

Supplementary Materials

N-[(1*R*)-1-(4-Chlorophenyl)ethyl]-cyanamide

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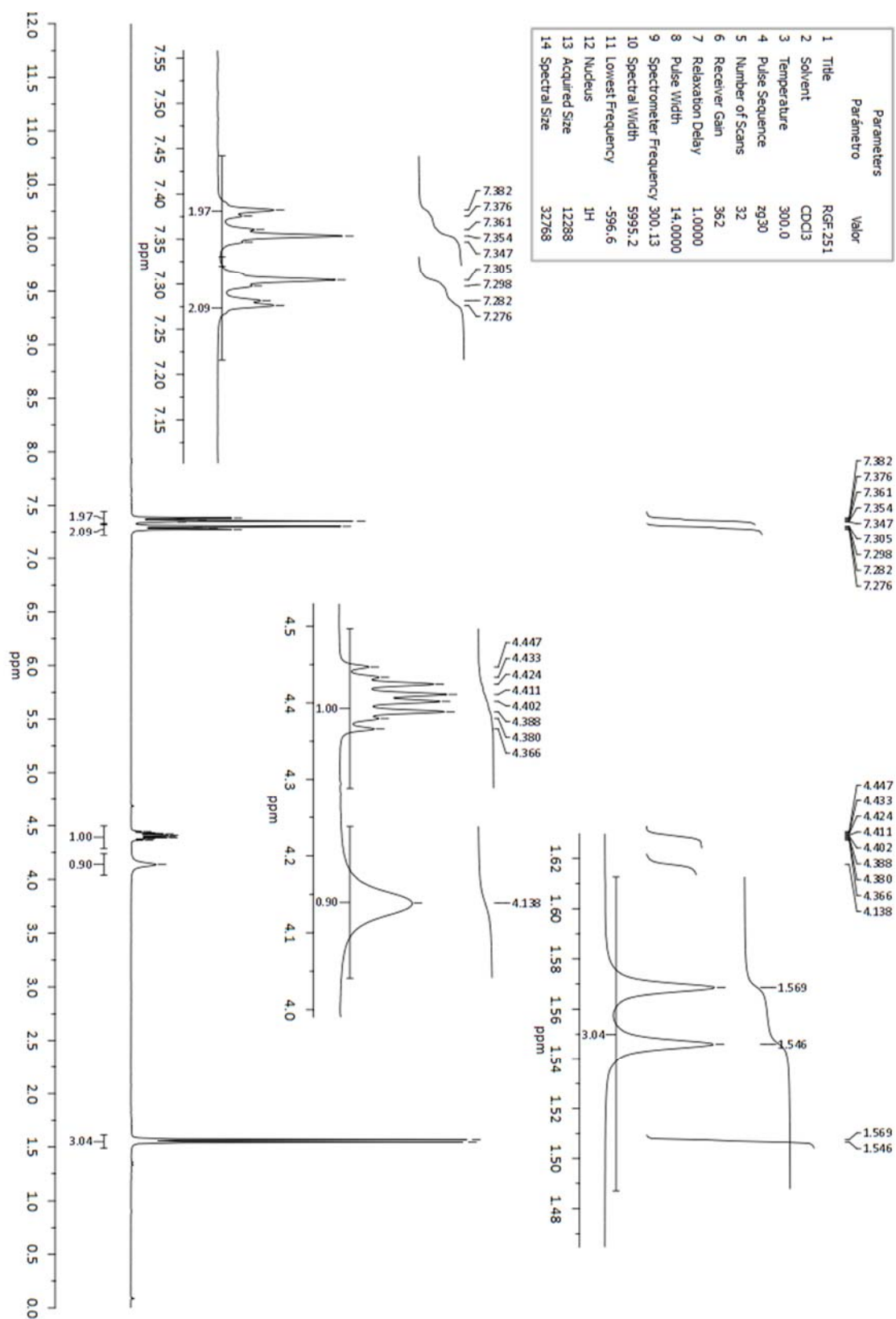


Figure S1: ¹H NMR spectrum (300 MHz, CDCl₃) of compound **2**.

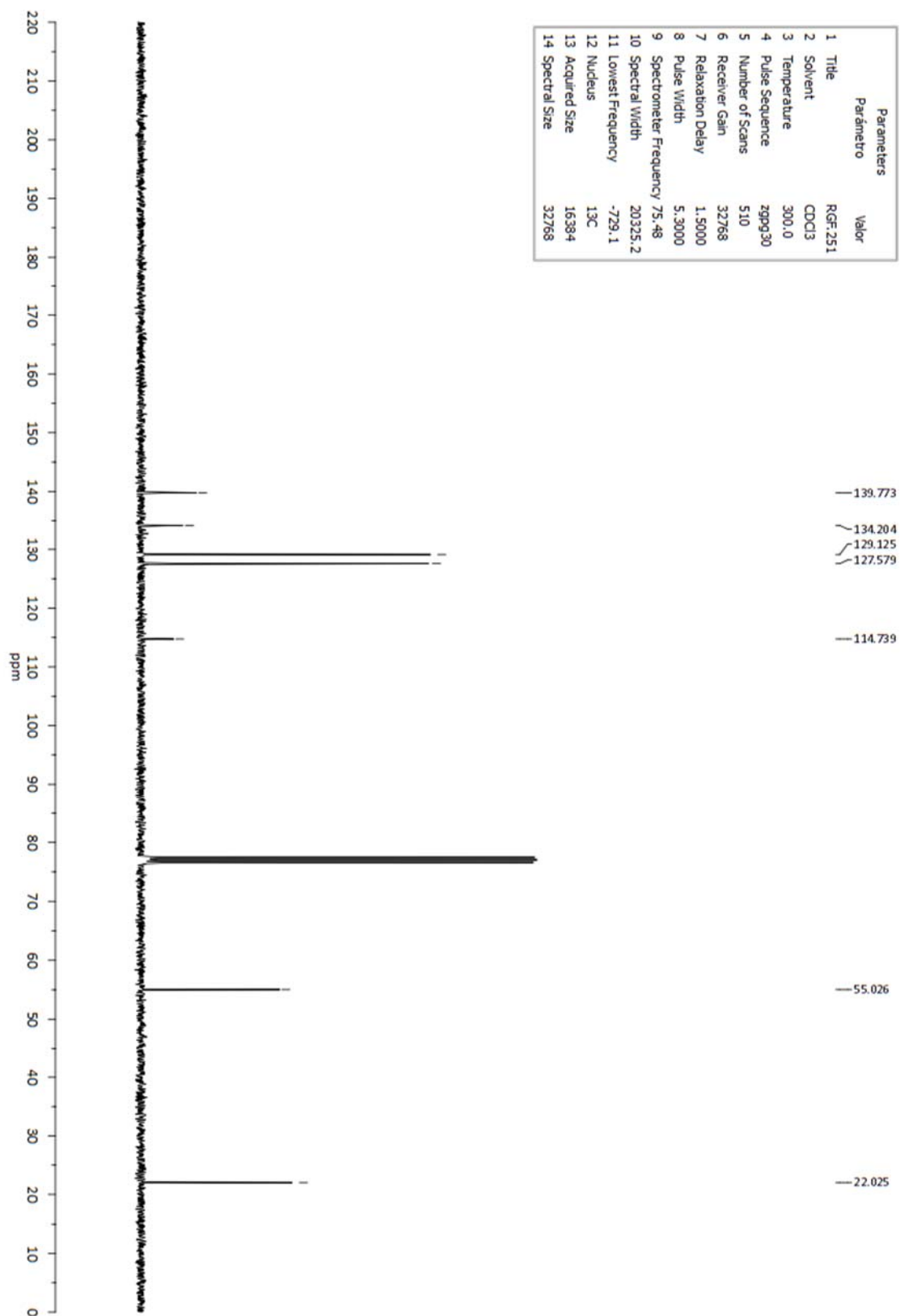


Figure S2: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (75 MHz, CDCl_3) of compound **2**.

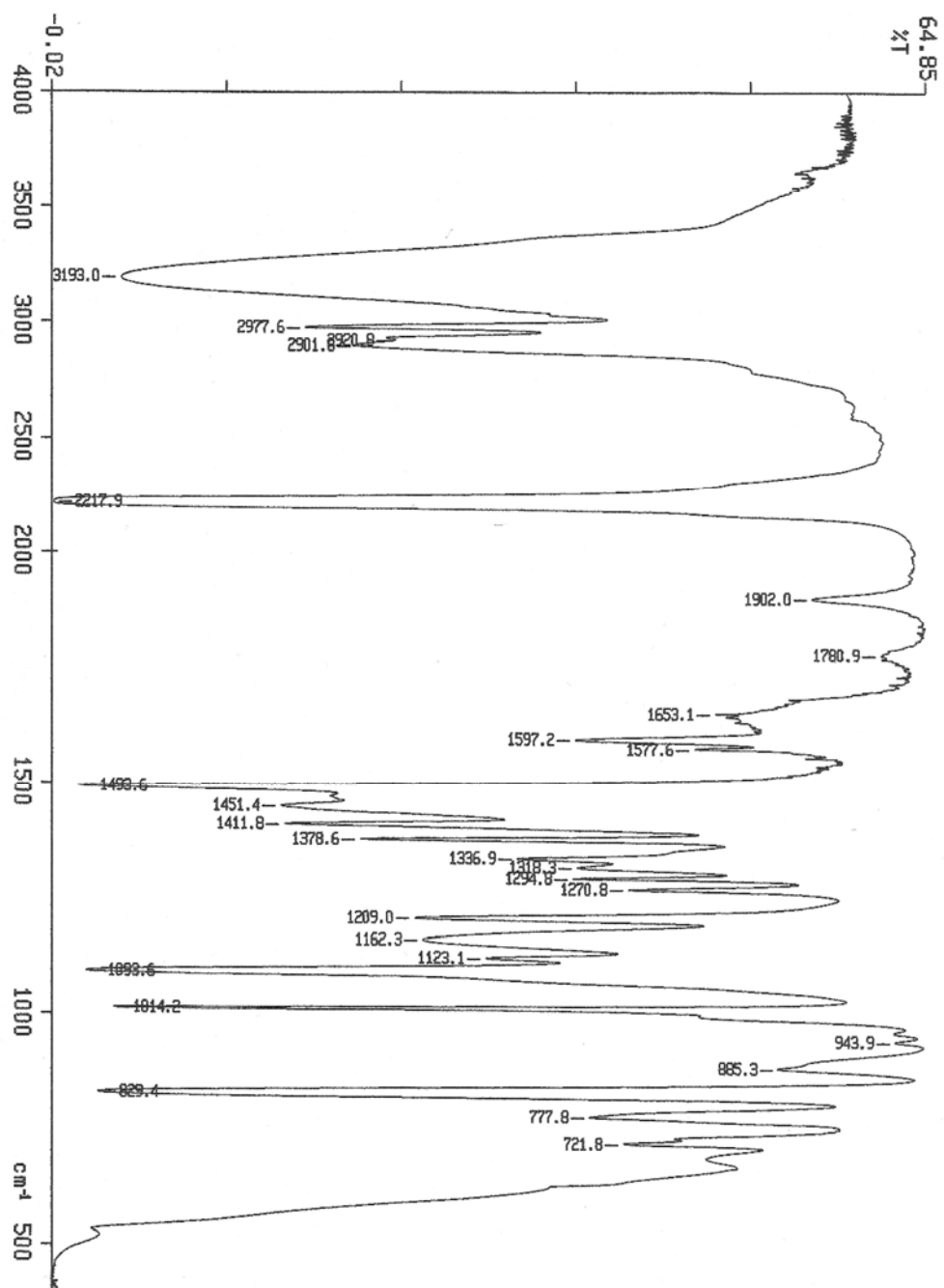


Figure S3: IR spectrum (neat) of compound 2.

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name D:\Data\Miguel\Comorca\180110\180110_RGF-251.d
Method MS 50-1000 orgánica.m
Sample Name 180110_RGF-251
Comment

Acquisition Date 10/01/2018 11:13:56

Operator Univ. Oviedo
Instrument impact II 1825265.10101

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.4 Bar
Focus	Active	Set Capillary	3000 V	Set Dry Heater	250 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C

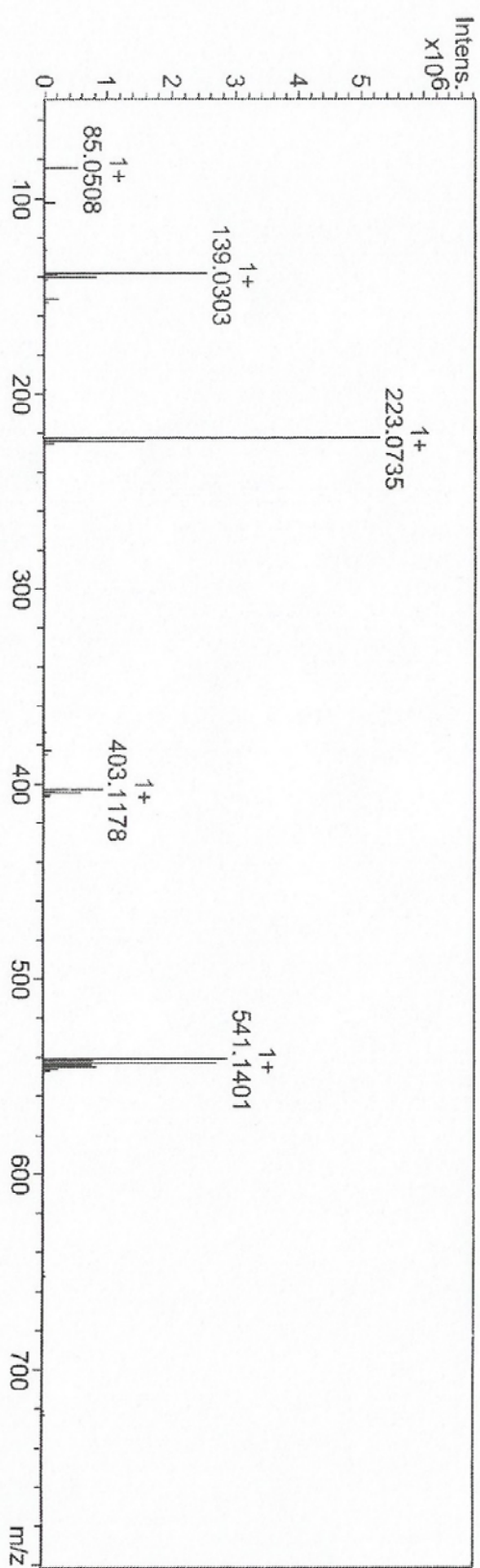
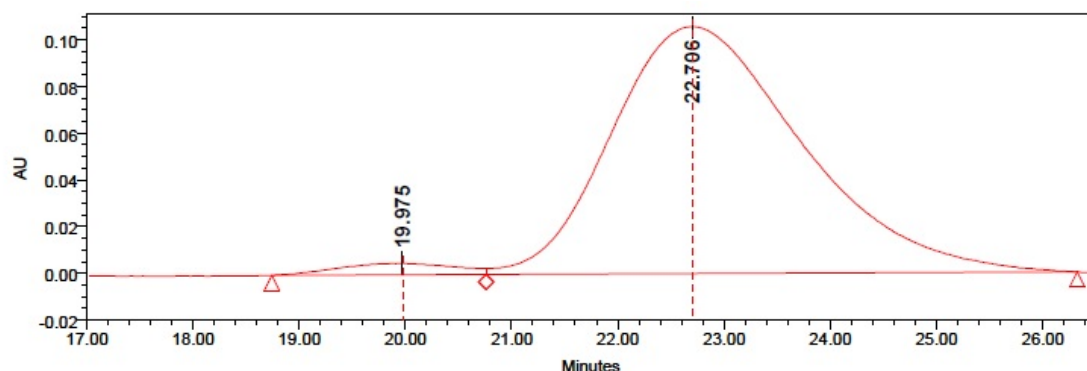


Figure S4: HRMS spectrum (ESI) obtained for compound 2.

Optical purity of compounds 1 and 2.

HPLC analyses to determine the optical purity of starting amine **1** and the cyanamide **2** were performed at 30 °C on a Waters 2690 chromatograph using a Chiralcel OJ-H column (93:7 hexane/PrOH mixture as eluent with a flow of 1.0 mL/min). Detection of peaks (UV absorption) were performed at 254 nm. Optical purity found for (*R*)-4-chloro- α -methylbenzylamine **1** (97%) was consistent with the manufacturer (Sigma-Aldrich) specifications ($\geq 95\%$).

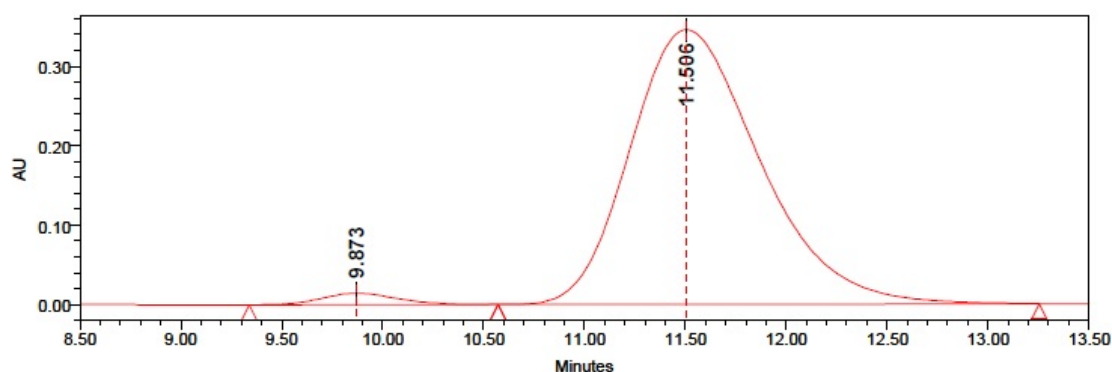
HPLC chromatogram of (*R*)-4-chloro- α -methylbenzylamine **1**.



Peak Results

	RT	Area	% Area
1	19.975	369469	2.74
2	22.706	13137240	97.26

HPLC chromatogram of *N*-[(1*R*)-1-(4-chlorophenyl)ethyl]-cyanamide **2**.



Peak Results

	RT	Area	% Area
1	9.873	379738	2.40
2	11.506	15463167	97.60