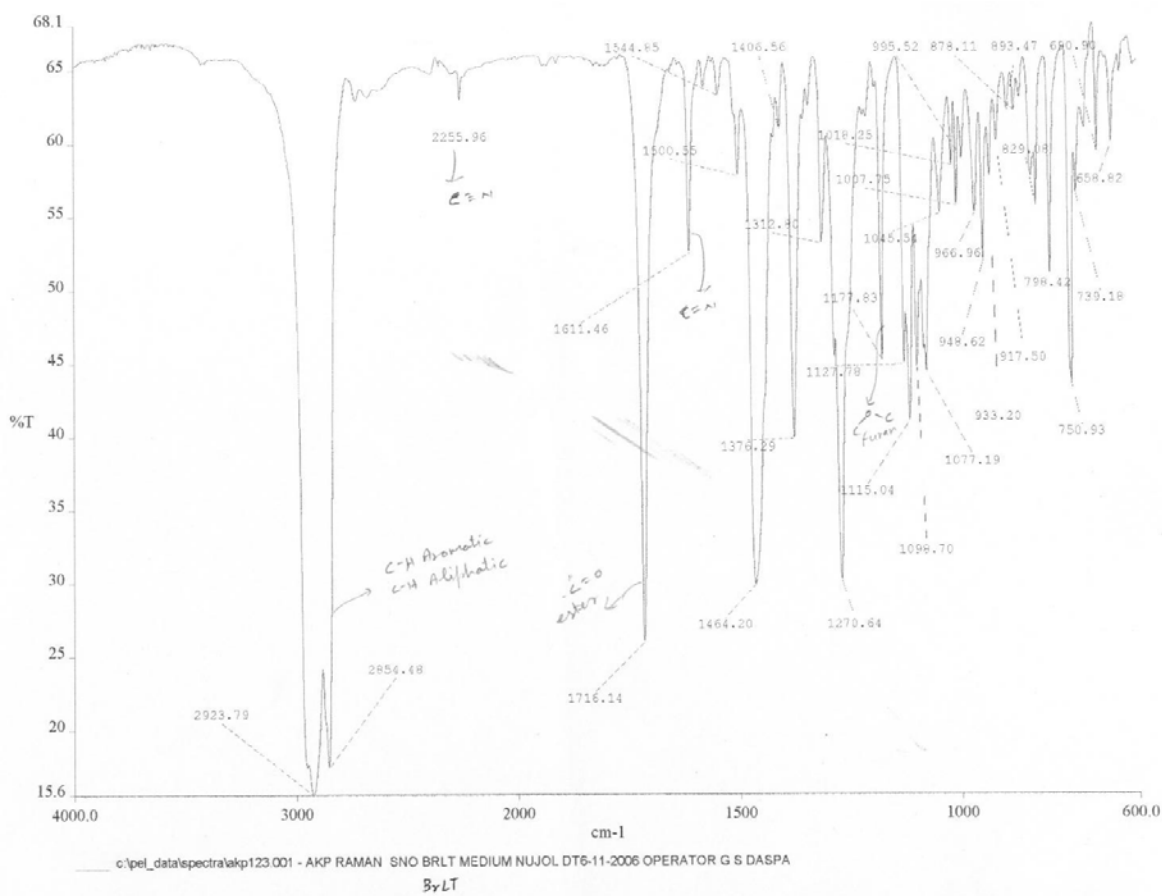
2'-Deoxy-1'-(5-cyanomethyl-3-*p*-bromophenyl)pyrazolyl-3',5'-di-*O*-toluoyl- β -D-ribofuranose (4e)



¹H NMR spectrum (Bruker, 300MHz, CDCl₃) of compound 4e

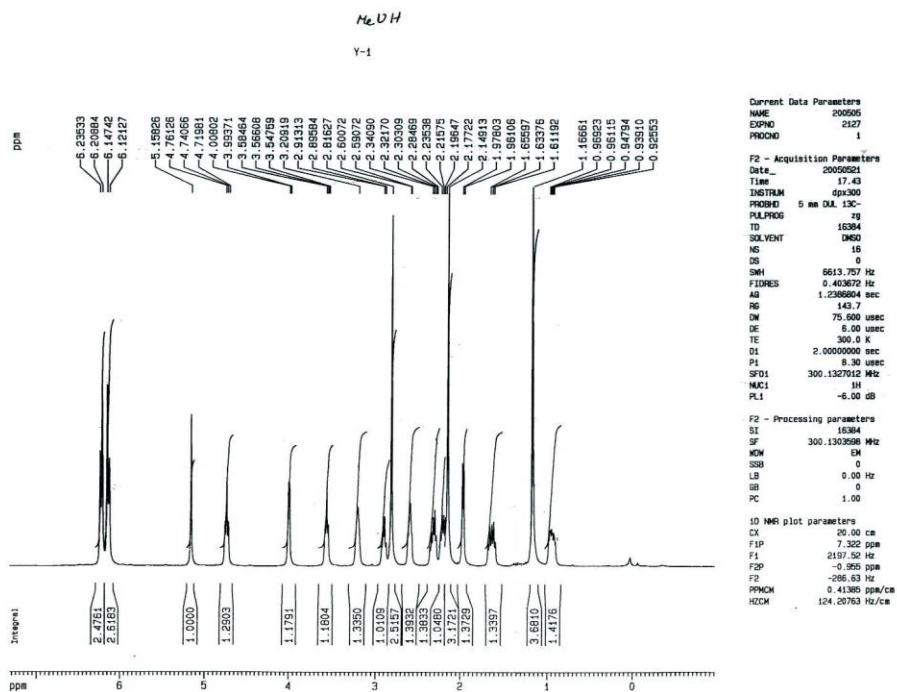


¹³C NMR spectrum (Bruker, 75.5MHz, CDCl₃) of compound 4e



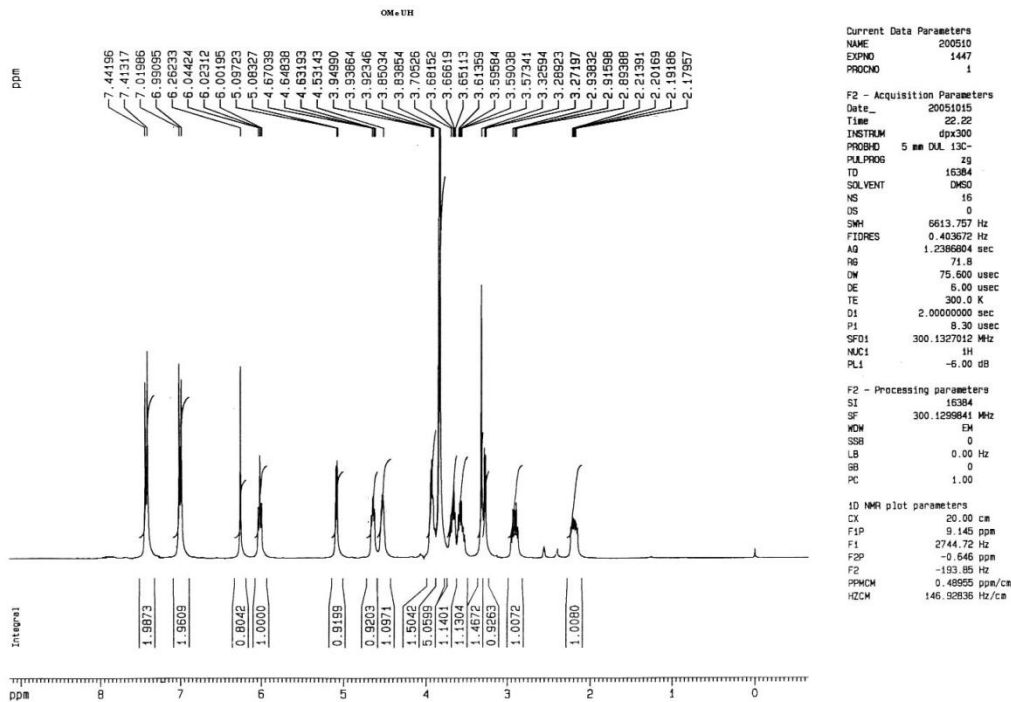
IR spectrum (Perkin-Elmer 2000 FT-IR spectrophotometer) of compound **4e**

2'-Deoxy-1'-(3-cyanomethyl-5-p-methylphenyl)pyrazolyl-β-D-ribofuranose (5a).

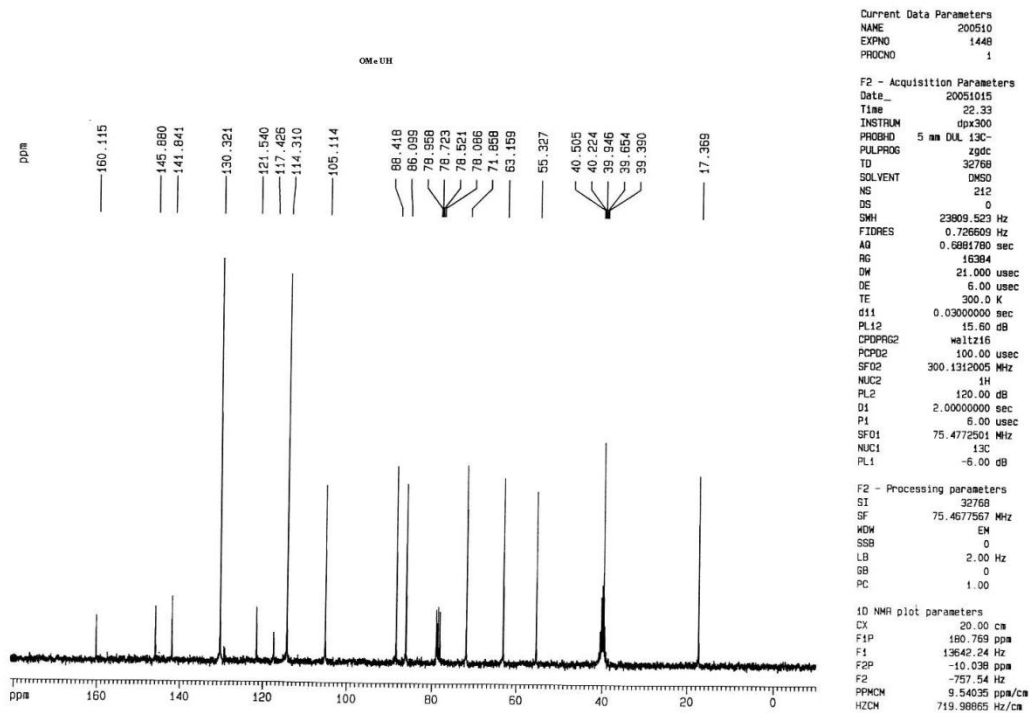


¹H NMR spectrum (Bruker, 300MHz, DMSO) of compound 5a

2'-Deoxy-1'-(3-cyanomethyl-5-p-methoxyphenyl)pyrazolyl-β-D-ribofuranose (5b).

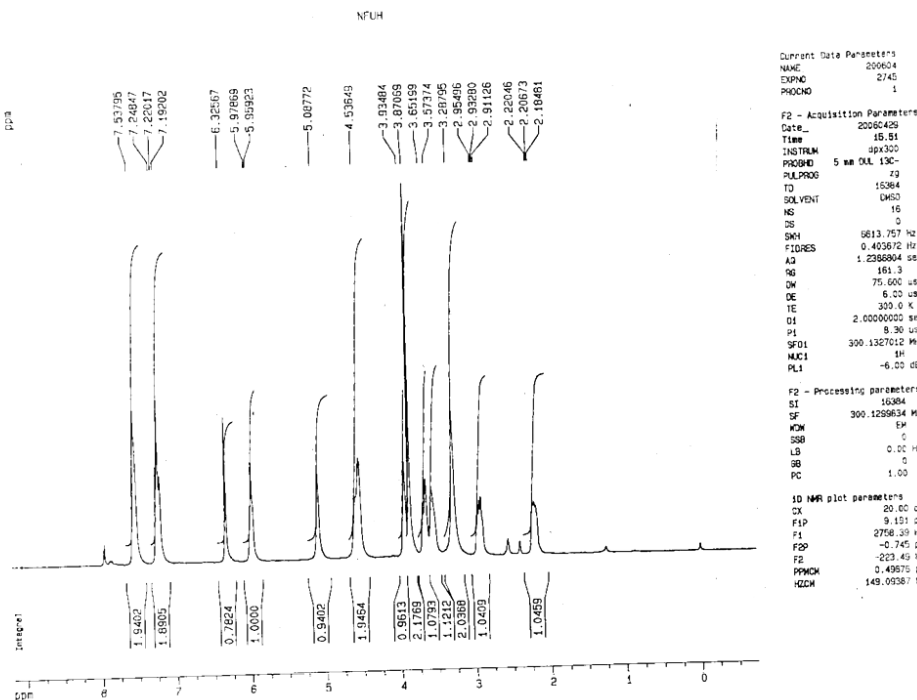


¹H NMR spectrum (Bruker, 300MHz, mixture of CDCl₃ & DMSO) of compound **5b**

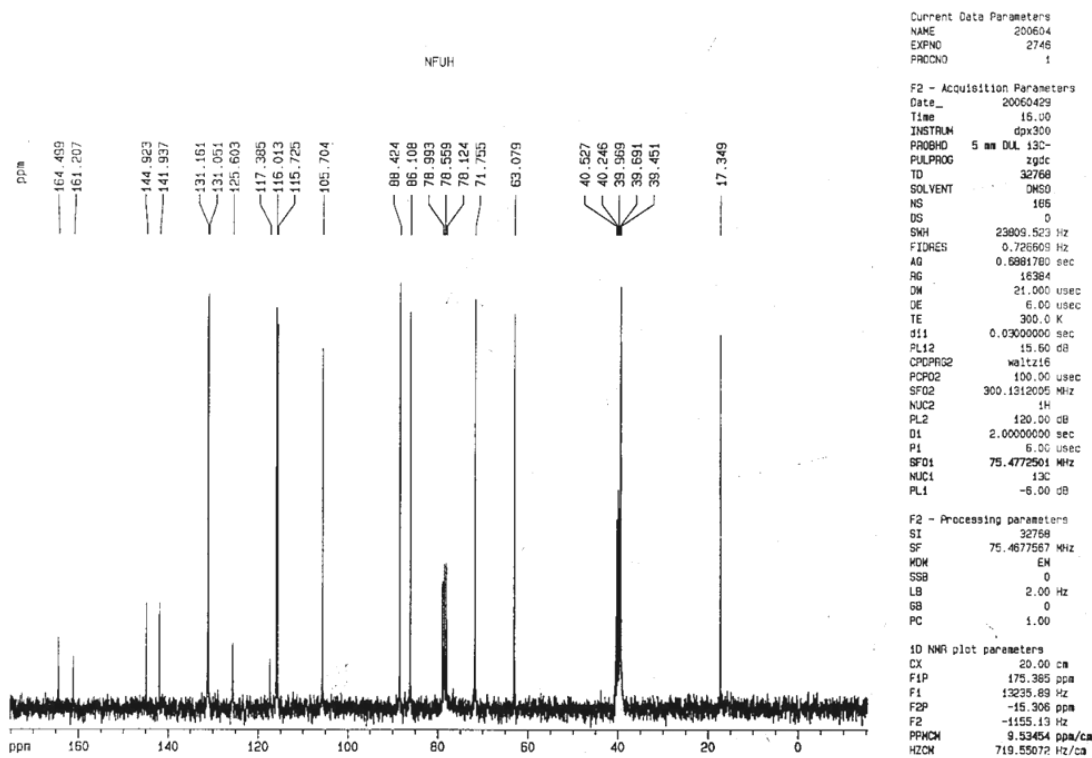


¹³C NMR spectrum (Bruker, 75.5MHz, mixture of CDCl₃ & DMSO) of compound **5b**

2'-Deoxy-1'-(3-cyanomethyl-5-p-fluorophenyl)pyrazolyl-β-D-ribofuranose (5c).

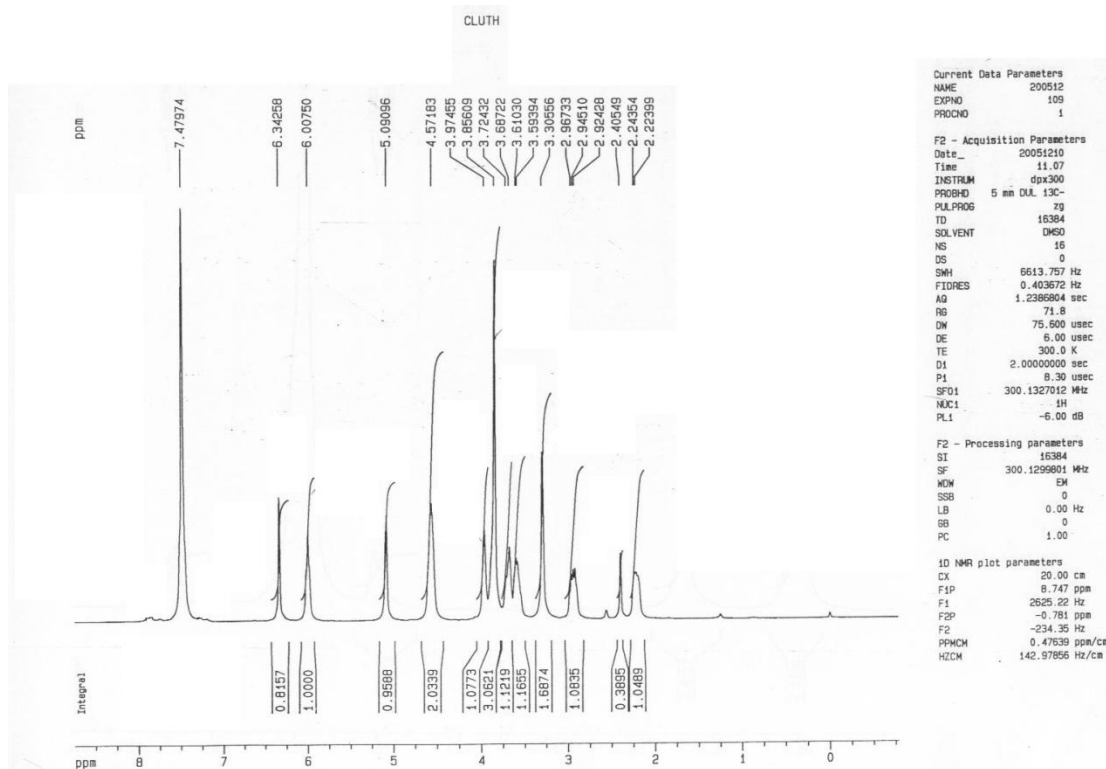


¹H NMR spectrum (Bruker, 300MHz, mixture of CDCl₃ & DMSO) of compound 5c

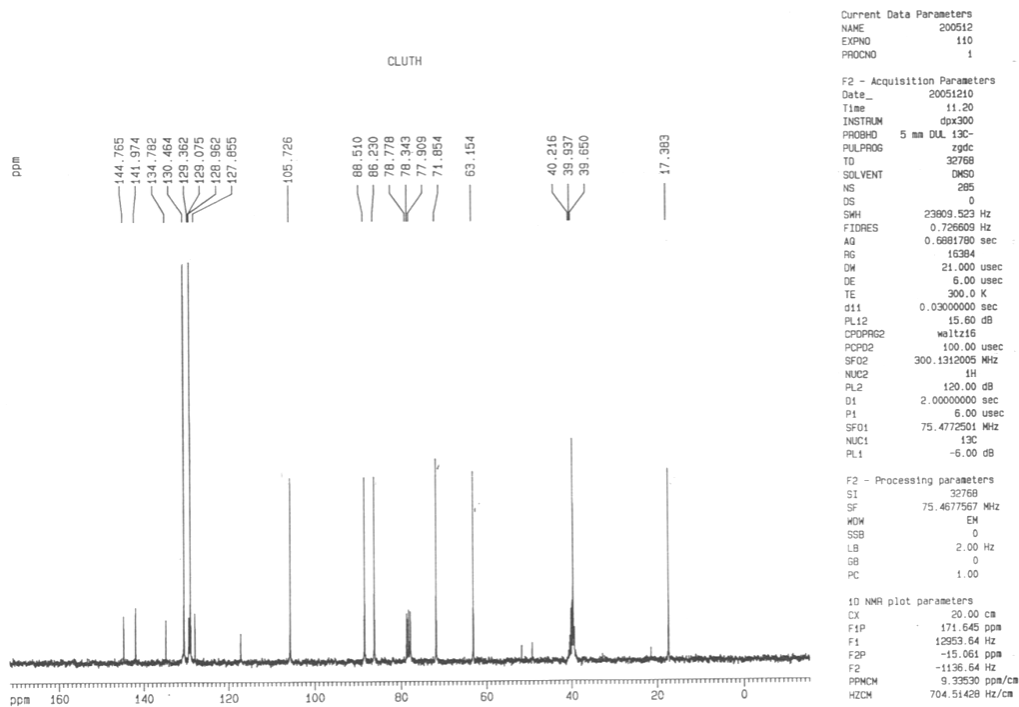


¹³C NMR spectrum (Bruker, 75.5MHz, mixture of CDCl₃ & DMSO) of compound 5c

2'-Deoxy-1'-(3-cyanomethyl-5-p-chlorophenyl)pyrazolyl-β-D-ribofuranose (5d)

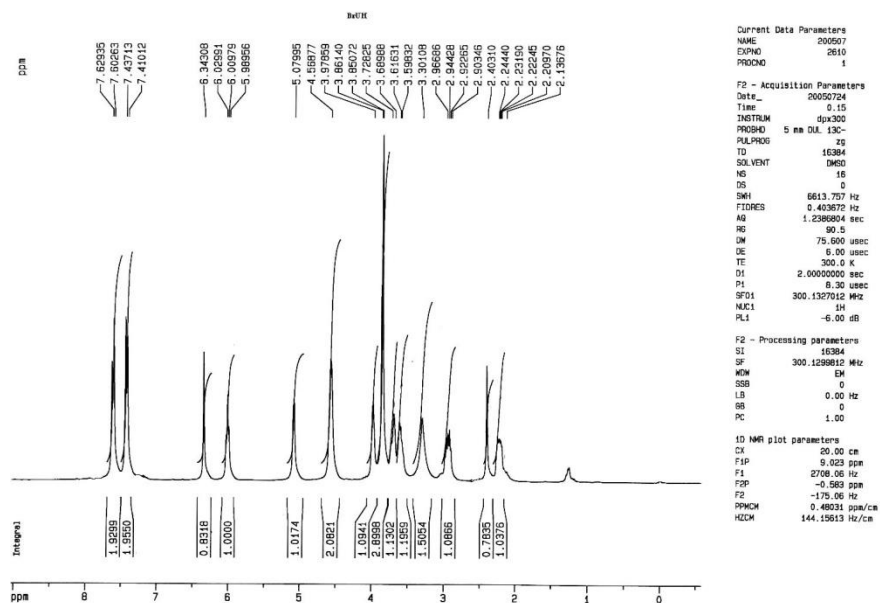


¹H NMR spectrum (Bruker, 300MHz, mixture of CDCl₃ & DMSO) of compound **5d**

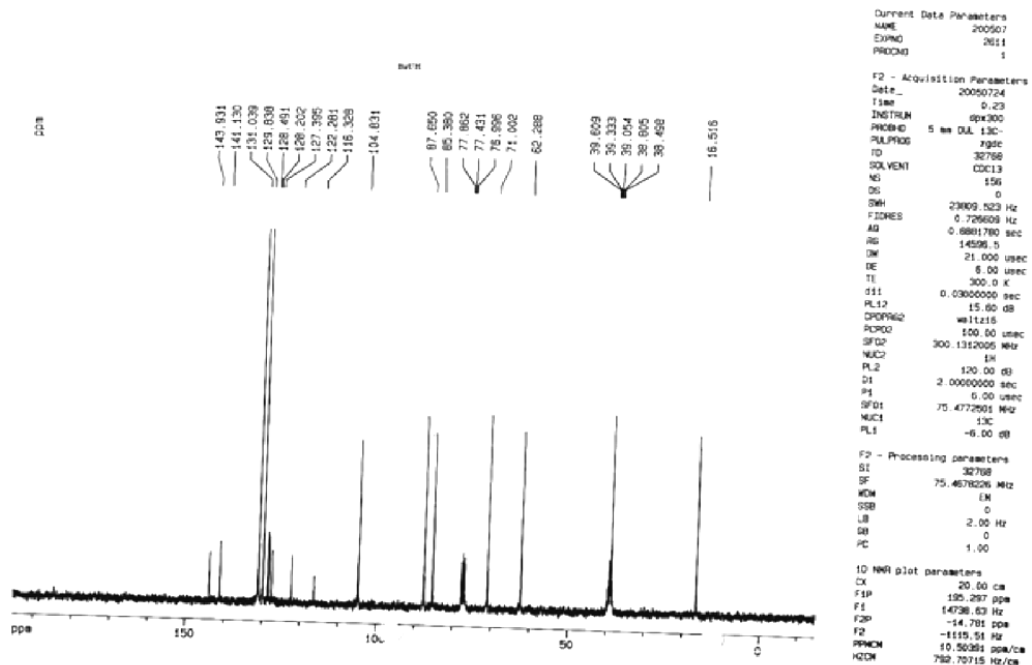


¹³C NMR spectrum (Bruker, 75.5MHz, mixture of CDCl₃ & DMSO) of compound **5d**

2'-Deoxy-1'-(3-cyanomethyl-5-p-bromophenyl)pyrazolyl-β-D-ribofuranose (5e).

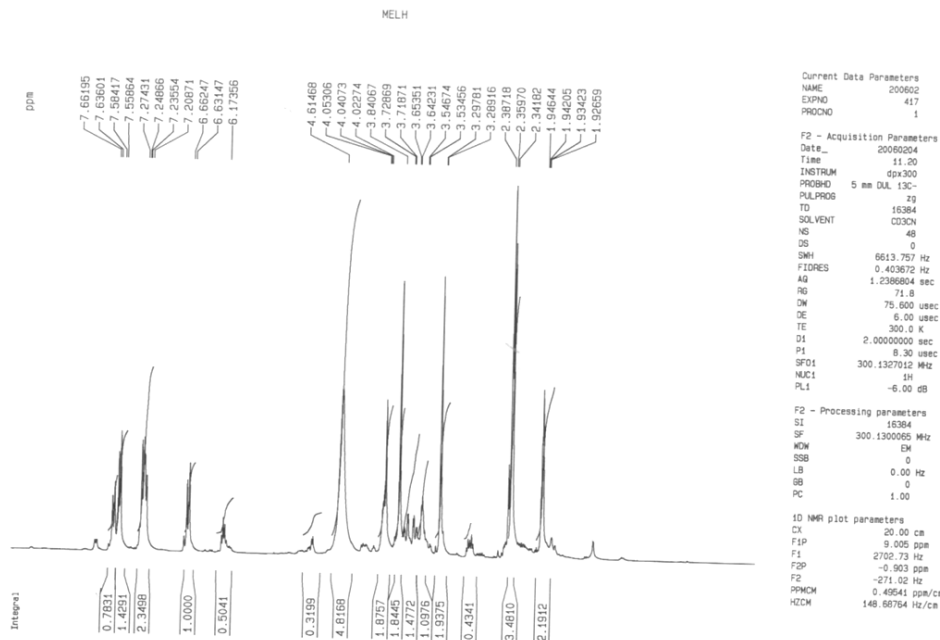


¹H NMR spectrum (Bruker, 300MHz, mixture of CDCl₃ & DMSO) of compound 5e

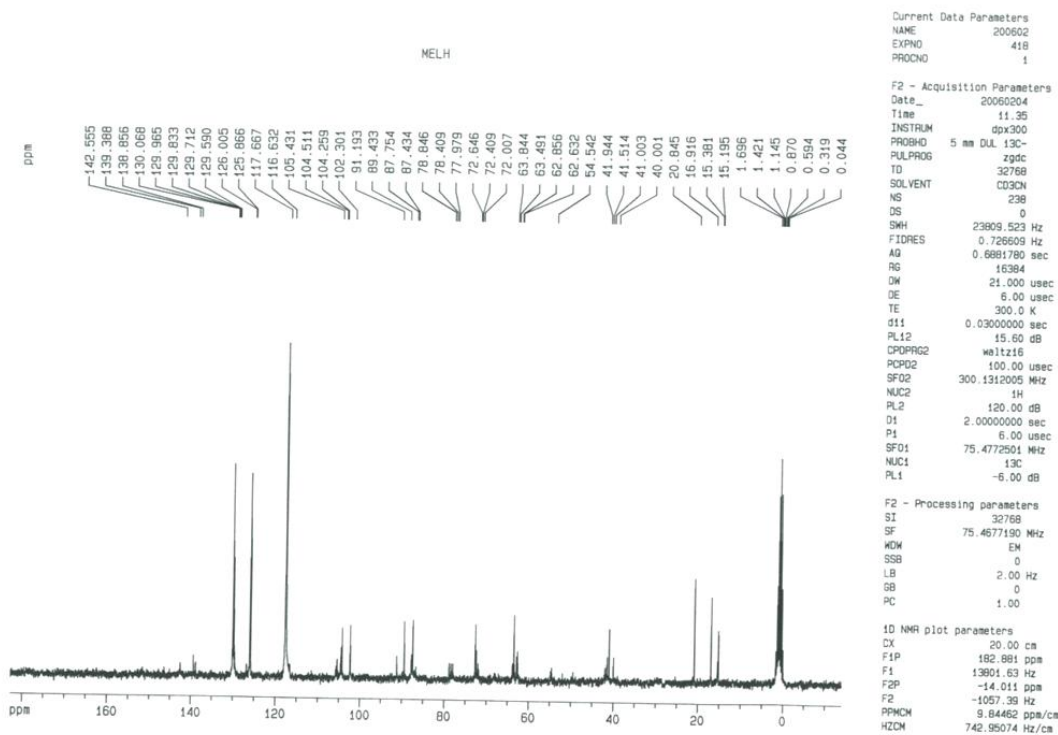


¹³C NMR spectrum (Bruker, 75.5MHz, mixture of CDCl₃ & DMSO) of compound 5d

2'-Deoxy-1'-(5-cyanomethyl-3-*p*-methylphenyl)pyrazolyl- β -D-ribofuranose (**6a**)

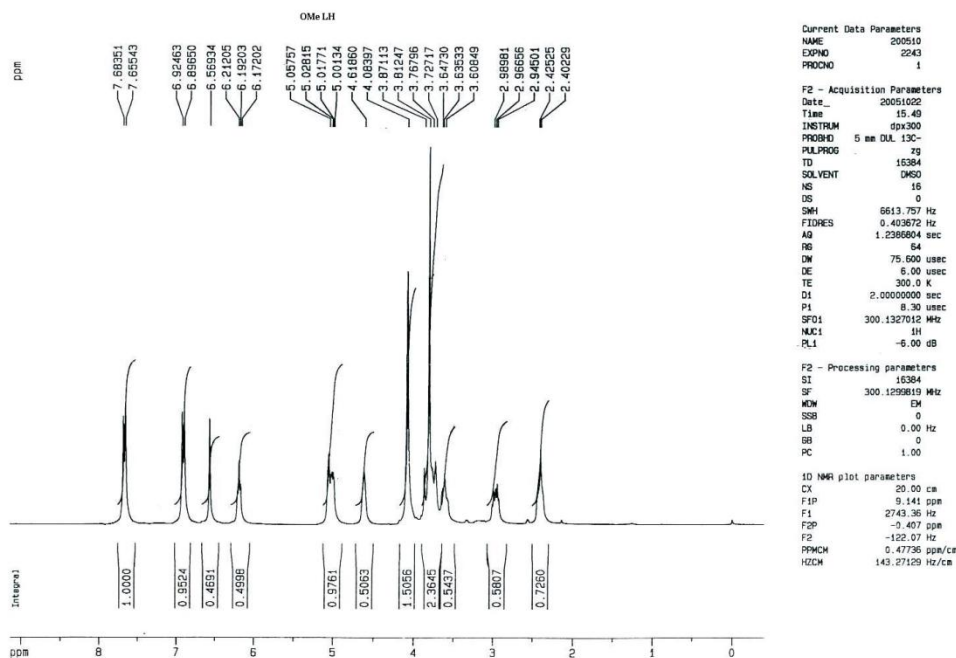


^1H NMR spectrum (Bruker, 300MHz, mixture of CD_3CN) of compound **6a**

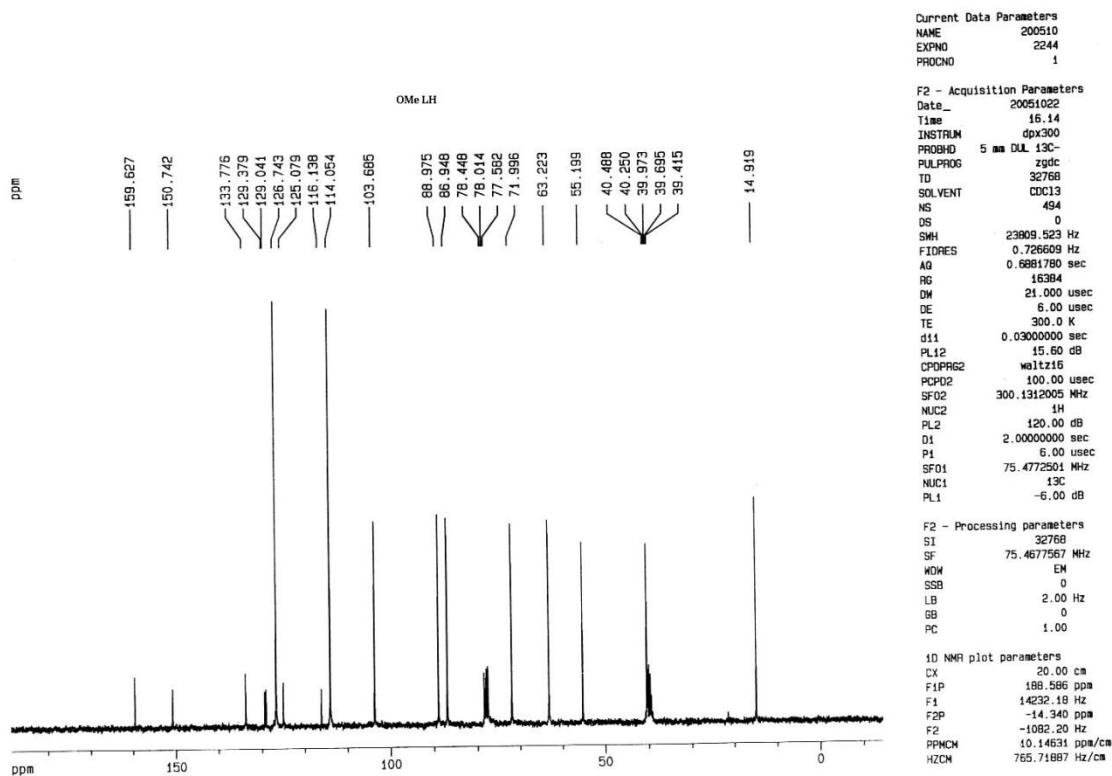


^{13}C NMR spectrum (Bruker, 75.5MHz, mixture of CD_3CN) of compound **6a**

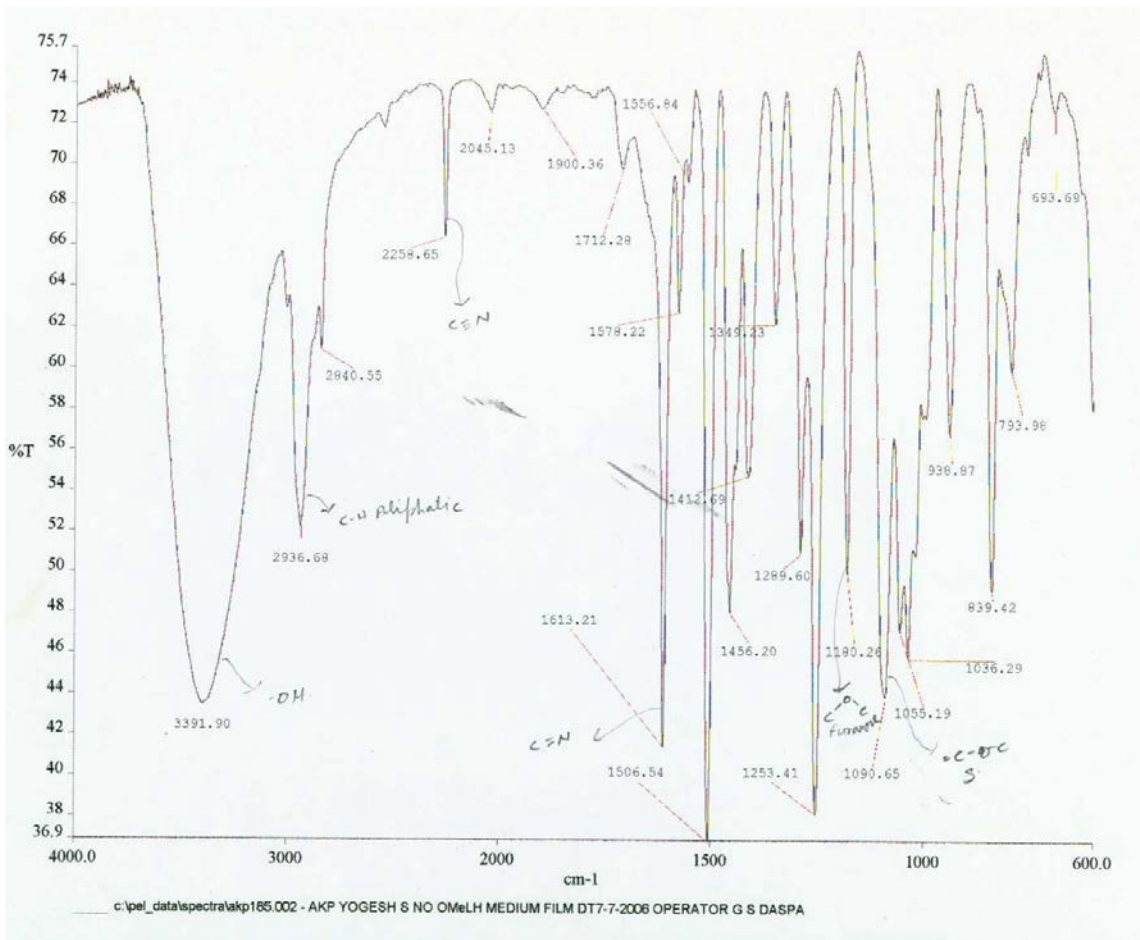
2'-Deoxy-1'-(3-cyanomethyl-5-*p*-methoxyphenyl)pyrazolyl- β -D-ribofuranose (**6b**)



^1H NMR spectrum (Bruker, 300MHz, mixture of CDCl_3 & DMSO) of compound **6b**

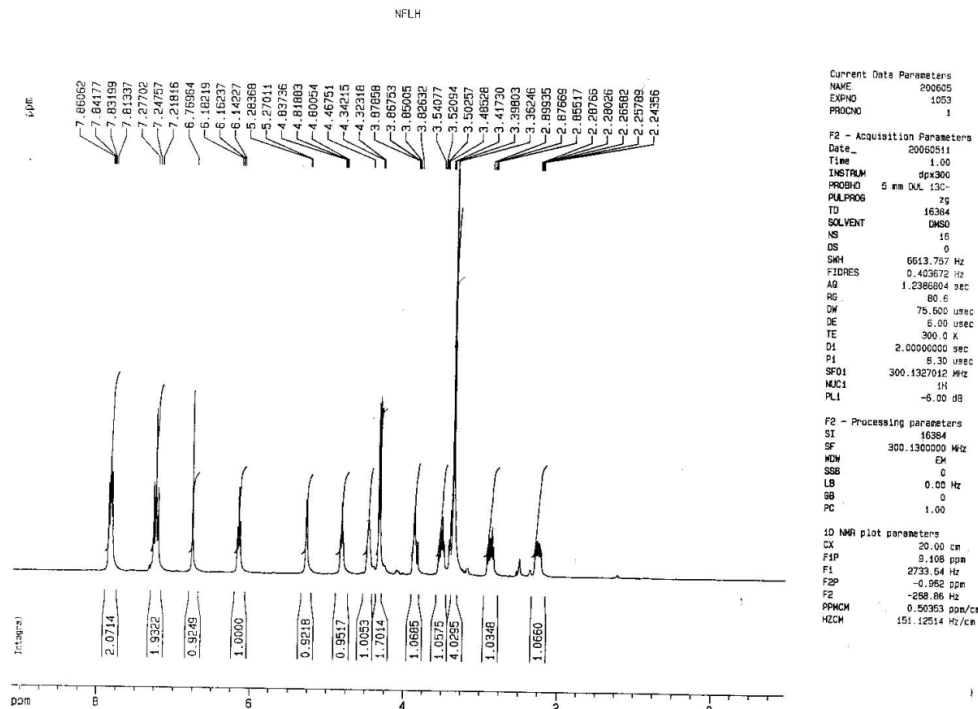


^{13}C NMR spectrum (Bruker, 75.5MHz, mixture of CDCl_3 & DMSO) of compound **6b**

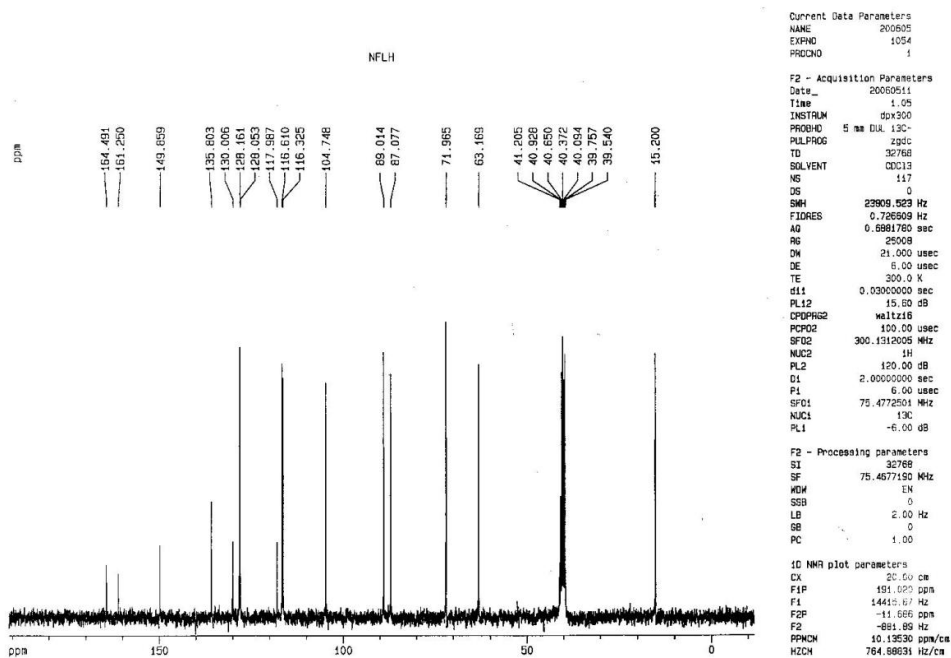


IR spectrum (Perkin-Elmer 2000 FT-IR spectrophotometer) of compound **6b**

2'-Deoxy-1'-(5-cyanomethyl-3-p-fluorophenyl)pyrazolyl-β-D-ribofuranose (6c)

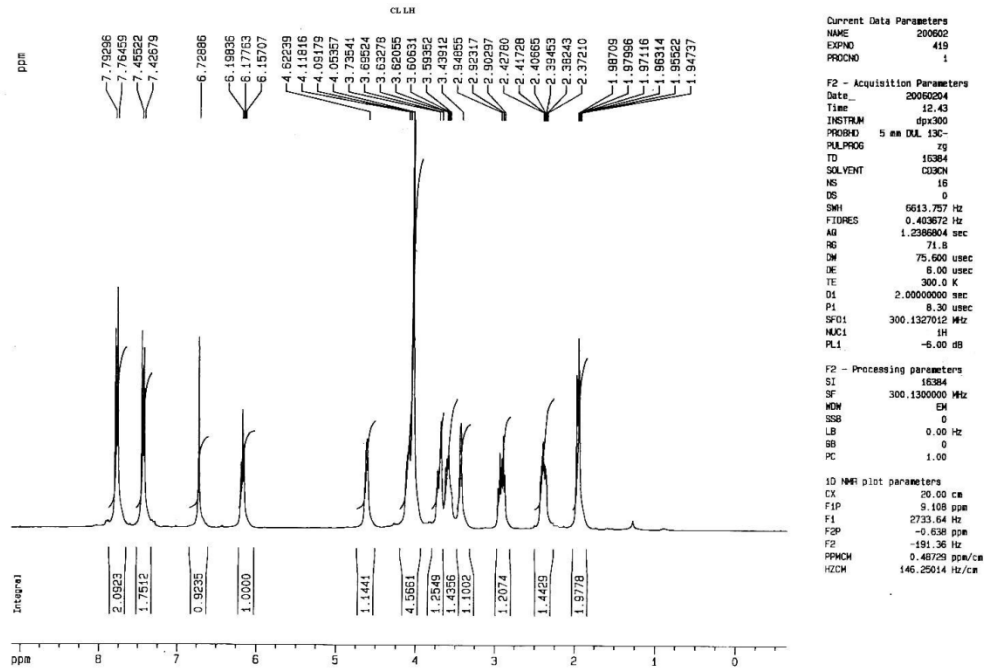


¹H NMR spectrum (Bruker, 300MHz, DMSO) of compound 6c

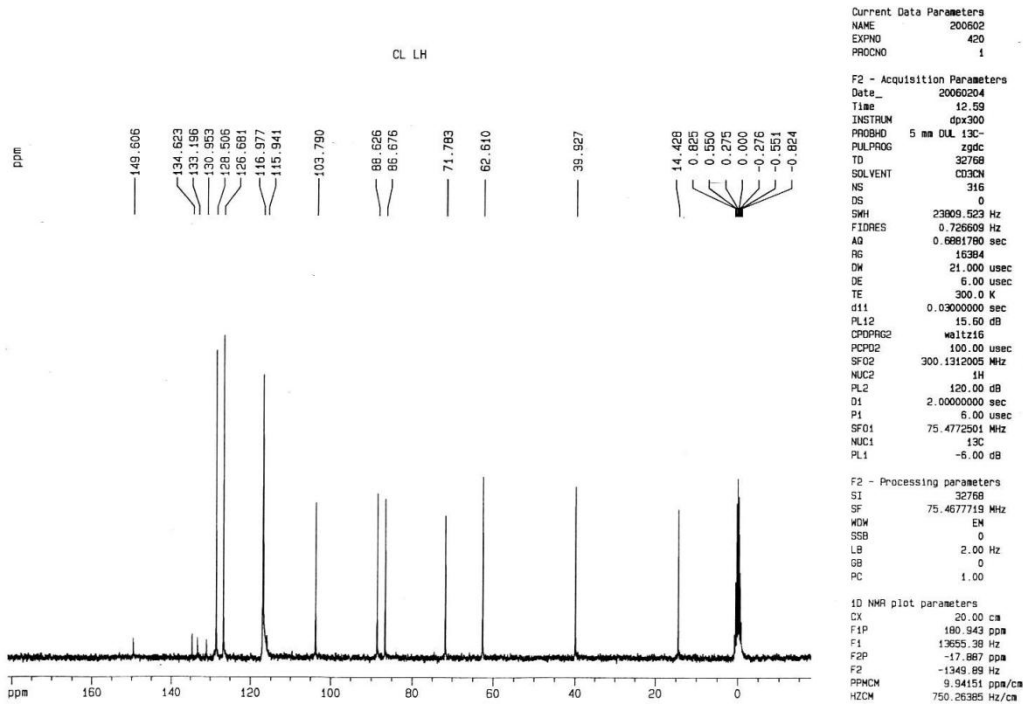


¹³C NMR spectrum (Bruker, 75.5MHz, CDCl₃) of compound 6c

2'-Deoxy-1'-(5-cyanomethyl-3-p-chlorophenyl)pyrazolyl-β-D-ribofuranose (6d).

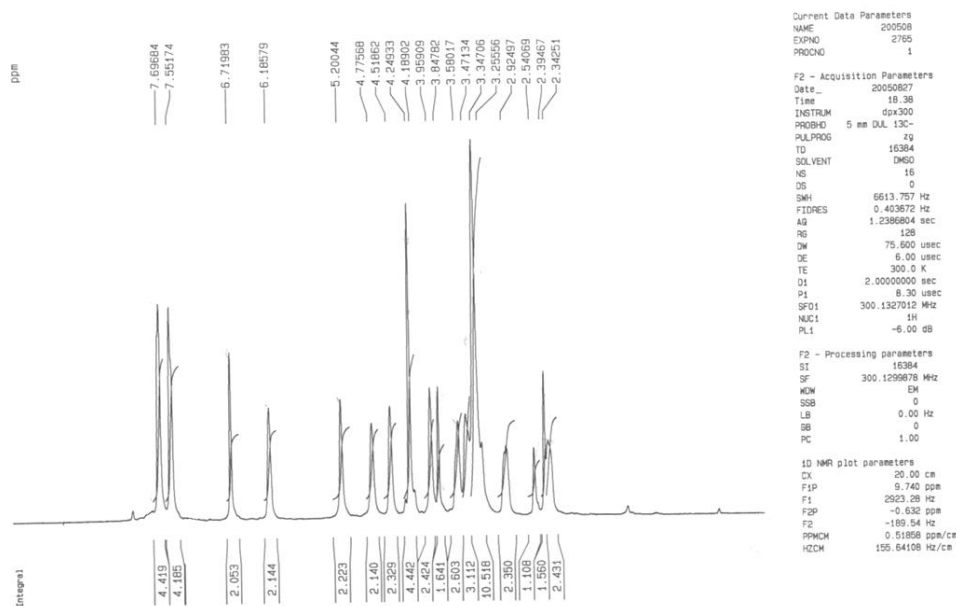


¹H NMR spectrum (Bruker, 300MHz, CD₃CN) of compound 6d



¹³C NMR spectrum (Bruker, 75.5MHz, CD₃CN) of compound 6d

2'-Deoxy-1'-(3-*p*-bromophenyl-5-cyanomethyl)pyrazolyl- β -D-ribofuranose (6e).



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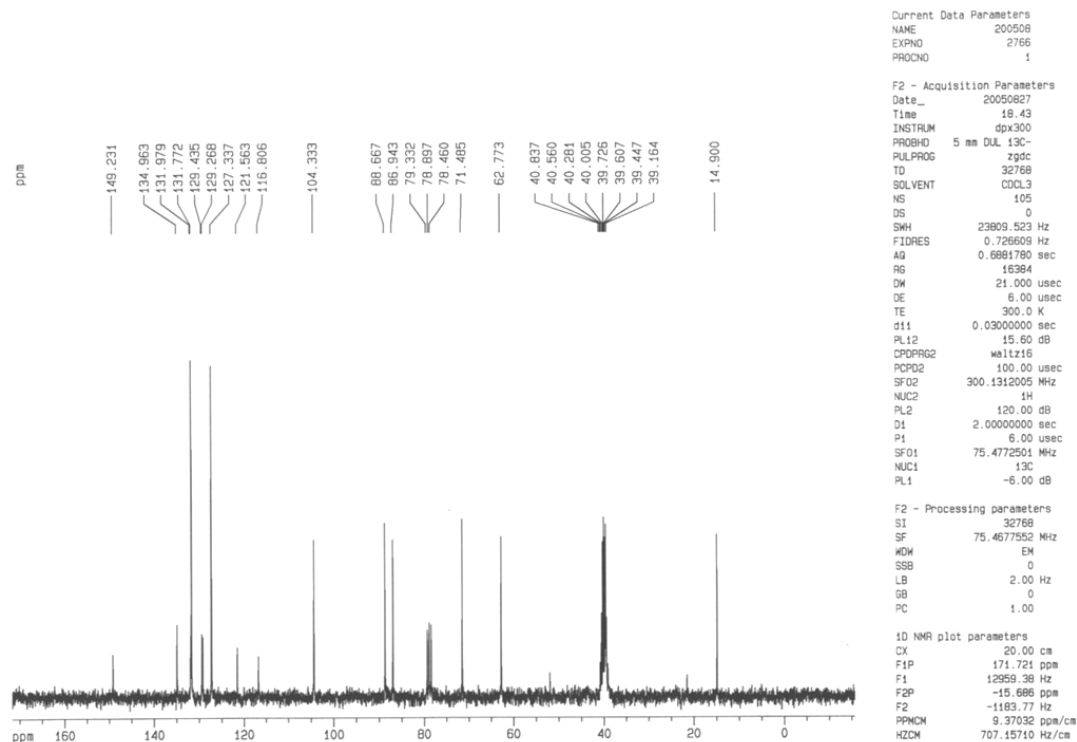
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¹H NMR spectrum (Bruker, 300MHz, mixture of CDCl₃ & DMSO) of compound **6e**



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¹³C NMR spectrum (Bruker, 75.5MHz, mixture of CDCl₃ & DMSO) of compound **6e**