Supporting Information for:

Systematic Evaluation of 2,6-Linked Pyridine-Thiophene Oligomers

Silvia Rocha and Nathaniel S. Finney*,[≠]

Institute of Organic Chemistry, University of Zurich

Winterthurerstrasse 190, 8057 Zurich, Switzerland

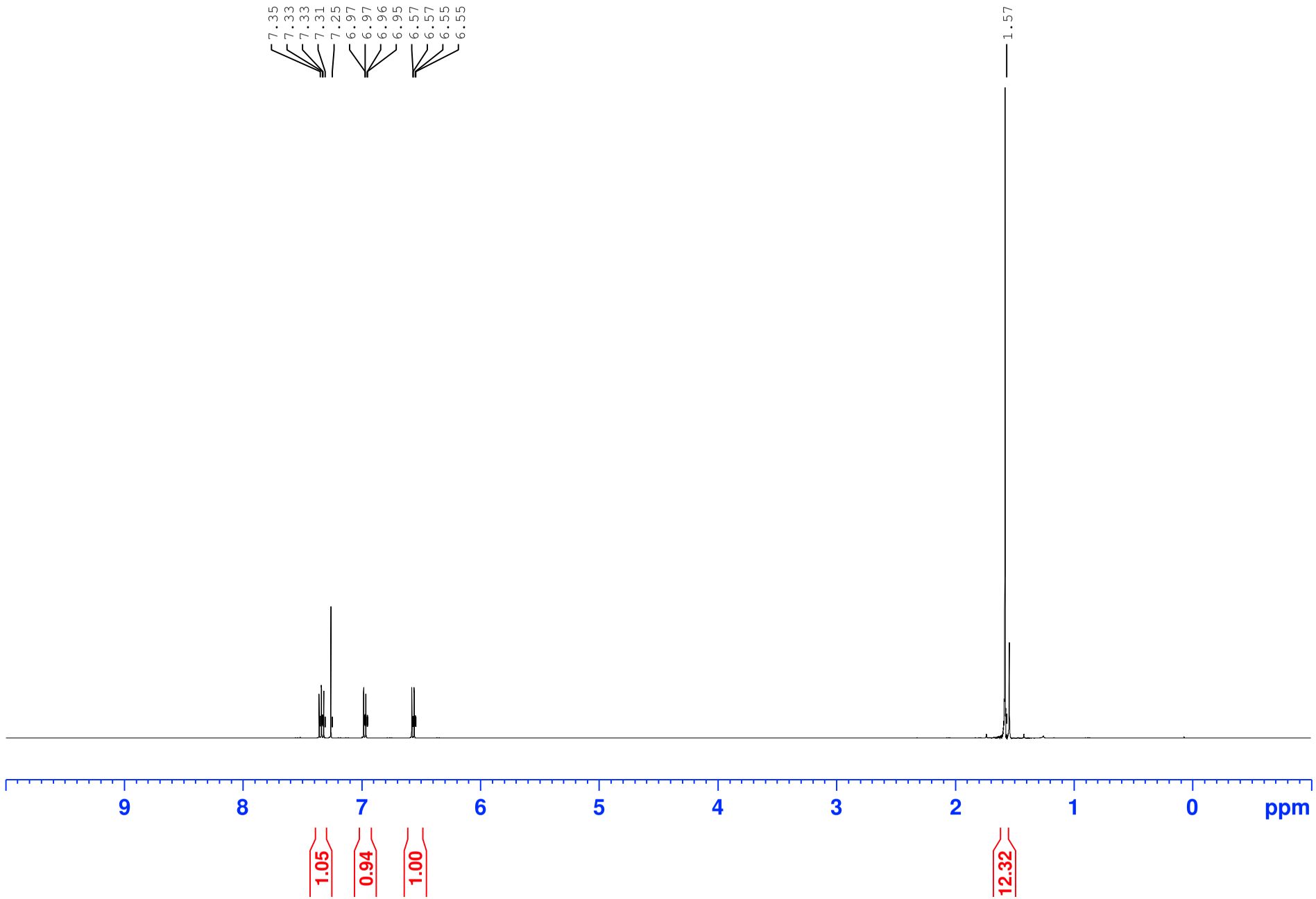
nsfinney@ncsu.edu

Table of Contents:

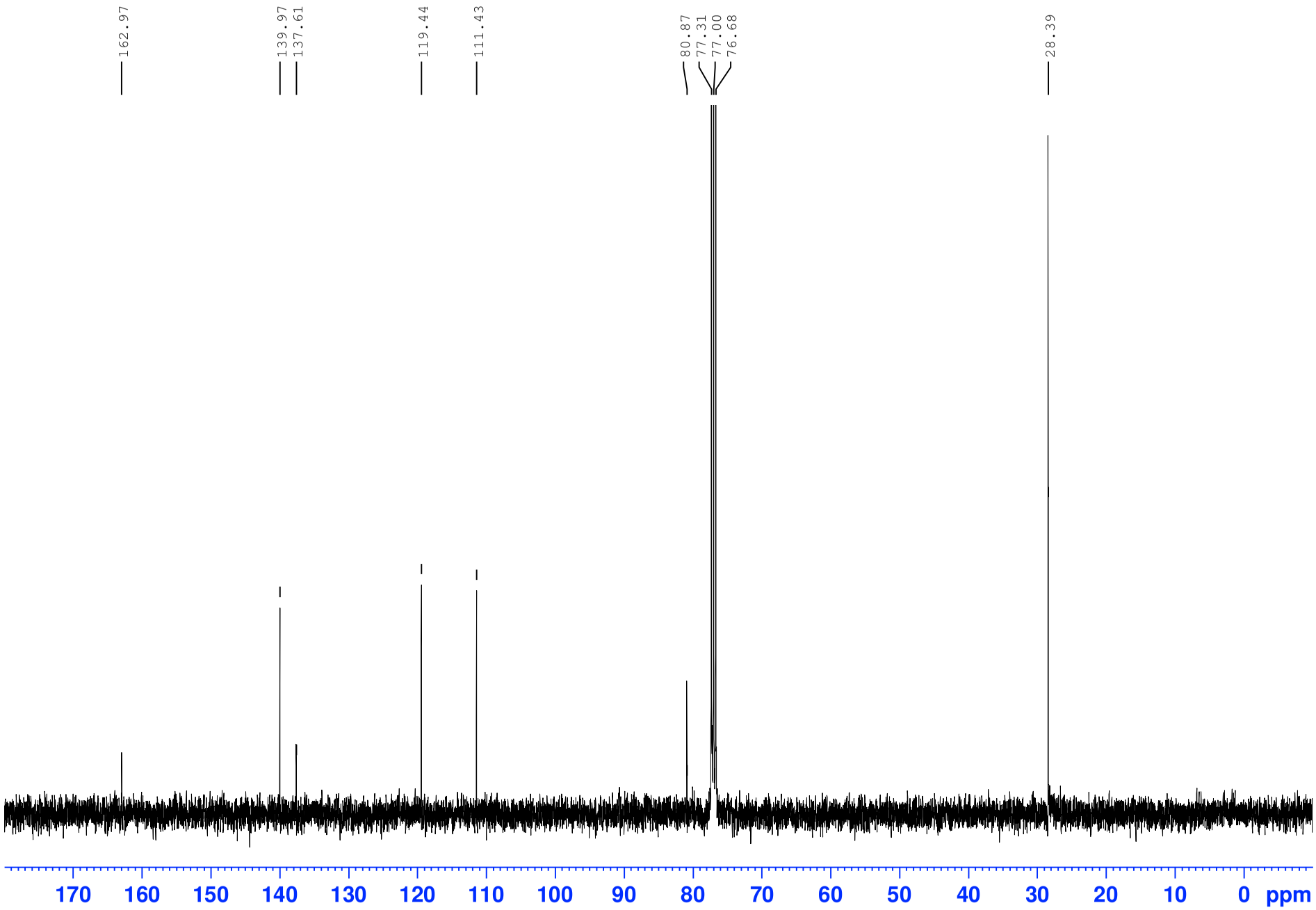
^{1}H-NMR spectra of 6-Bromo-2-(1,1-dimehylethoxy)pyridine	S2
^{13}C{^{1}H}-NMR spectra of 6-Bromo-2-(1,1-dimehylethoxy)pyridine	S3
^{1}H-NMR spectra of **26a**	S4
^{13}C{^{1}H}-NMR spectra of **26a**	S5
^{1}H-NMR spectra of **26aOH**	S6
^{13}C{^{1}H}-NMR spectra of **26aOH**	S7
^{1}H-NMR spectra of **26aTf**	S8
^{13}C{^{1}H}-NMR spectra of **26aTf**	S9
^{1}H-NMR spectra of **26b**	S10
^{13}C{^{1}H}-NMR spectra of **26b**	S11
^{1}H-NMR spectra of **26bOH**	S12
^{13}C{^{1}H}-NMR spectra of **26bOH**	S13
^{1}H-NMR spectra of **26bTf**	S14
^{13}C{^{1}H}-NMR spectra of **26bTf**	S15
^{1}H-NMR spectra of **26c**	S16
^{13}C{^{1}H}-NMR spectra of **26c**	S17
^{1}H-NMR spectra of **26d**	S18
^{13}C{^{1}H}-NMR spectra of **26d**	S19
^{1}H-NMR spectra of **26TPT-H**	S20
^{13}C{^{1}H}-NMR spectra of **26TPT-H**	S21
^{1}H-NMR spectra of **26TPT-CN**	S22
^{13}C{^{1}H}-NMR spectra of **26TPT-CN**	S23
Figure 1: ORTEP Representation of **26TPT-CN**	S24
Table 1: Crystallographic Data for **26TPT-CN**	S25

[≠]Present address: Department of Chemistry, North Carolina State University

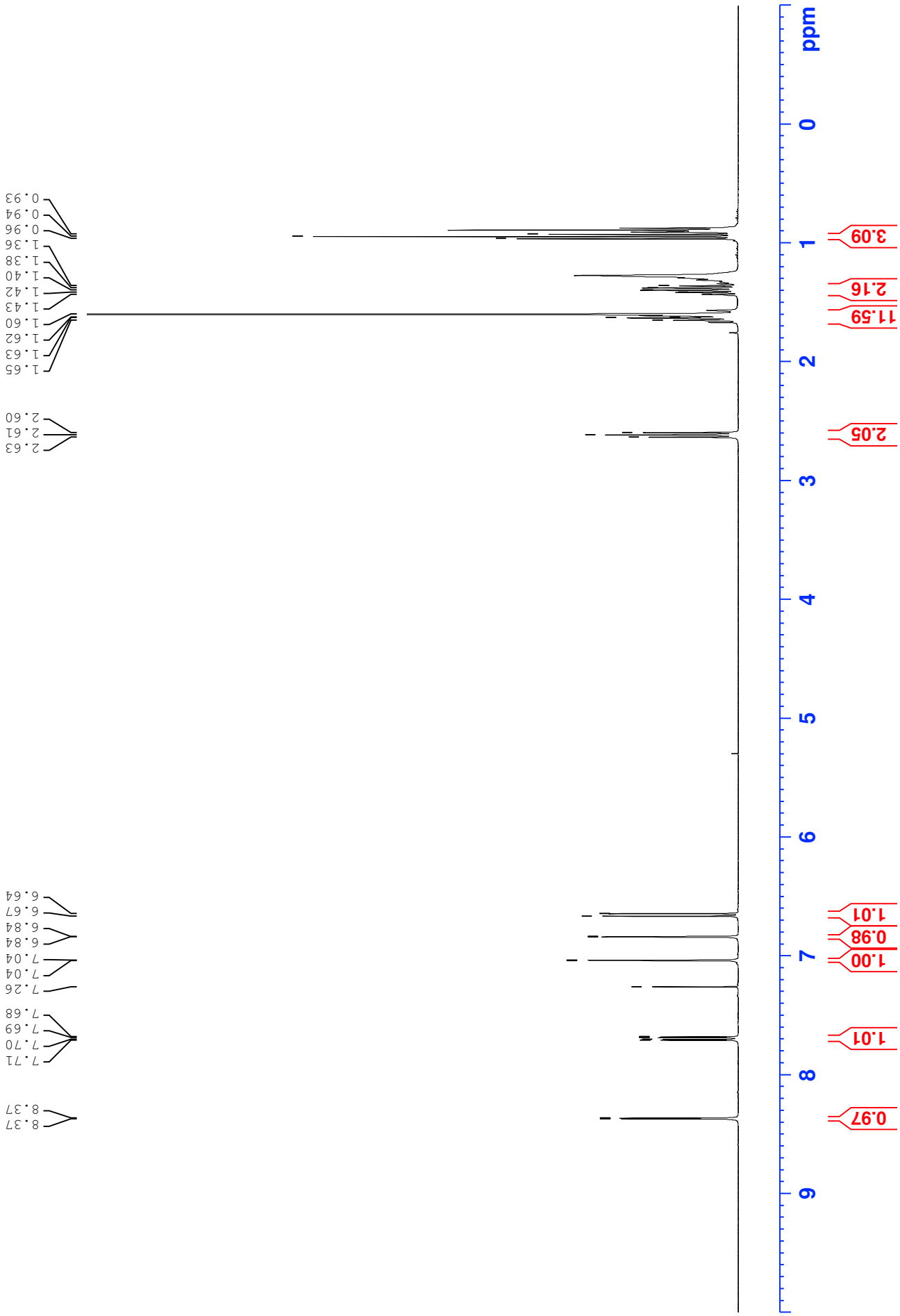
400 MHz 1H-NMR of 6-Bromo-2-(1,1-dimethylethoxy)pyridine, 300 K, CDCl3



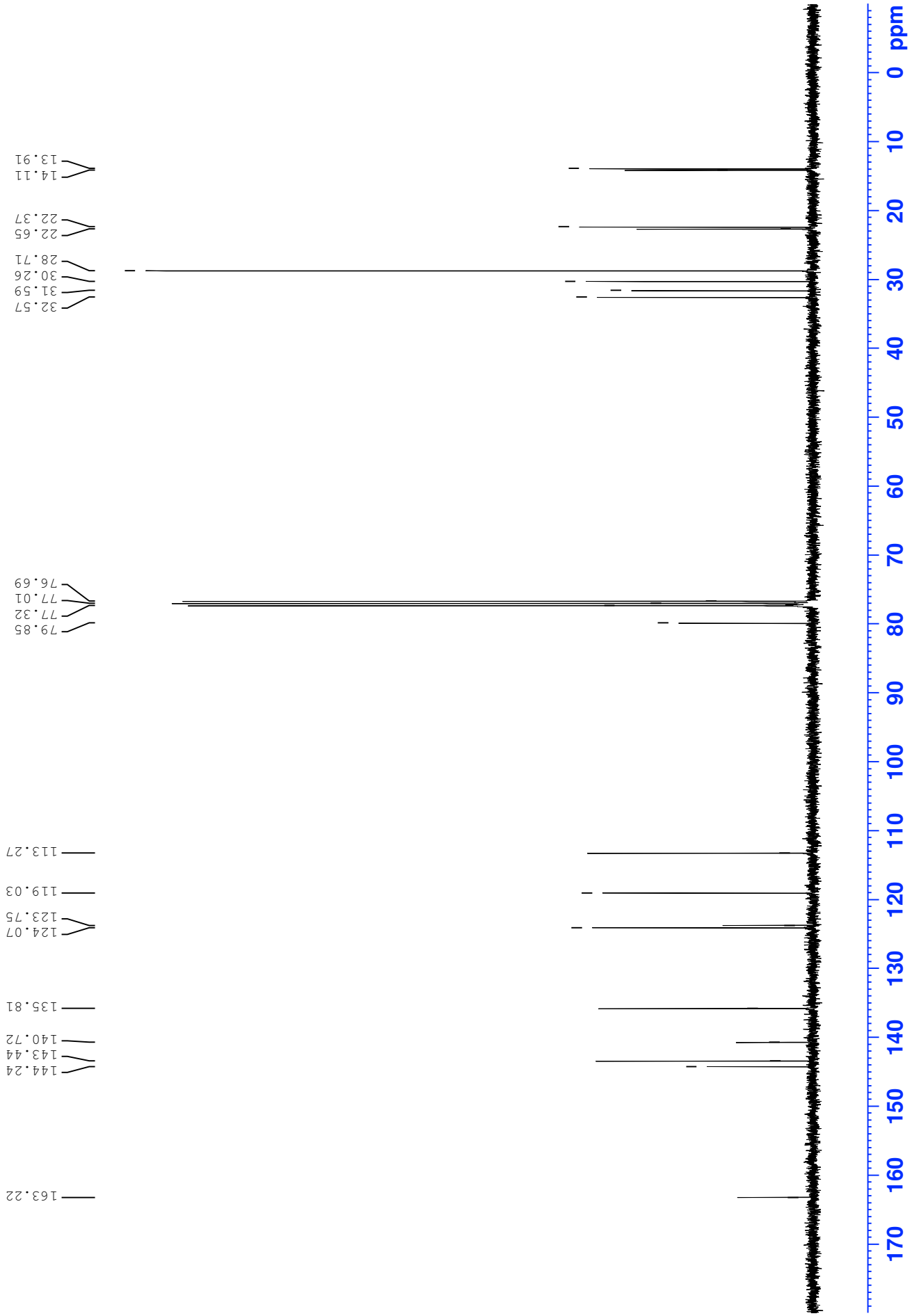
100 MHz 13C{1H}-NMR of 6-Bromo-2-(1,1-dimethylethoxy)pyridine, 300 K, CDCl3



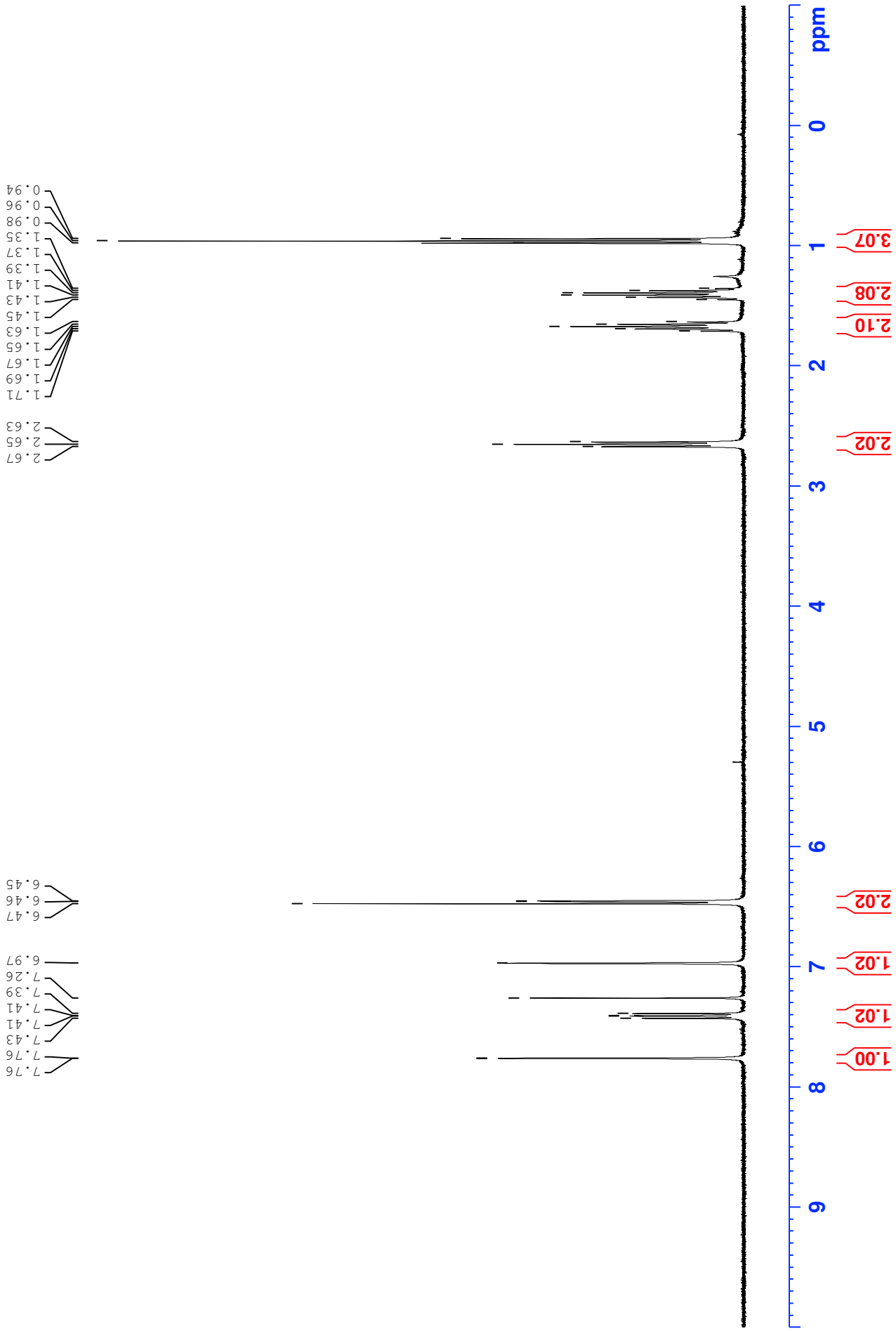
400 MHz ^{1}H–NMR spectra of **26a**, 300 K, $CDCl_3$.



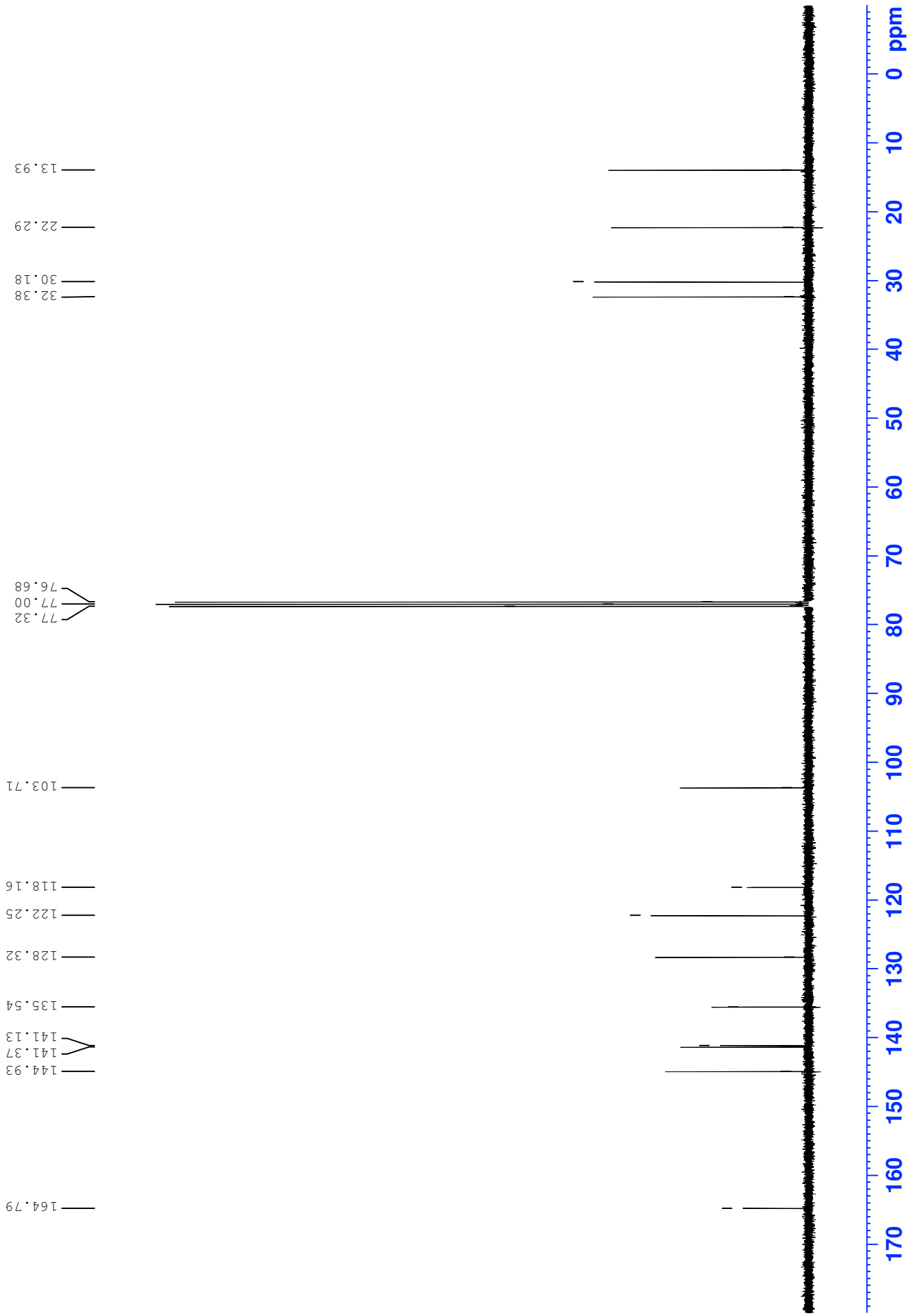
100 MHz 13C{1H}–NMR spectra of **26a**, 300 K, $CDCl_3$.



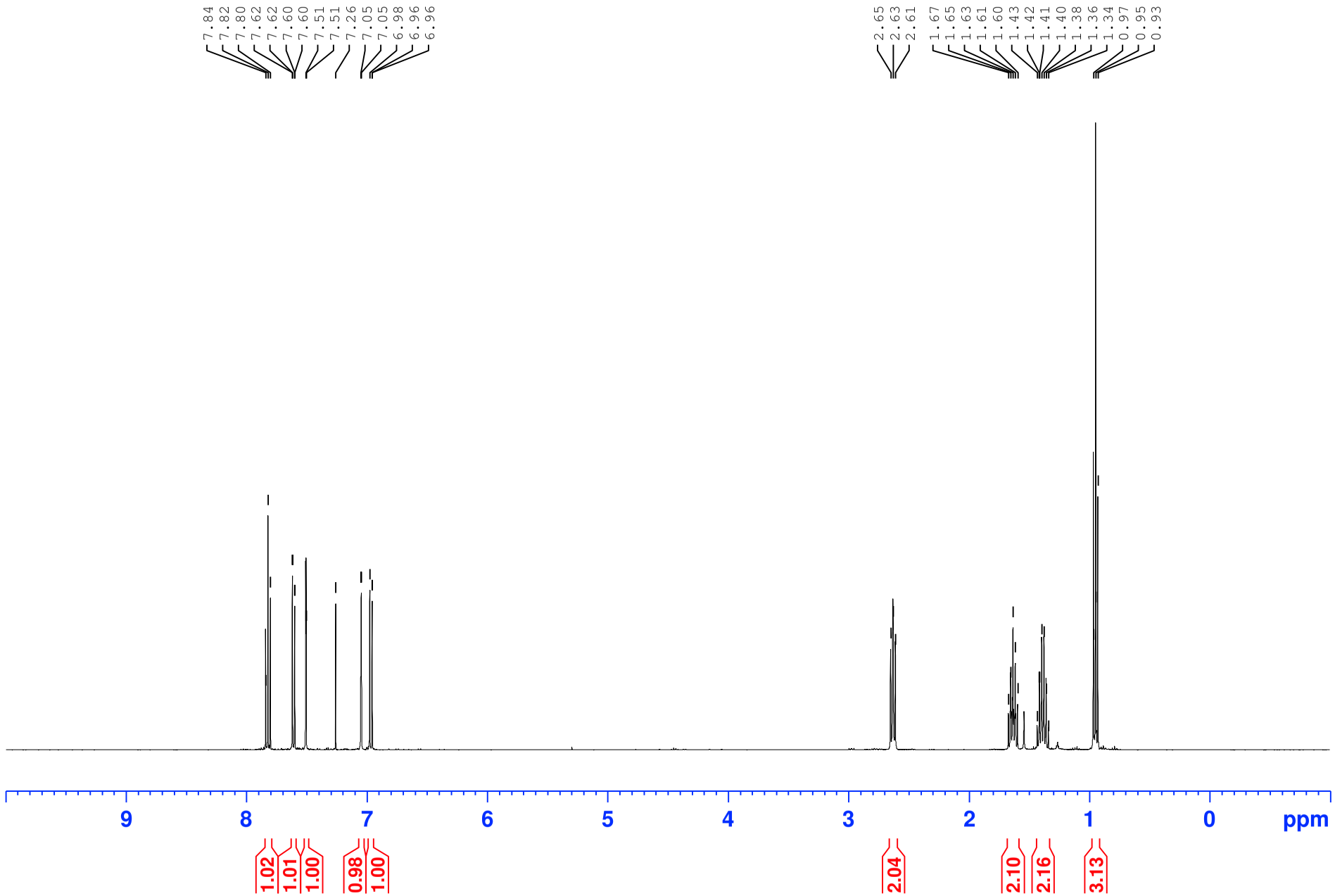
400 MHz ^{1}H–NMR spectra of **26aOH**, 300 K, $CDCl_3$.



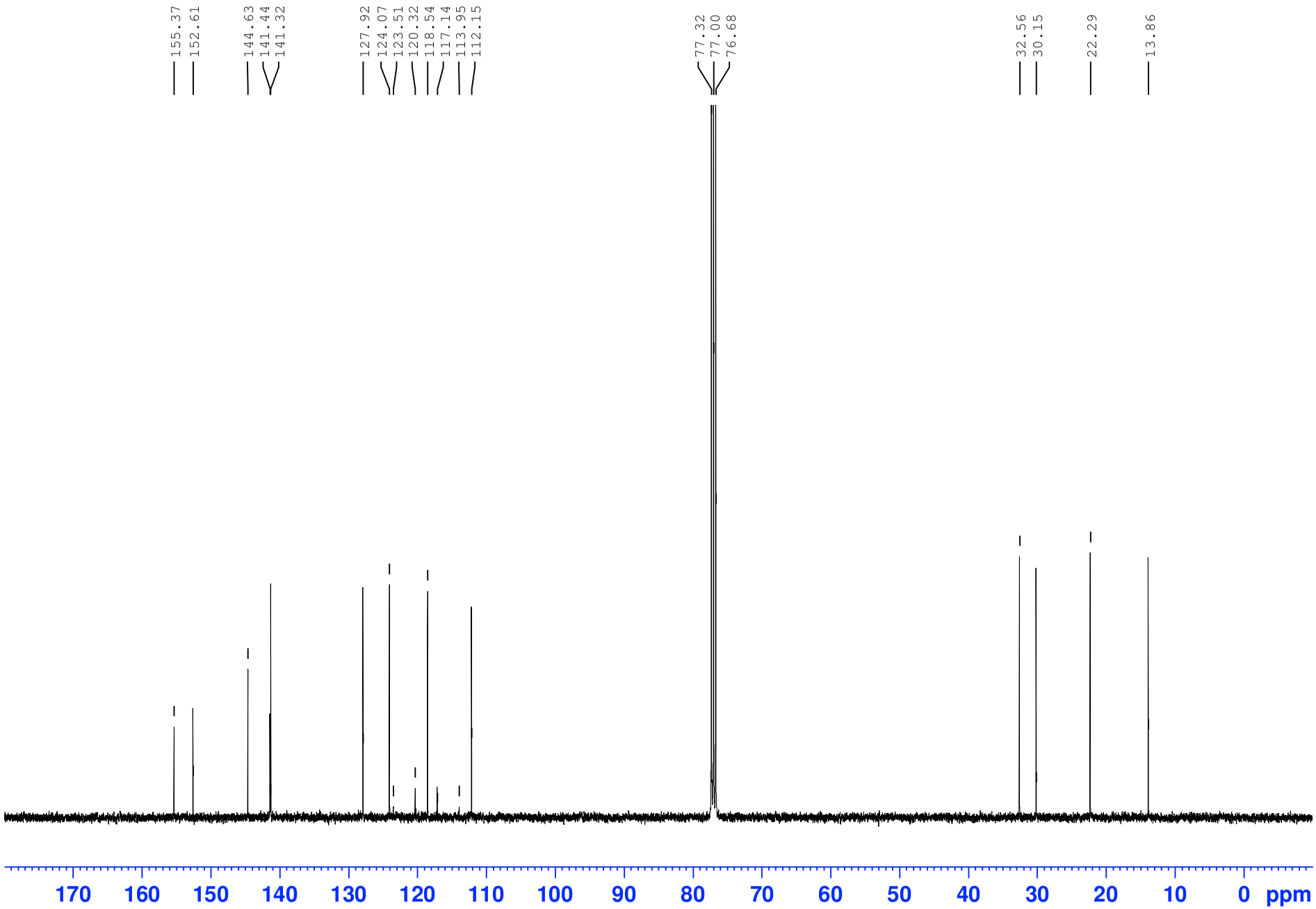
100 MHz 13C{1H}–NMR spectra of **26aOH**, 300 K, $CDCl_3$.



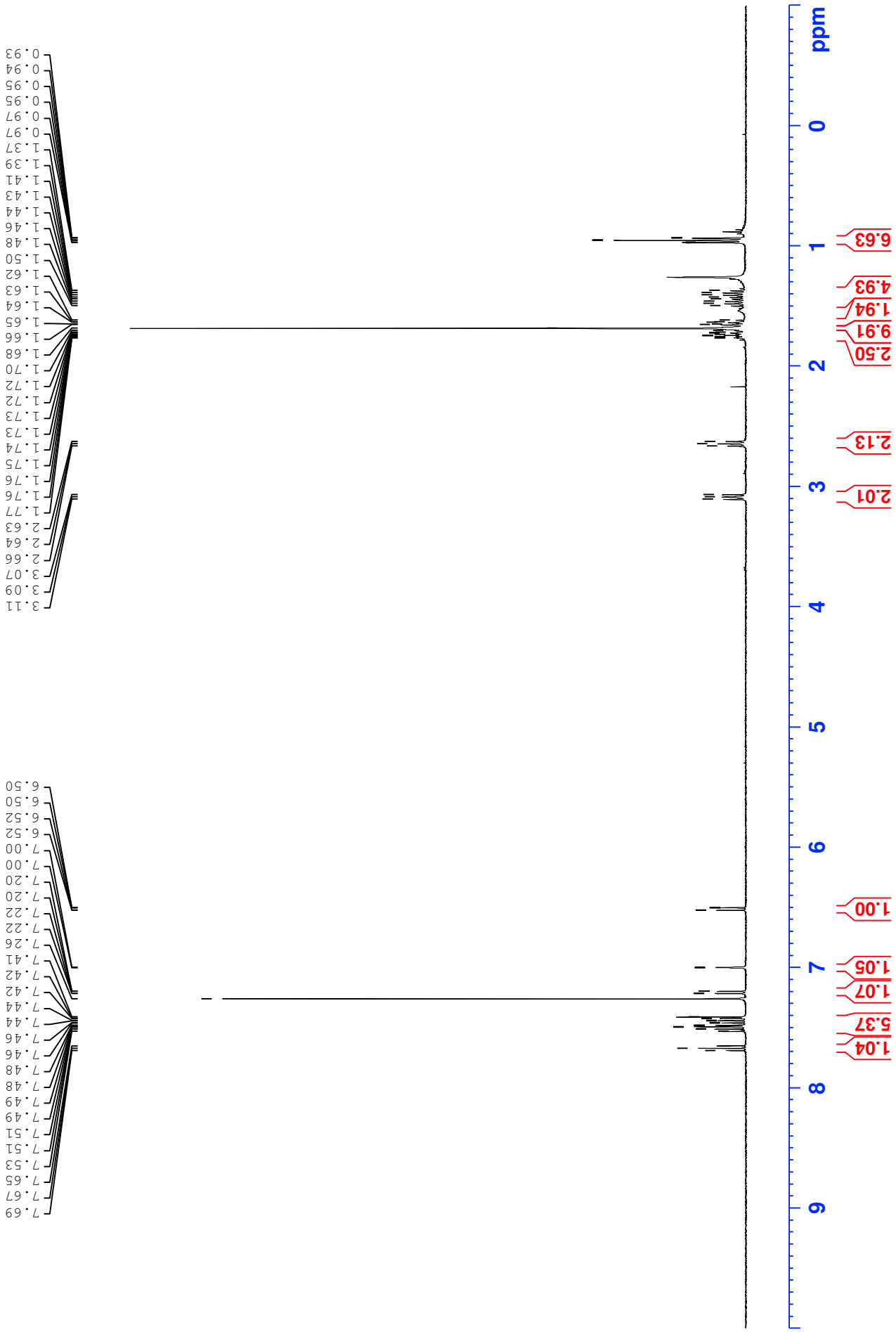
400 MHz ^{1}H–NMR spectra of **26aTf**, 300 K, $CDCl_3$.



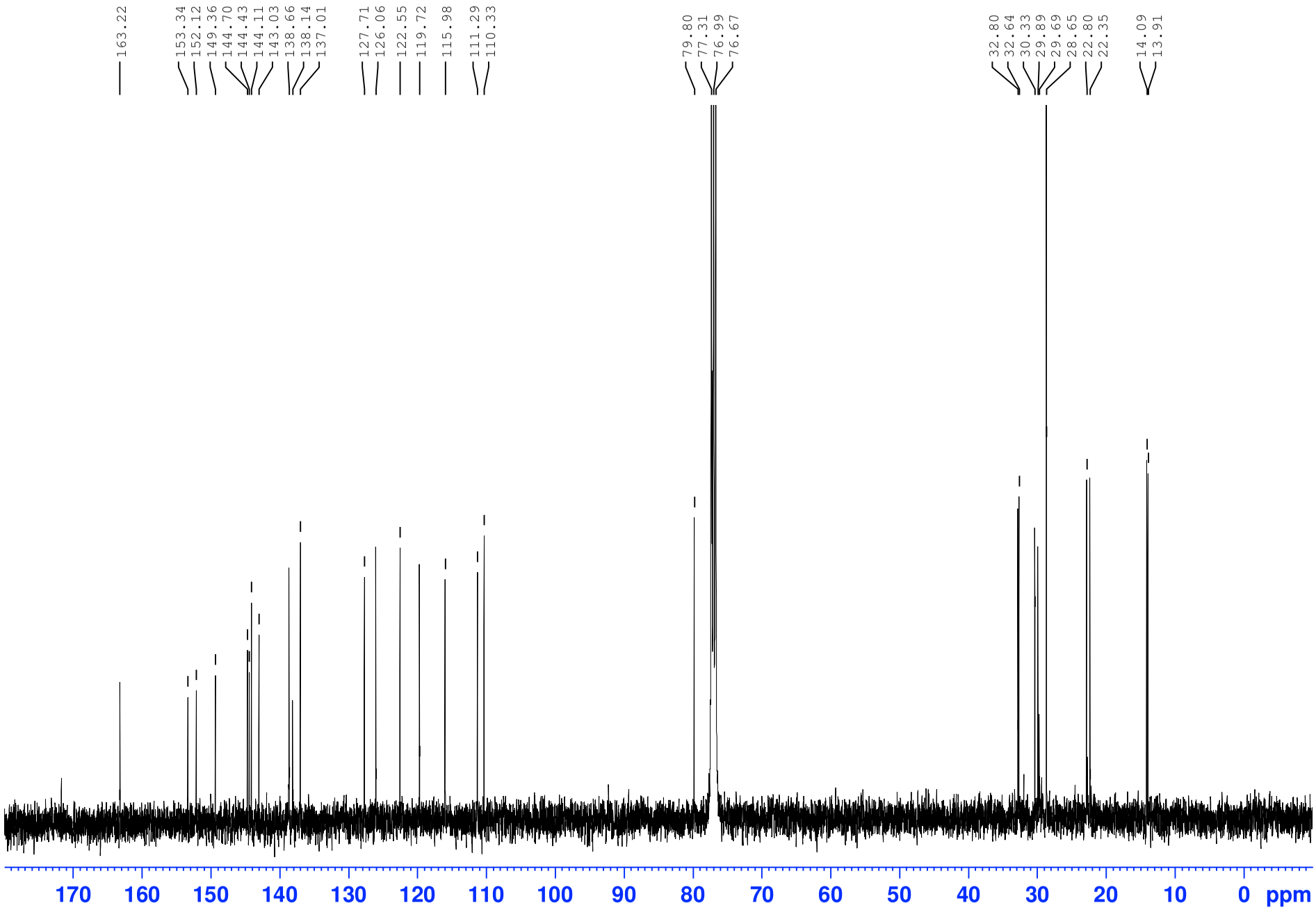
100 MHz 13C{^{1}H}–NMR spectra of **26aTf**, 300 K, $CDCl_3$.



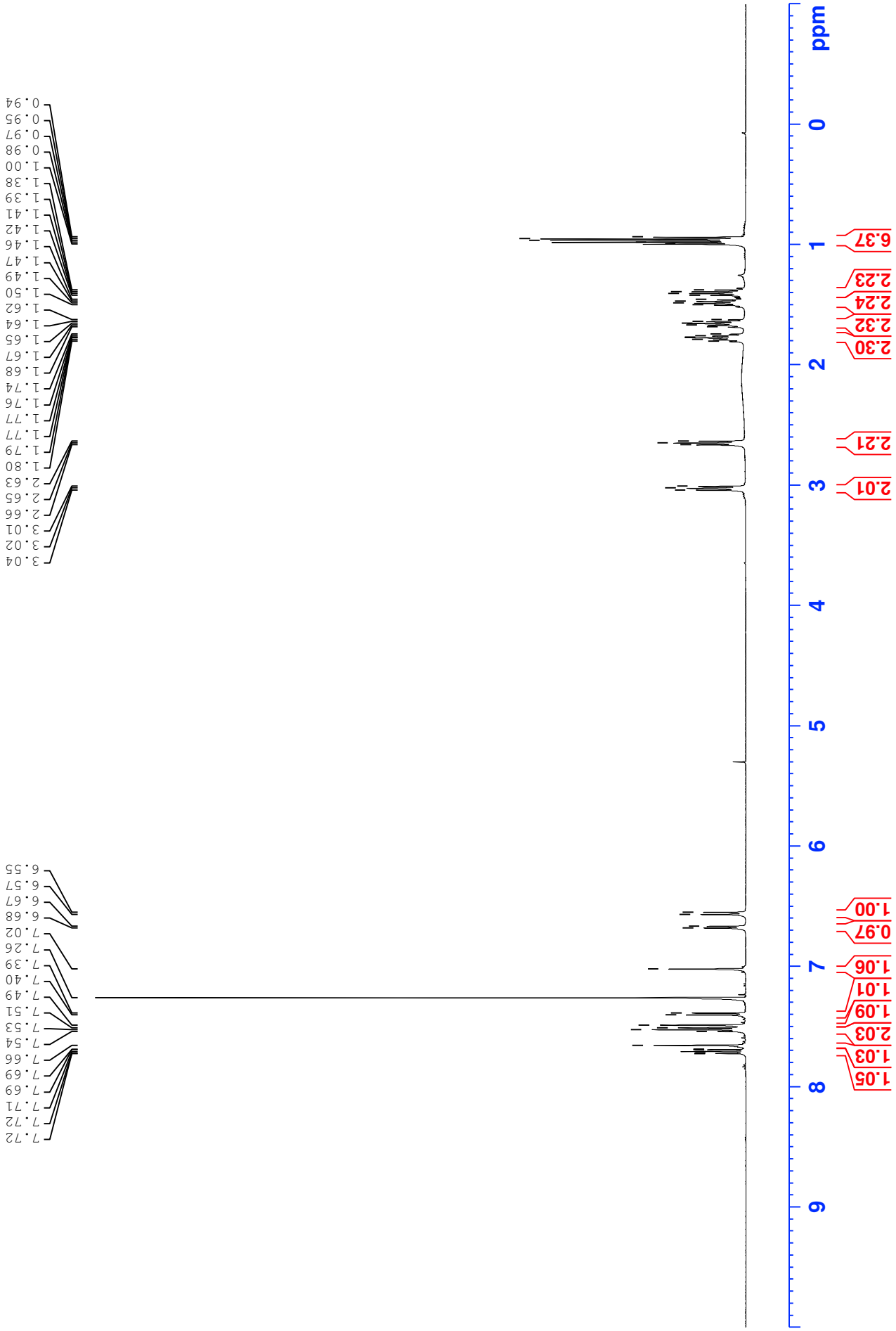
400 MHz ^{1}H–NMR spectra of **26b**, 300 K, $CDCl_3$.



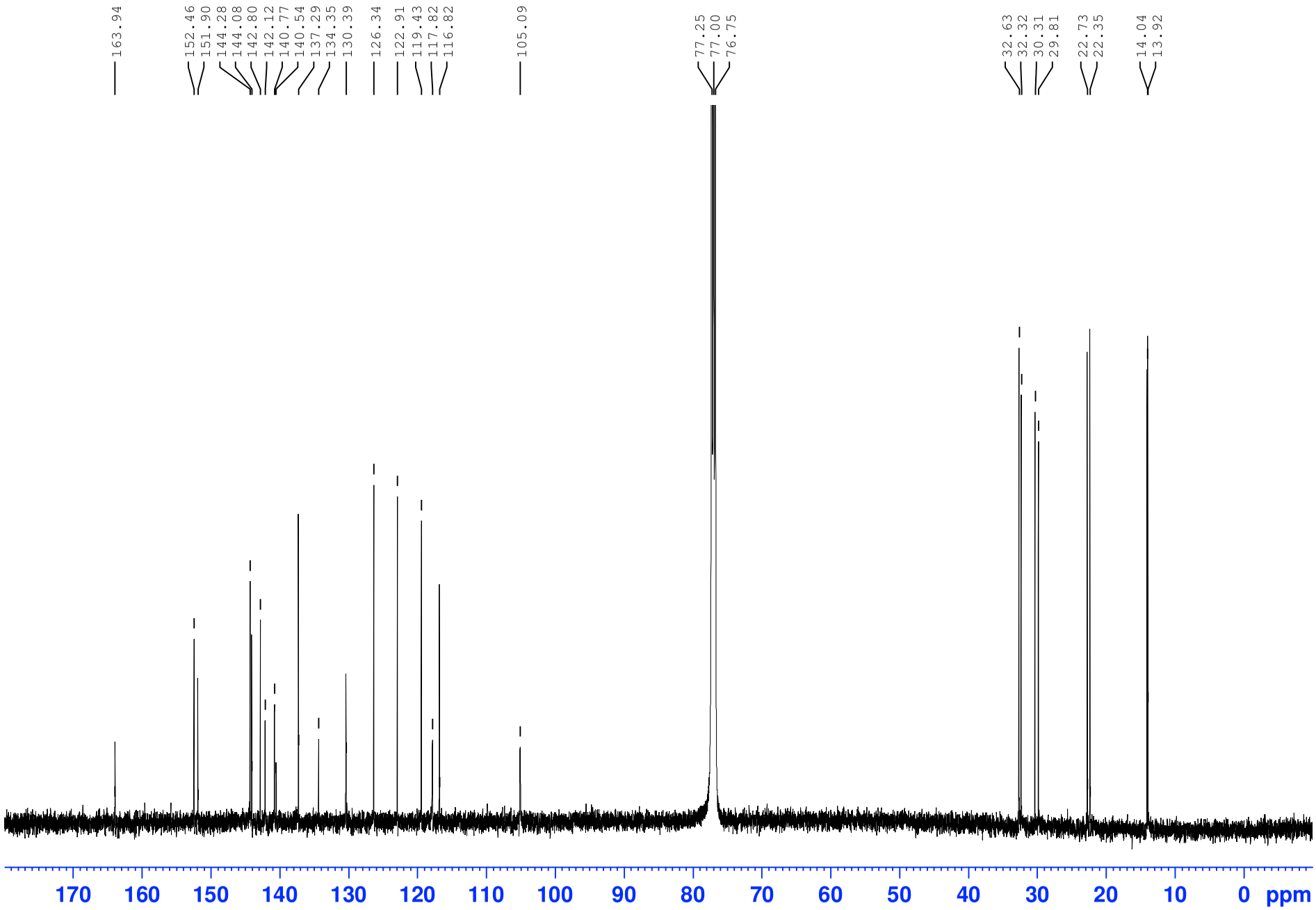
100 MHz 13C{^{1}H}–NMR spectra of **26b**, 300 K, $CDCl_3$.



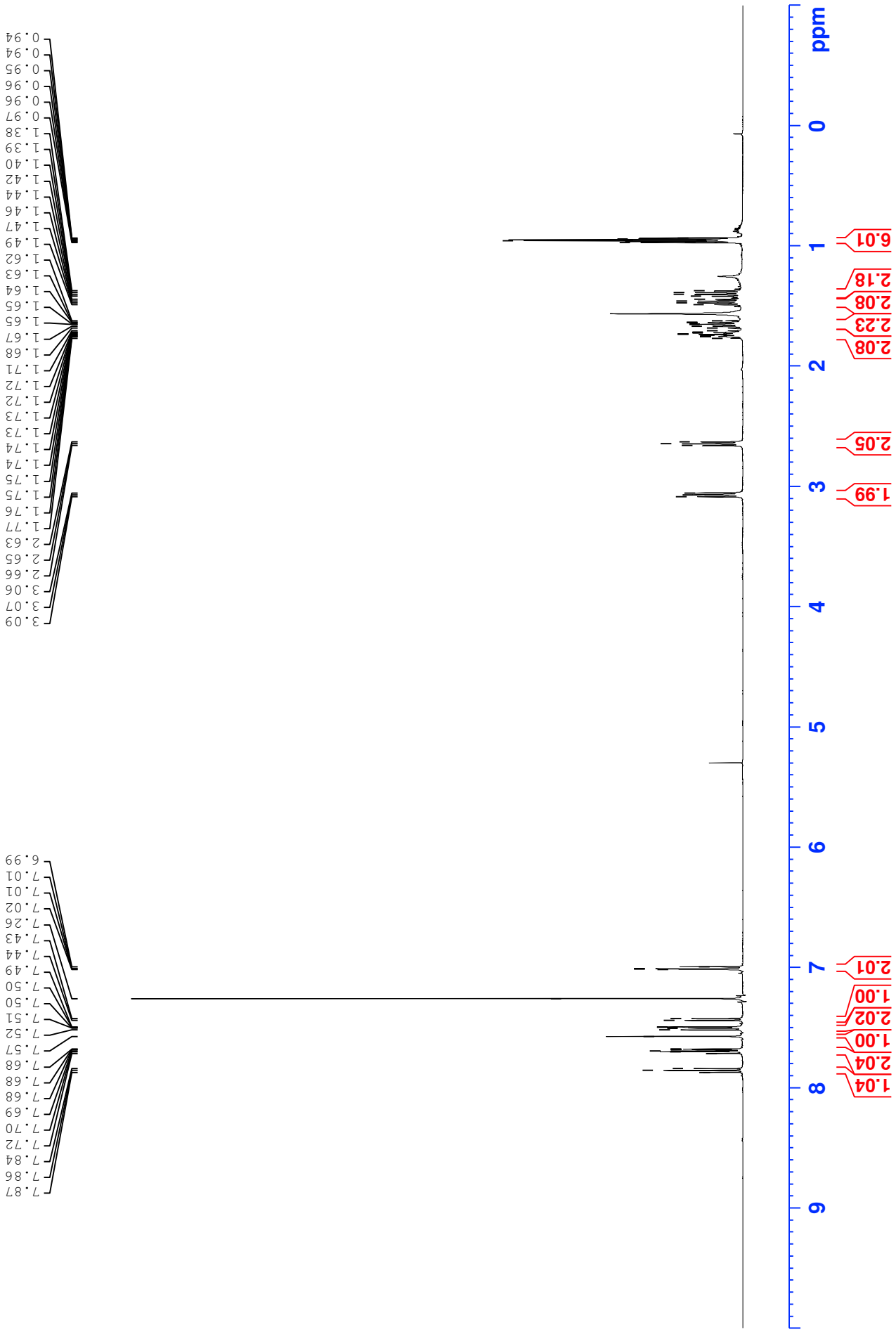
500 MHz ^{1}H–NMR spectra of **26bOH**, 300 K, $CDCl_3$.



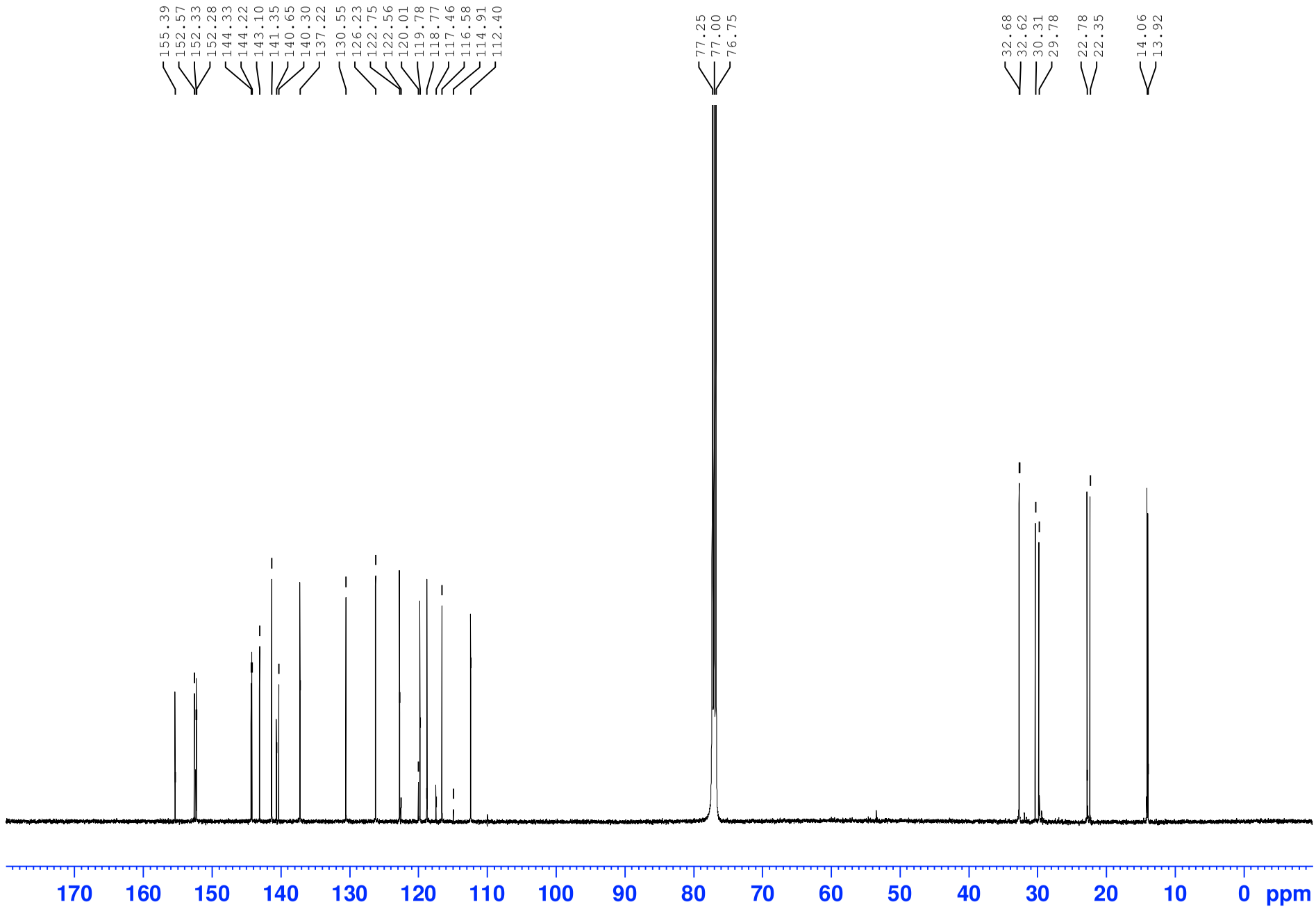
125 MHz 13C{^{1}H}–NMR spectra of **26bOH**, 300 K, $CDCl_3$.



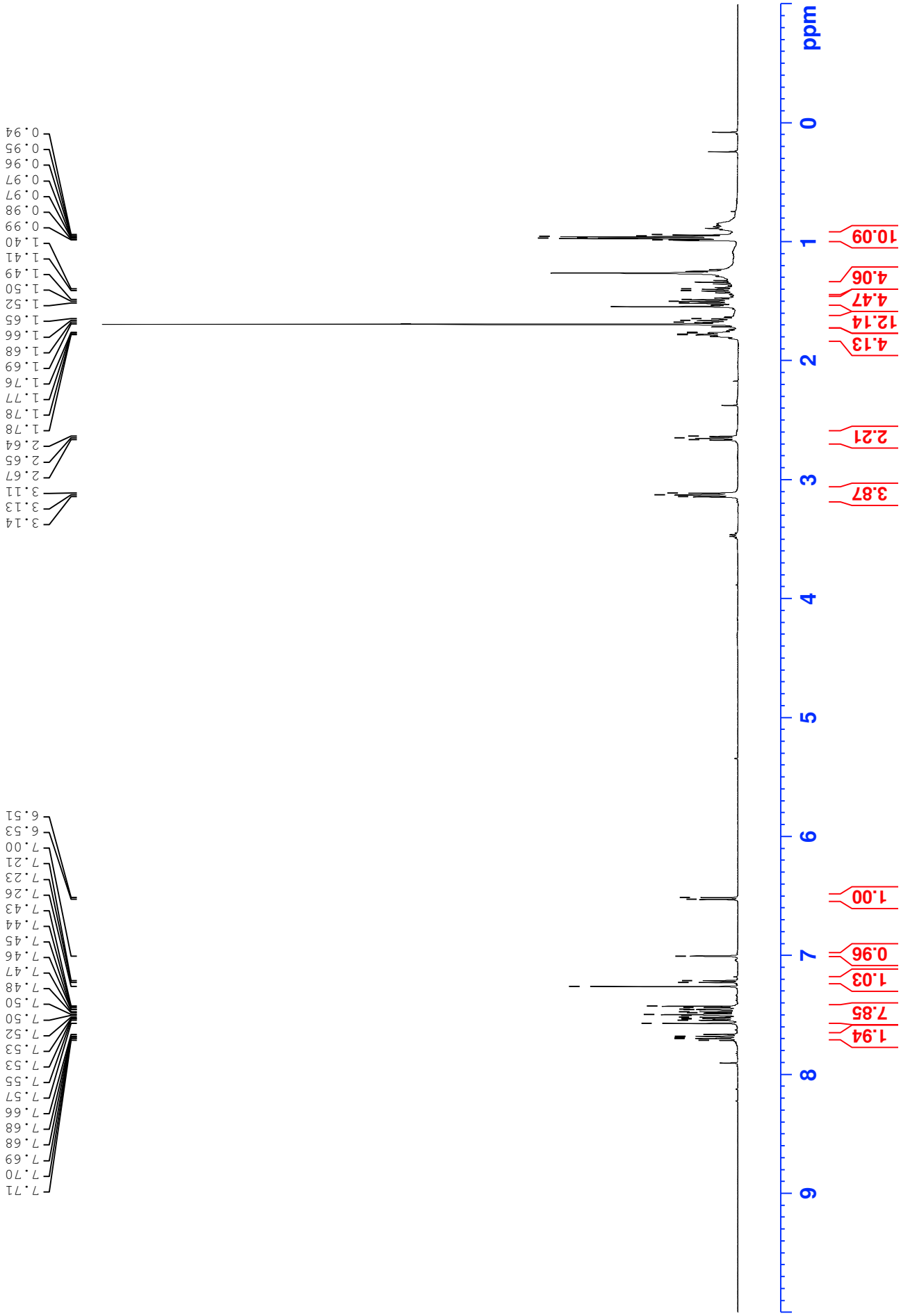
500 MHz ^{1}H–NMR spectra of **26bTf**, 300 K, $CDCl_3$.



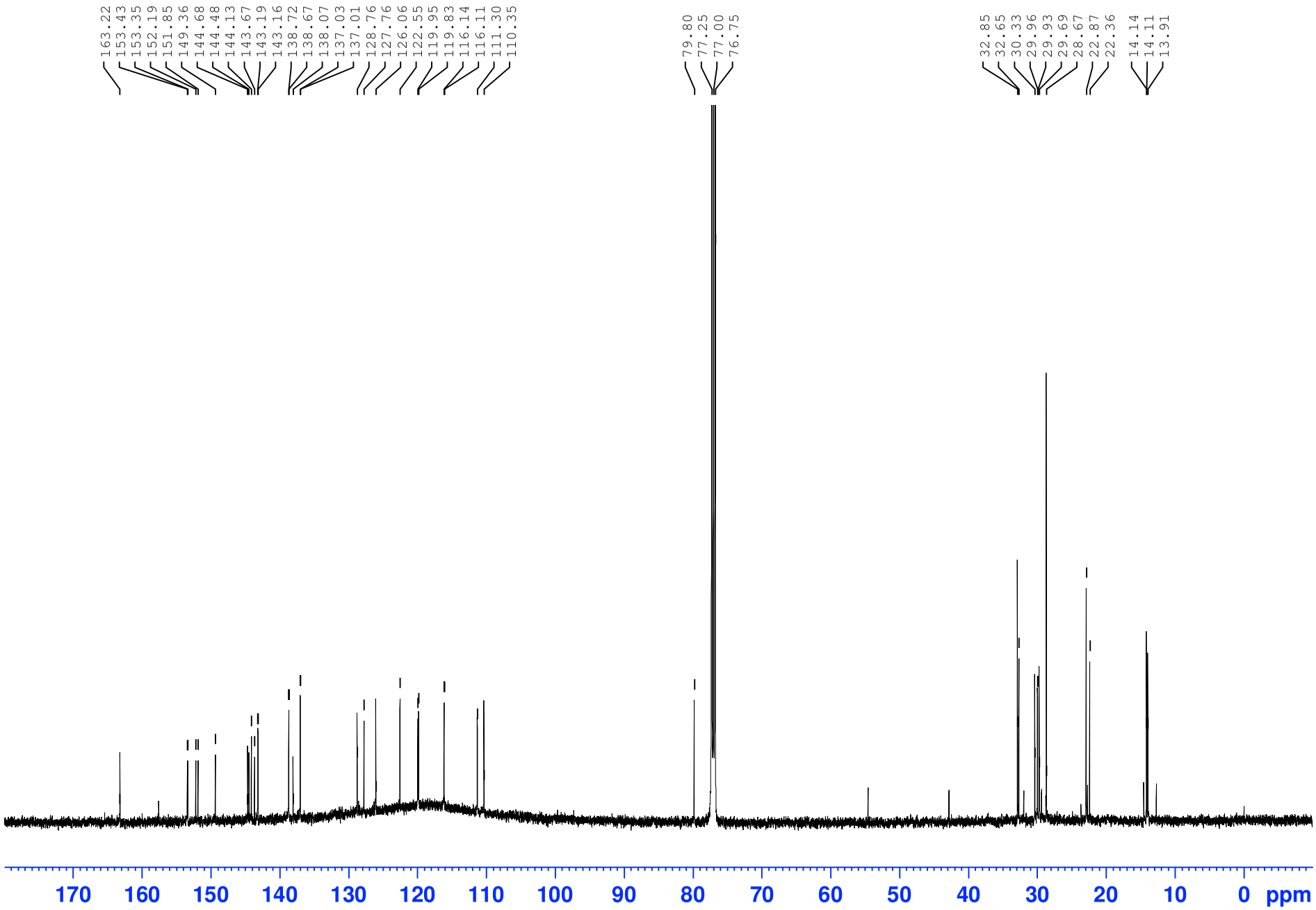
125 MHz 13C{^{1}H}–NMR spectra of **26bTf**, 300 K, $CDCl_3$.



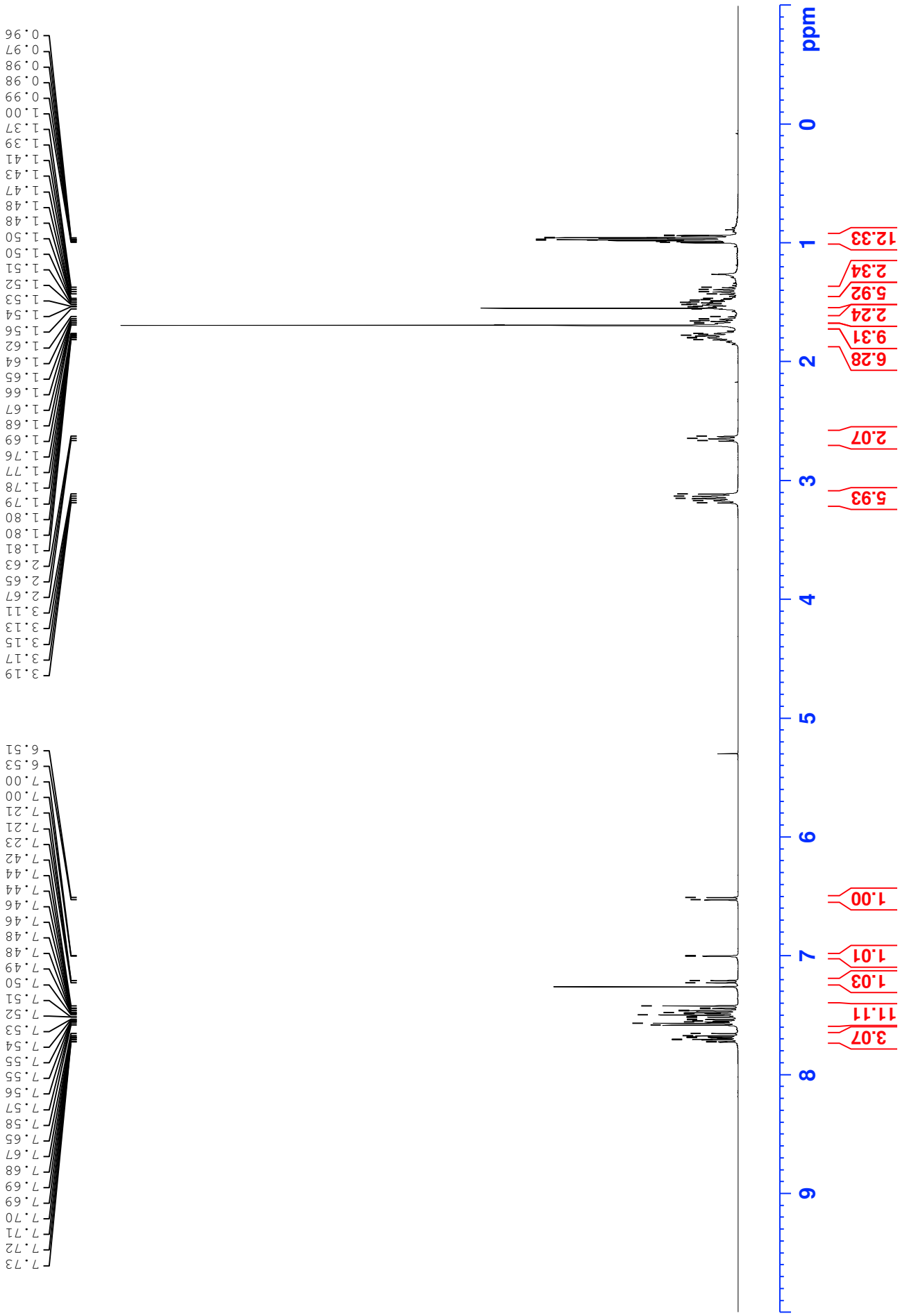
500 MHz ^{1}H–NMR spectra of **26c**, 300 K, $CDCl_3$.



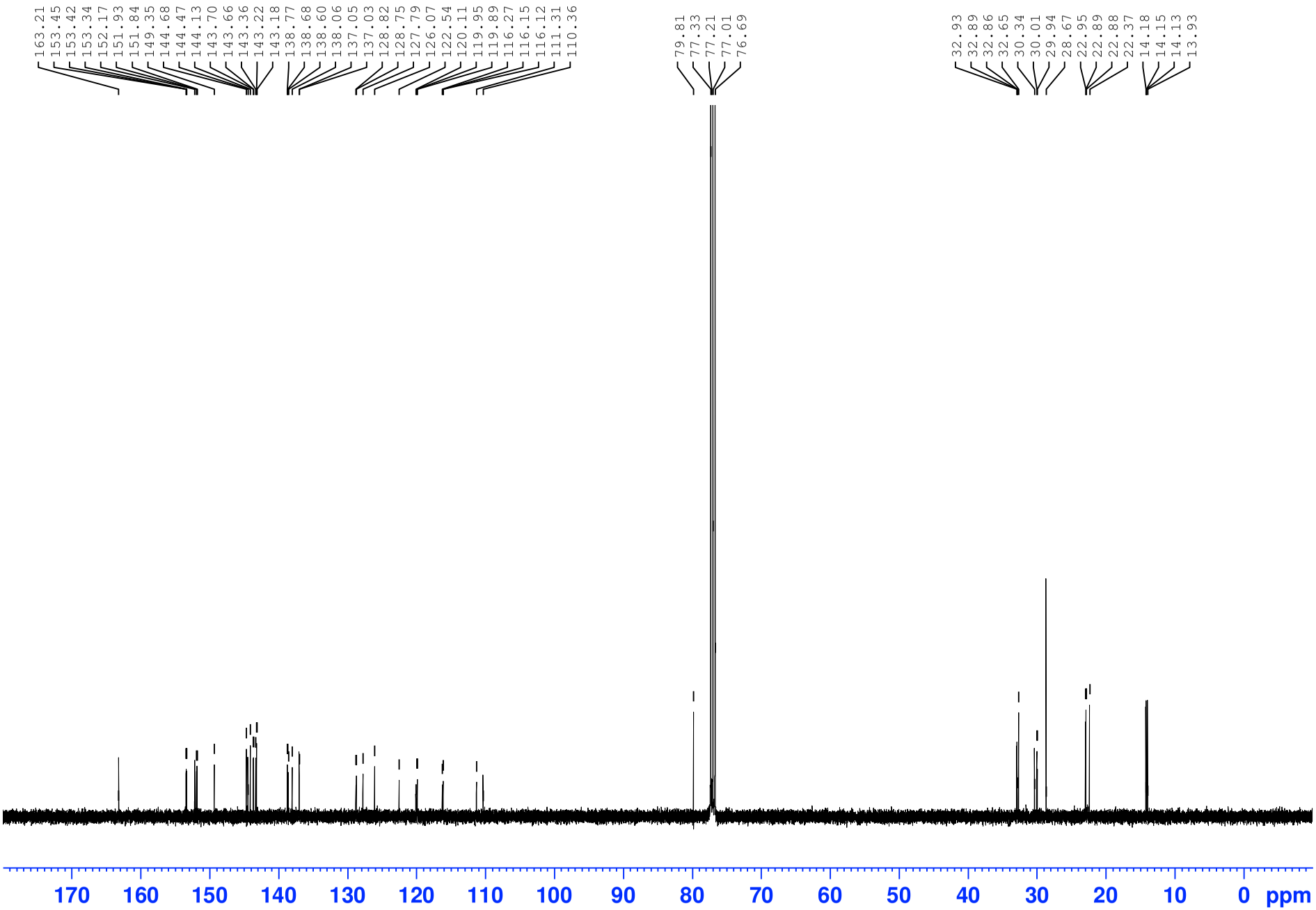
125 MHz 13C{^{1}H}–NMR spectra of **26c**, 300 K, $CDCl_3$.



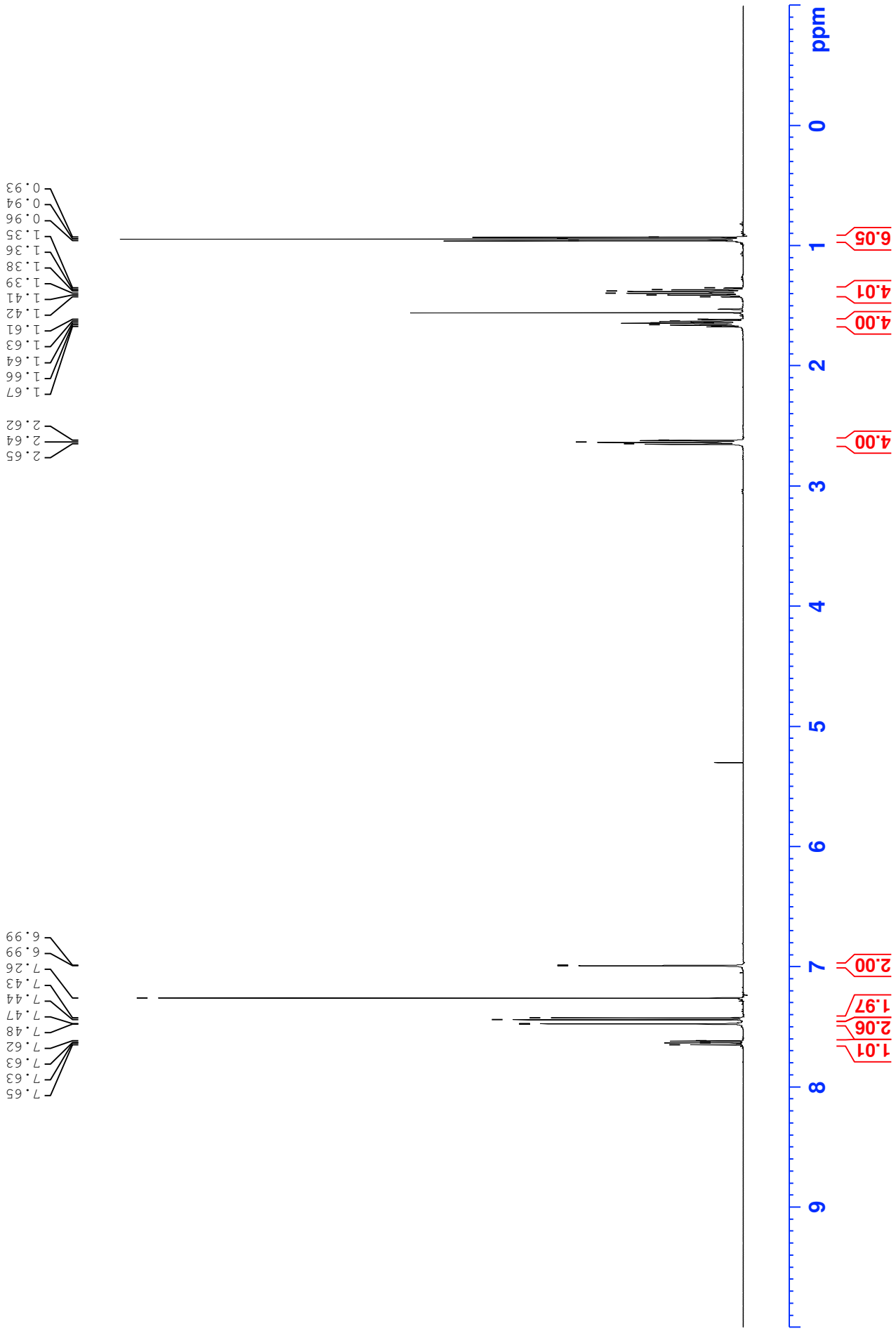
400 MHz ^{1}H–NMR spectra of **26d**, 300 K, $CDCl_3$.



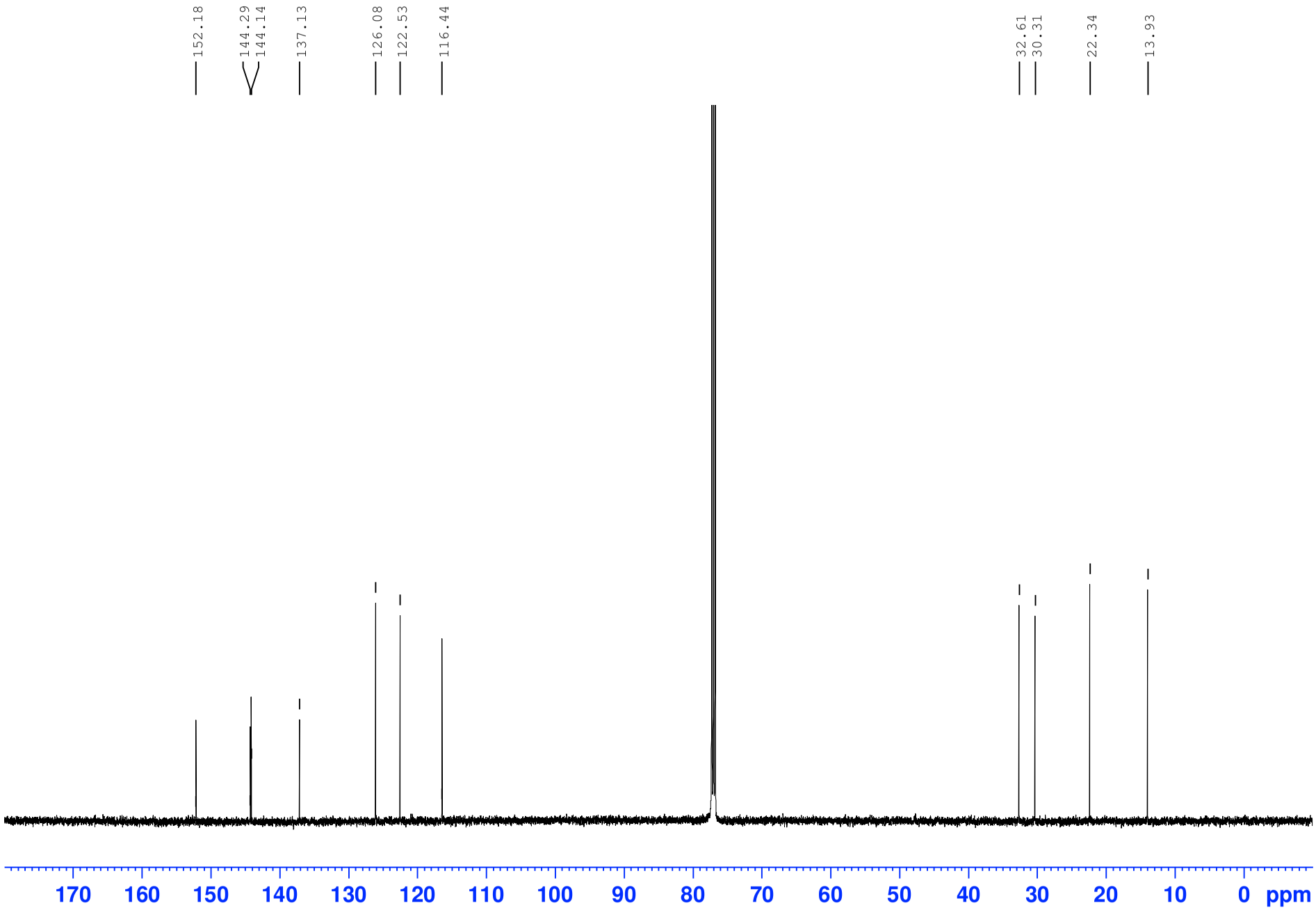
100 MHz 13C{^{1}H}–NMR spectra of **26d**, 300 K, $CDCl_3$.



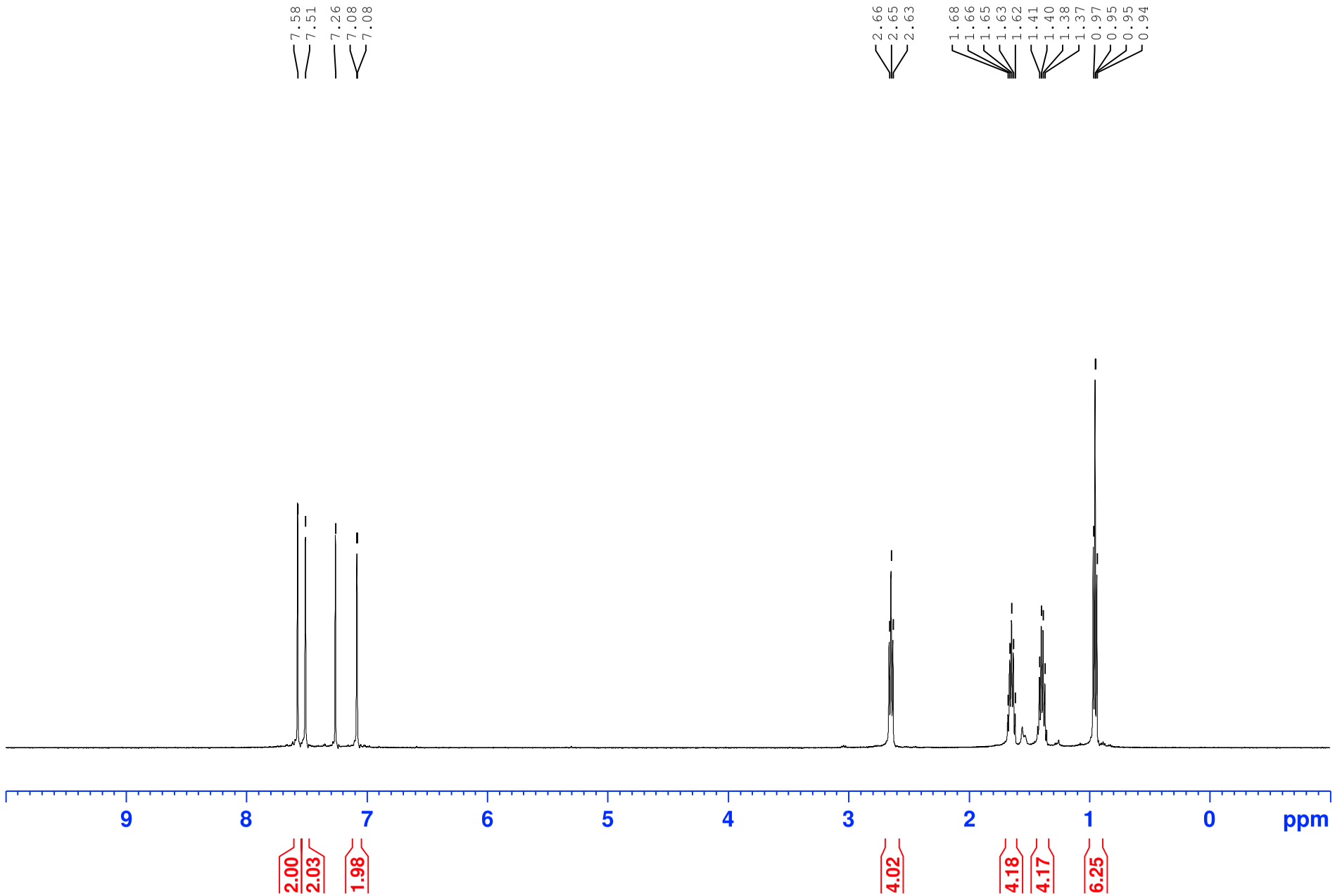
500 MHz ^{1}H–NMR spectra of **26TPT-H**, 300 K, $CDCl_3$.



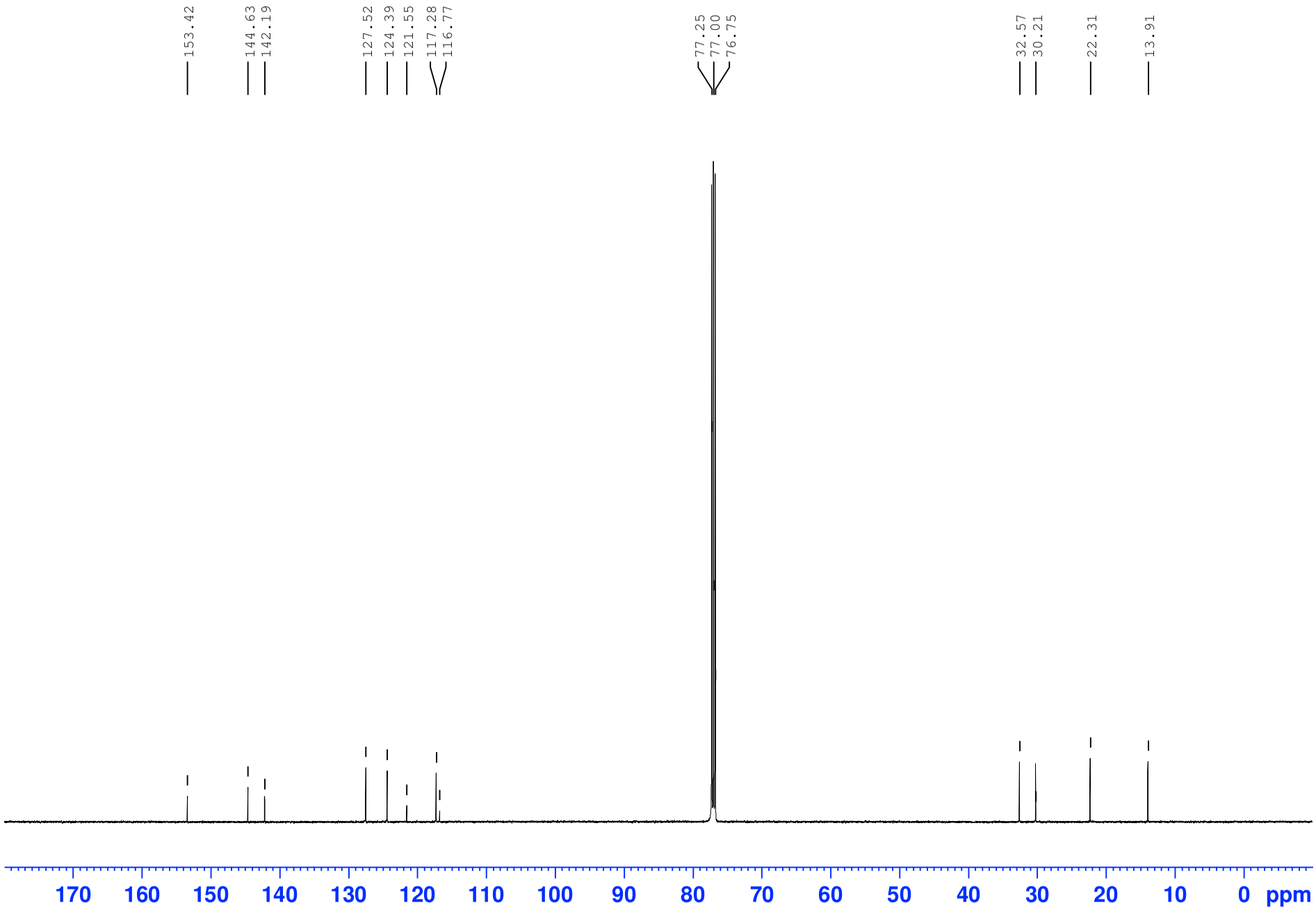
125 MHz 13C{^{1}H}–NMR spectra of **26TPT-H**, 300 K, $CDCl_3$.



500 MHz ^{1}H–NMR spectra of **26TPT-CN**, 300 K, $CDCl_3$.



125 MHz 13C{^{1}H}–NMR spectra of **26TPT-CN**, 300 K, $CDCl_3$.



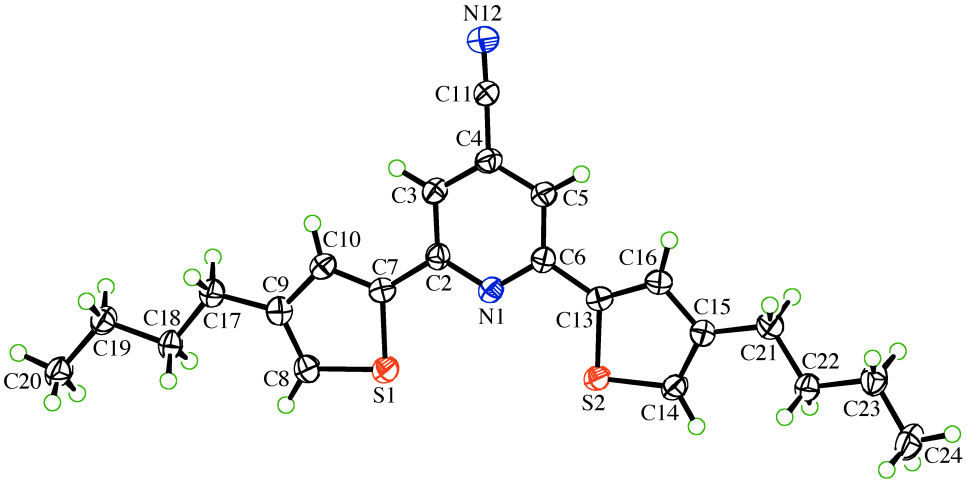


Figure 1: *ORTEP representation of the molecule,* ***26TPT-CN*** *(50% probability ellipsoids; H-atoms given arbitrary displacement parameters for clarity).*

Table 1. *Crystallographic Data for* ***26TPT-CN***

Crystallised from	CH_2Cl_2 / hexane	
Empirical formula	$C_{22}H_{24}N_2S_2$	
Formula weight [g mol^{-1}]	380.57	
Crystal colour, habit	colourless, prism	
Crystal dimensions [mm]	0.12 × 0.22 × 0.35	
Temperature [K]	160(1)	
Crystal system	triclinic	
Space group	$P\bar{1}$ (#2)	
Z	2	
Reflections for cell determination	7747	
2θ range for cell determination [°]	4–50	
Unit cell parameters	a [Å]	10.3552(6)
b [Å]	10.7211(7)	
c [Å]	11.3768(5)	
α [°]	64.950(3)	
β [°]	63.749(4)	
γ [°]	70.394(3)	
V [Å^3]	1009.0(1)	
F(000)	404	
D_x [g cm^{-3}]	1.253	
μ(Mo $K\alpha$) [mm^{-1}]	0.272	
Scan type	ω	
2θ(max) [°]	50	
Transmission factors (min; max)	0.882; 0.969	
Total reflections measured	12890	
Symmetry independent reflections	3537	
R_{int}	0.080	
Reflections with $I > 2\sigma(I)$	2444	
Reflections used in refinement	3537	
Parameters refined	238	
Final	$R(F)$ [$I > 2\sigma(I)$ reflections]	0.0470
	$wR(F^2)$ (all data)	0.1283
Weights:	$w = [\sigma^2(F_o^2) + (0.0667P)^2 + 0.0085P]^{-1}$ where $P = (F_o^2 + 2F_c^2)/3$	
Goodness of fit	1.036	
Final Δ_{max}/σ	0.001	
$\Delta\rho$ (max; min) [e Å^{-3}]	0.29; -0.36	
$\sigma(d(C-C))$ [Å]	0.003 – 0.004	