Electronic Supporting Information

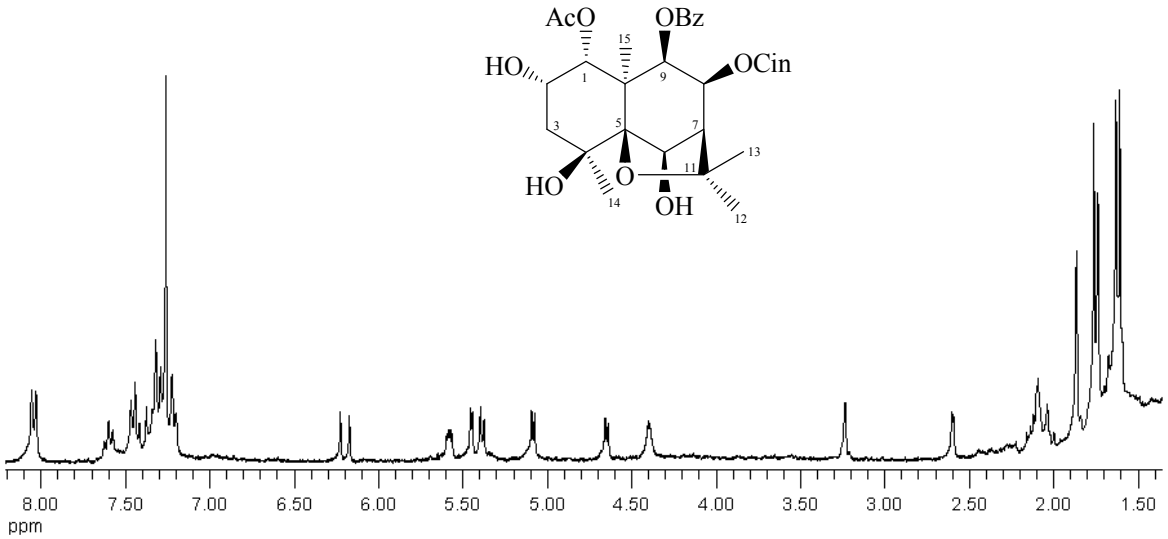
Novel dihydro-β-agarofuran sesquiterpenes as potent modulators of human P-glycoprotein dependent multidrug resistance†

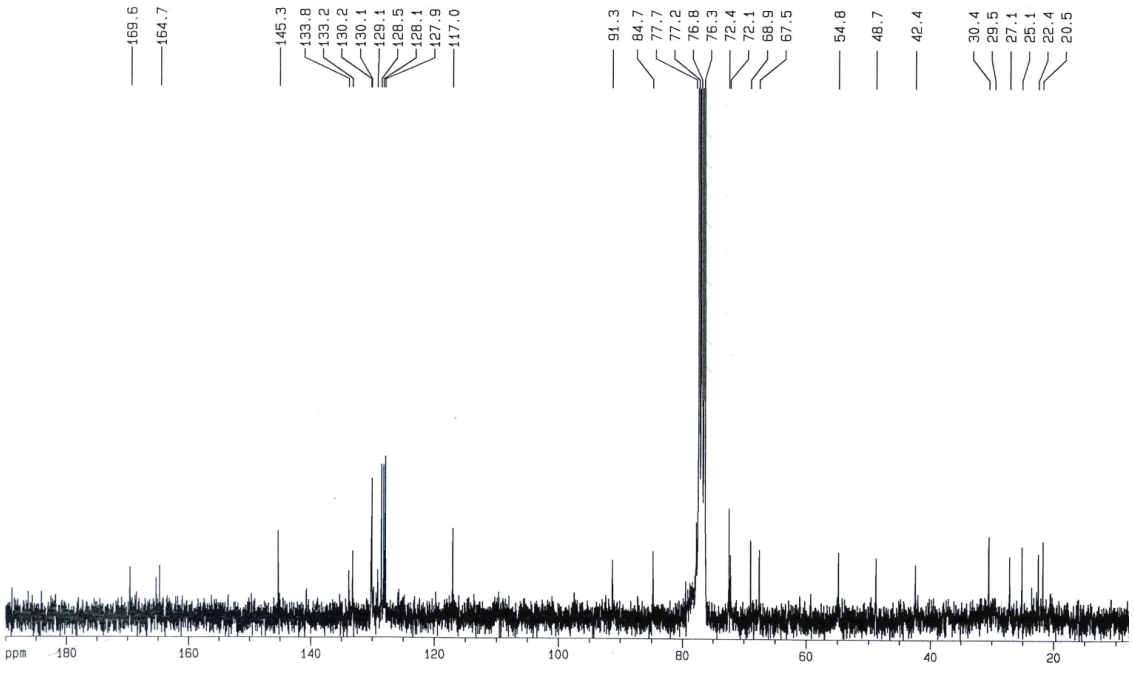
David Torres-Romero,[a] Francisco Muñoz-Martínez,[b] Ignacio A. Jiménez,[c] Santiago Castanys,[b] Francisco Gamarro,*[b] and Isabel L. Bazzocchi*[c]

[a]*Departamento de Bioquímica y Contaminación Ambiental, Facultad de Quiímica y Farmacia, Universidad de El Salvador, Final 25 Avenida Norte, El Salvador.*
[b]*Instituto de Parasitología y Biomedicina "López-Neyra", Consejo Superior de Investigaciones Científicas, Parque Tecnológico de Ciencias de la Salud, Avda. del Conocimiento s/n, 18100 Armilla, Granada, Spain.*
[c]*Instituto Universitario de Bio-Orgánica "Antonio González", Universidad de La Laguna and Instituto Canario de Investigación del Cáncer, Avenida Astrofísico Francisco Sánchez 2, 38206 La Laguna, Tenerife, Spain*

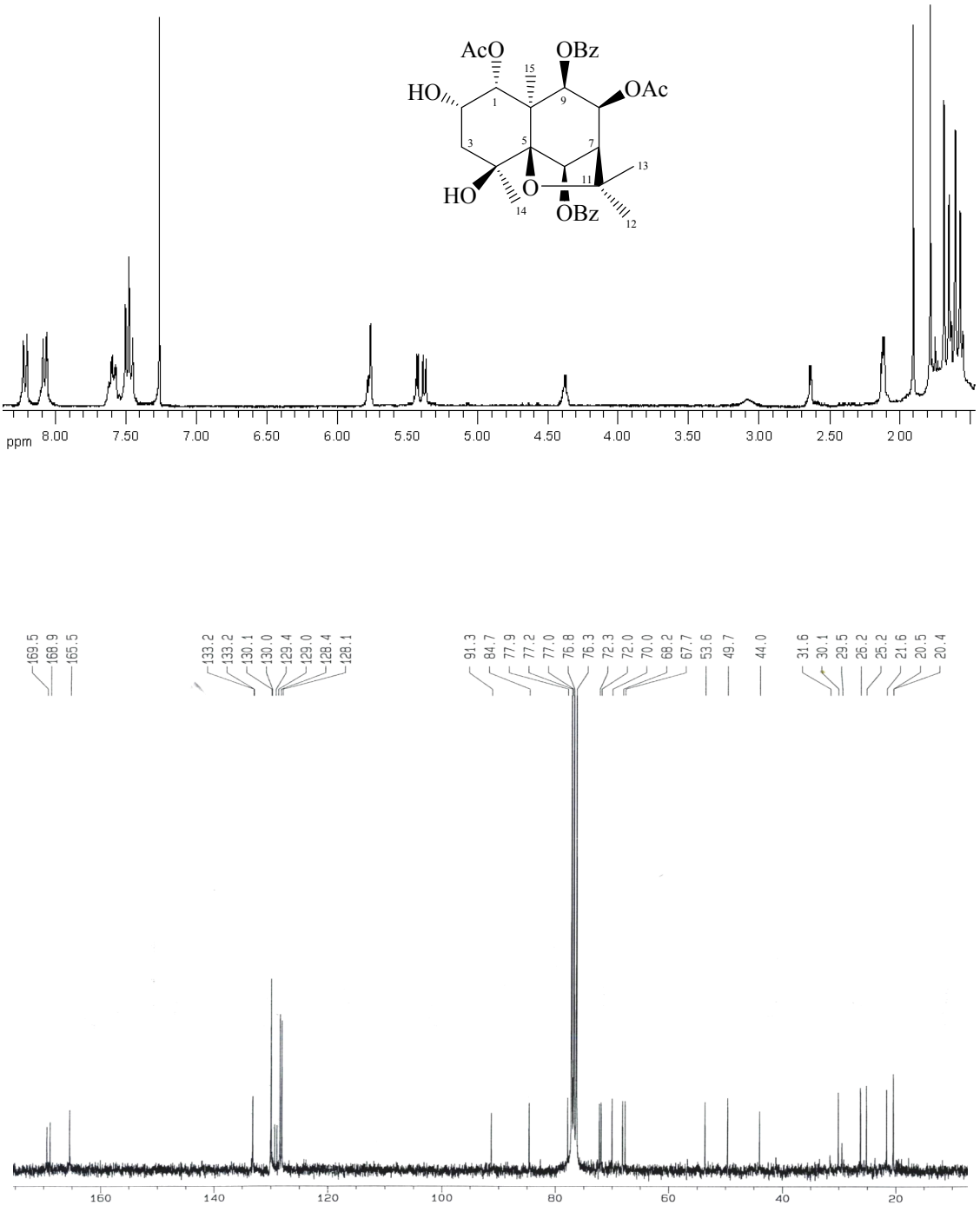
† Electronic Supplementary Information (ESI) available: ^{1}H and ^{13}C NMR spectra for compounds **1-5**, **9-11** and **13**, DC spectrum for compound **1**, and purity criteria for isolated compounds.

Contents

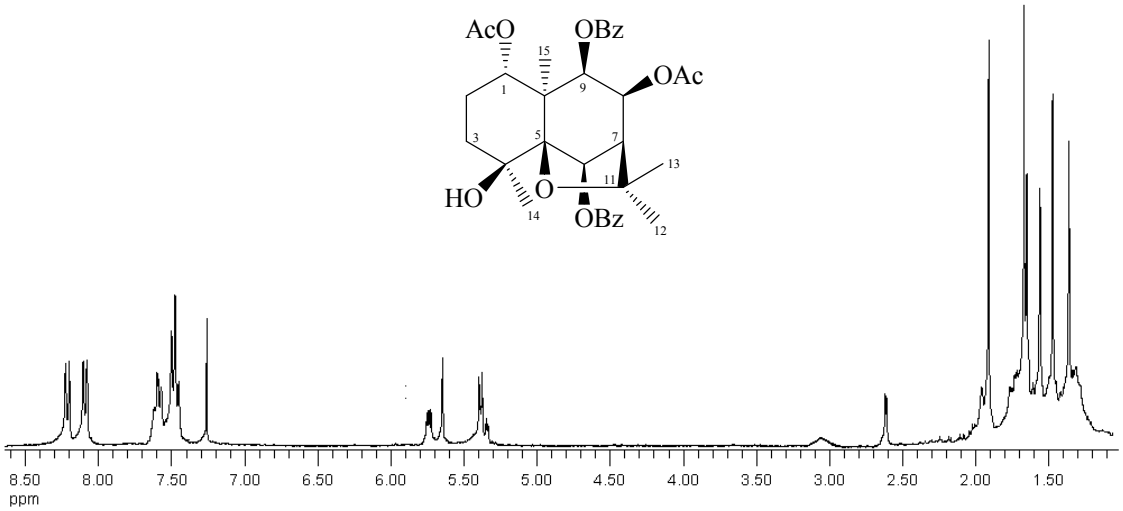


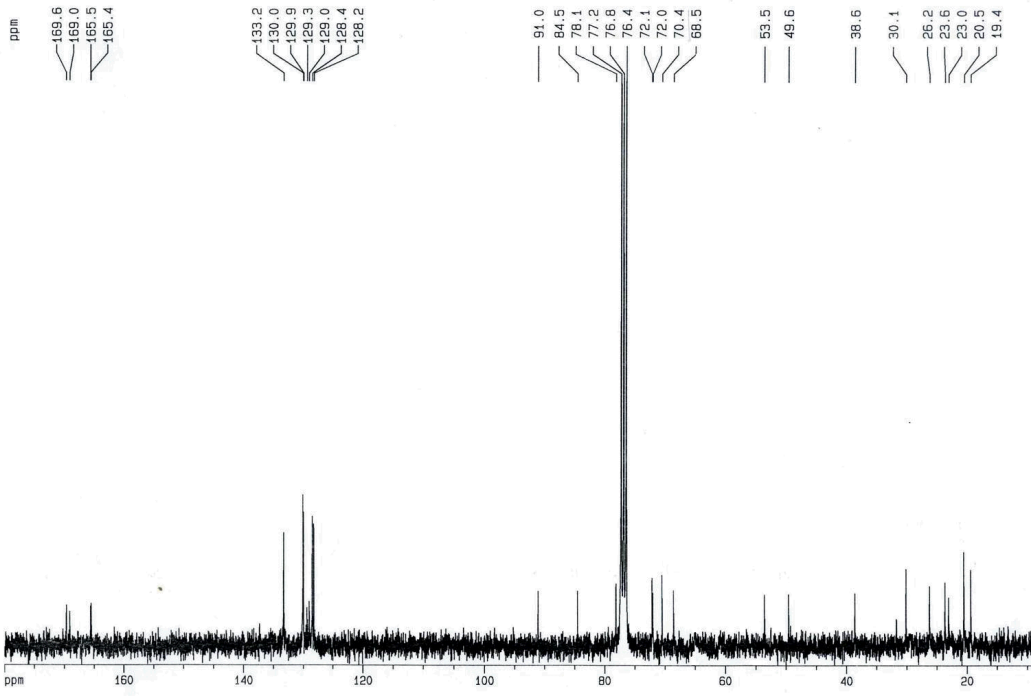


Spectra S1.
^{1}H NMR and ^{13}C NMR spectra of compound **1** (400 MHz, 100 MHz, solvent $CDCl_3$)

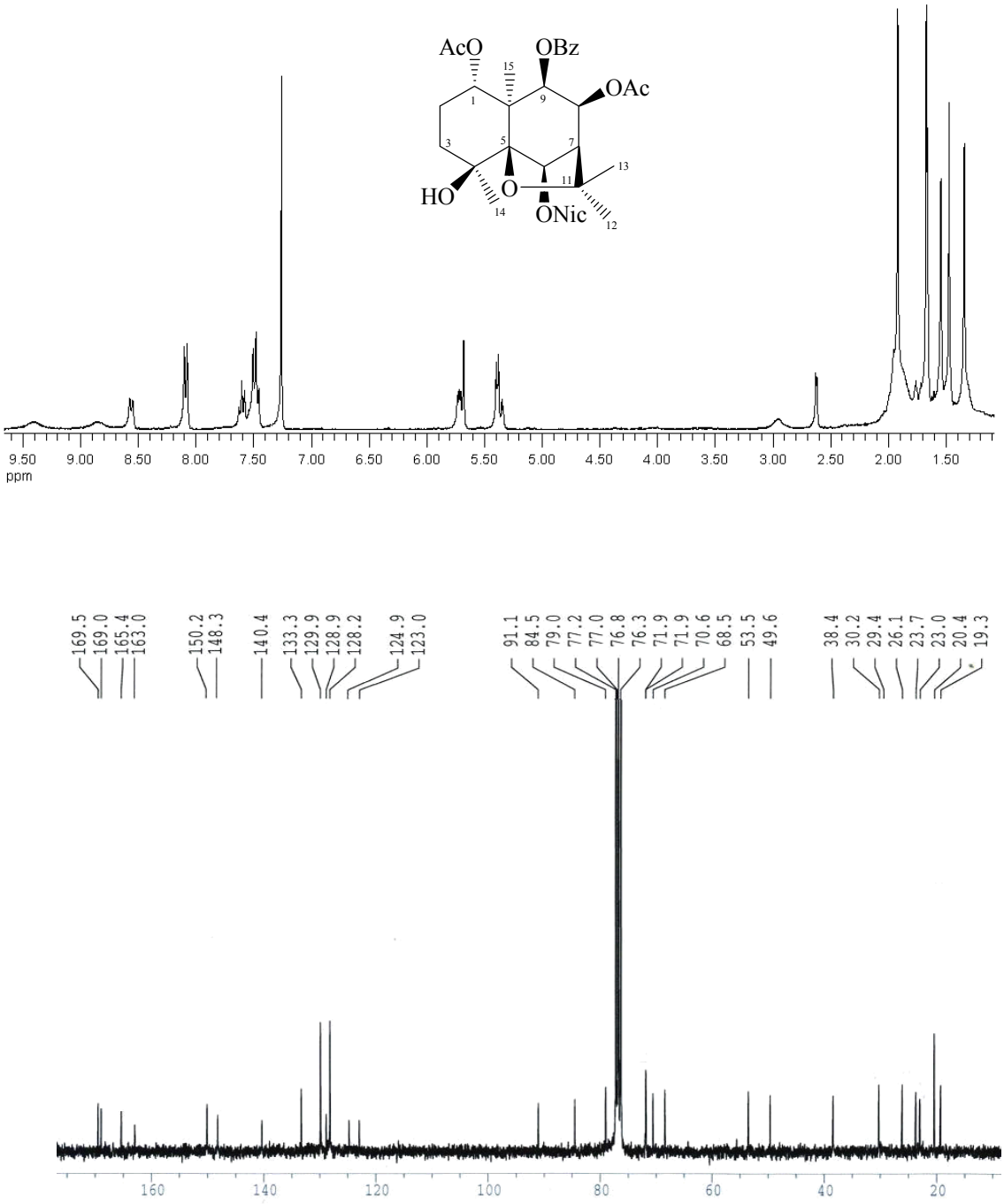


Spectra S2.
^{1}H NMR and ^{13}C NMR spectra of compound **2** (400 MHz, 100 MHz, solvent $CDCl_3$)

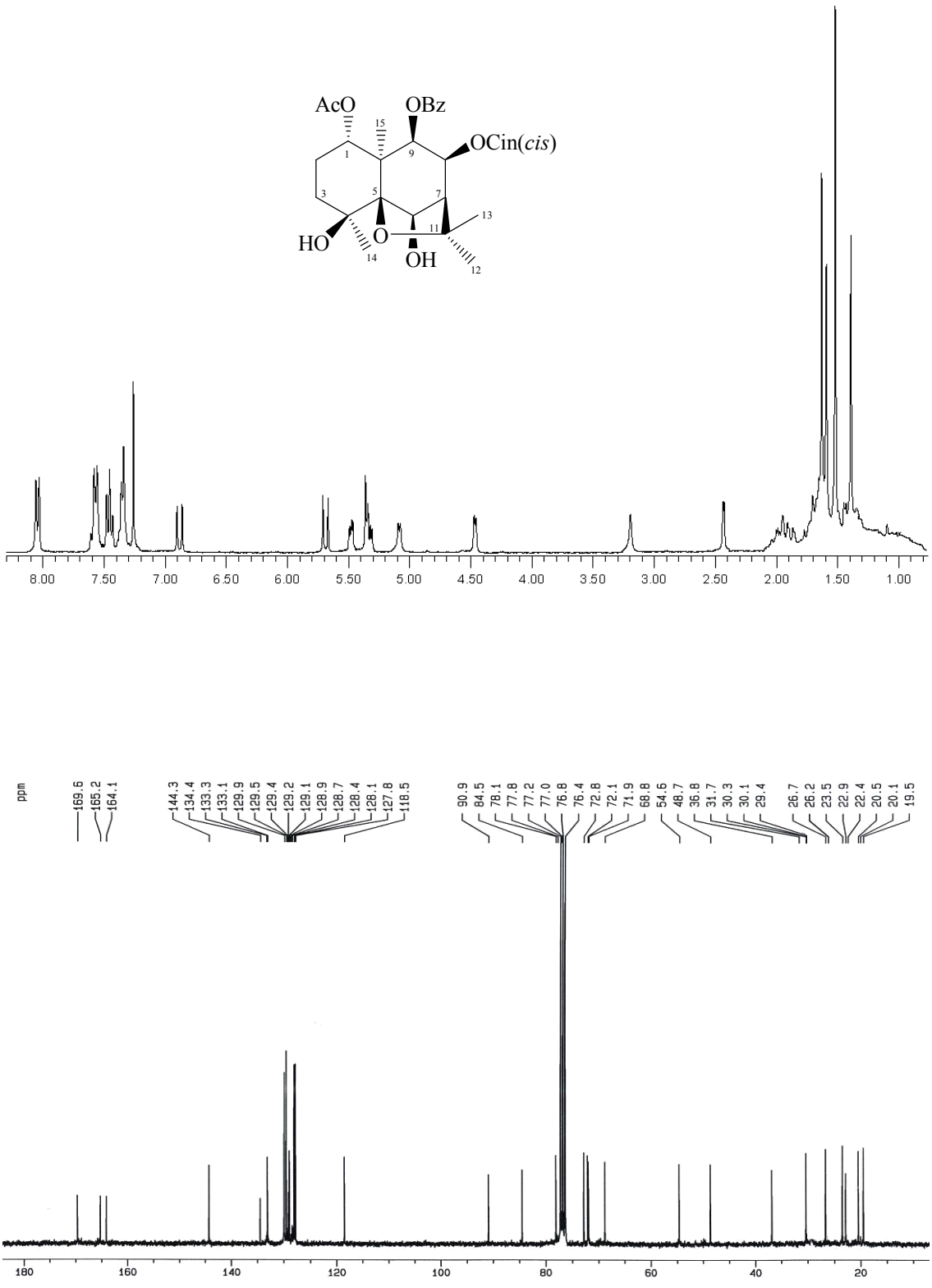




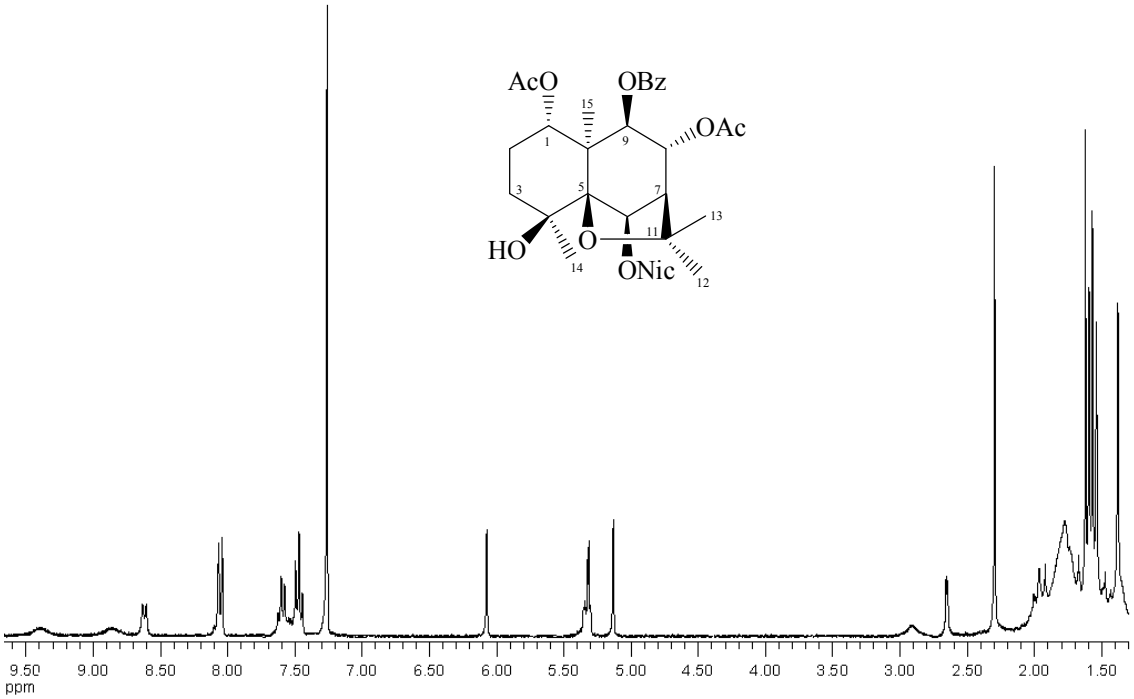
Spectra S3.
^{1}H NMR and ^{13}C NMR spectra of compound **3** (400 MHz, 100 MHz, solvent $CDCl_3$)

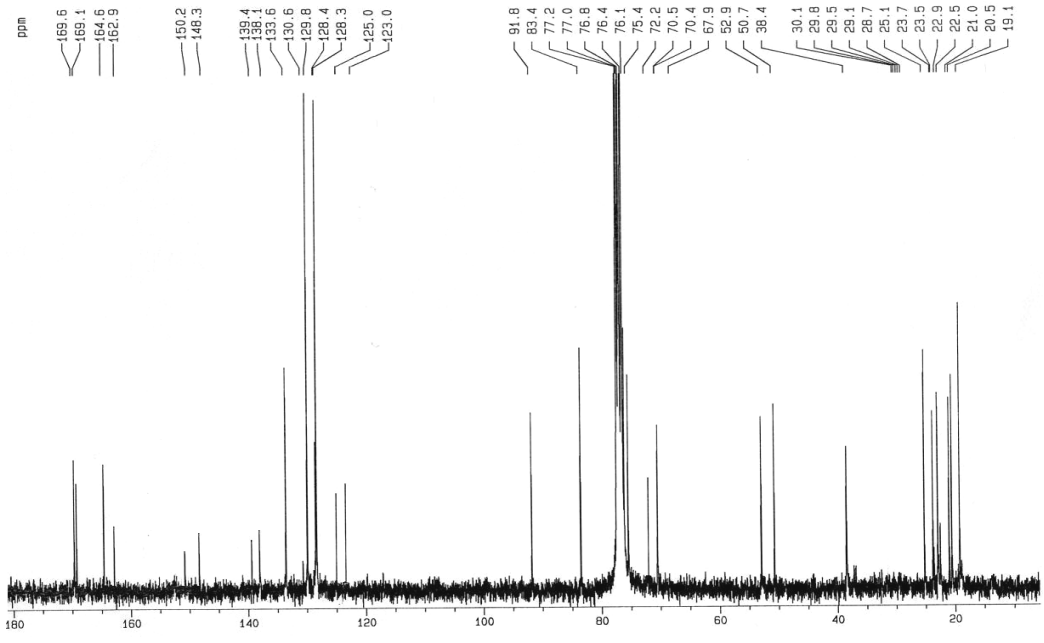


Spectra S4.
^{1}H NMR and ^{13}C NMR spectra of compound **4** (400 MHz, 100 MHz, solvent $CDCl_3$)

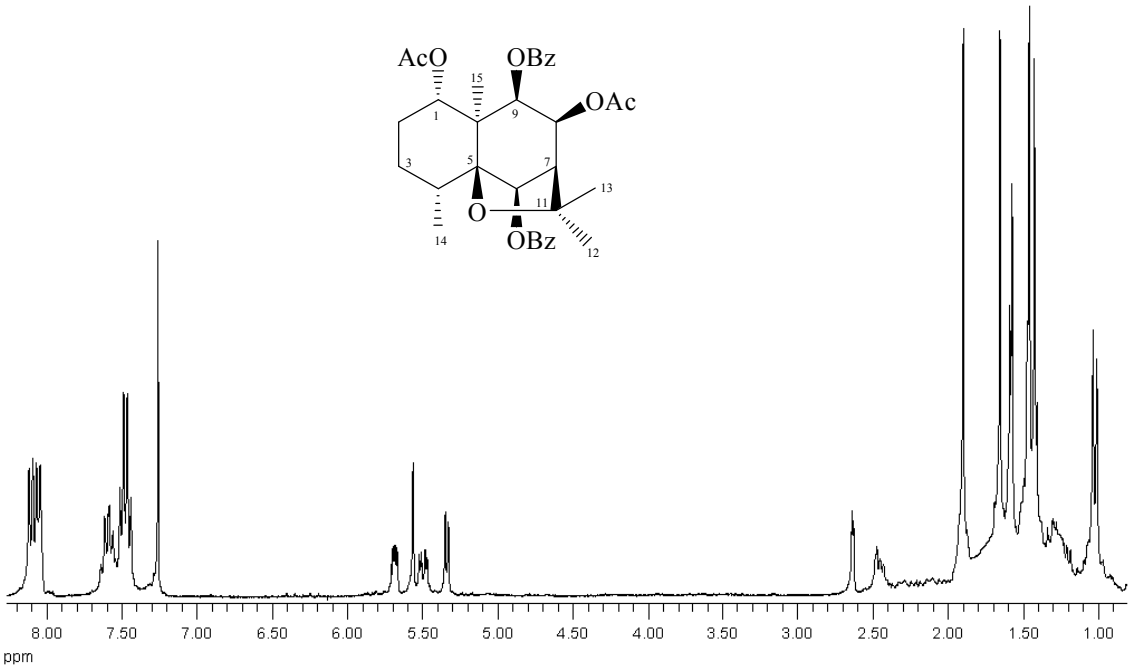


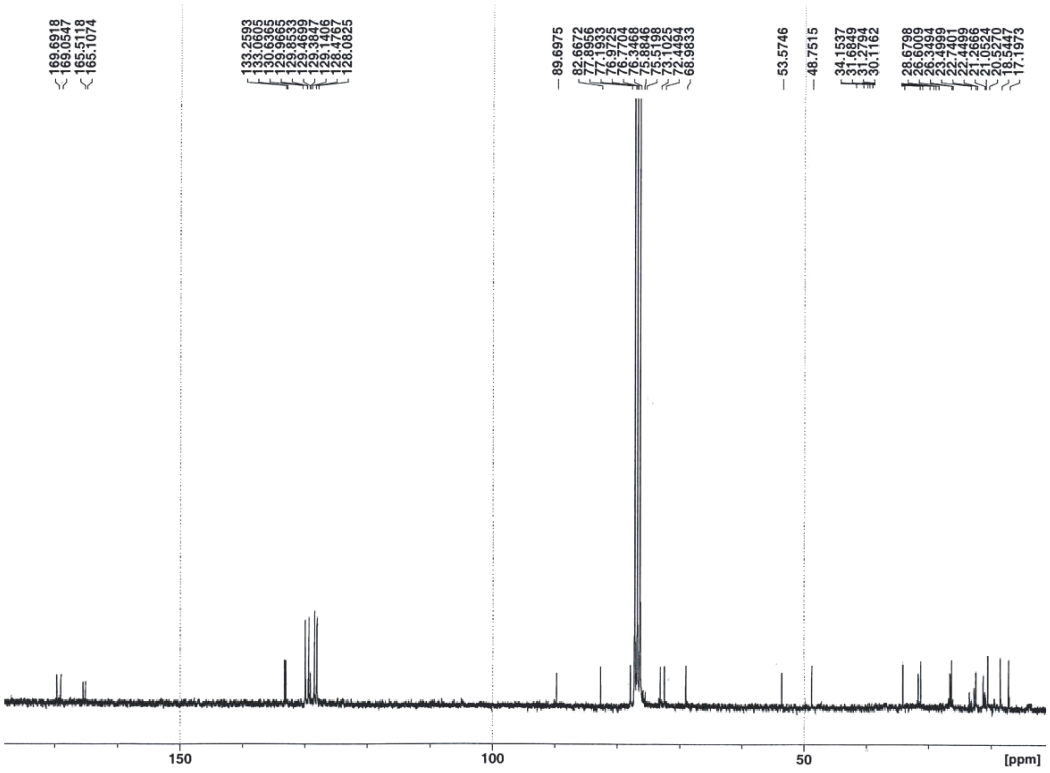
Spectra S5.
^{1}H NMR and ^{13}C NMR spectra of compound **5** (400 MHz, 100 MHz, solvent $CDCl_3$)



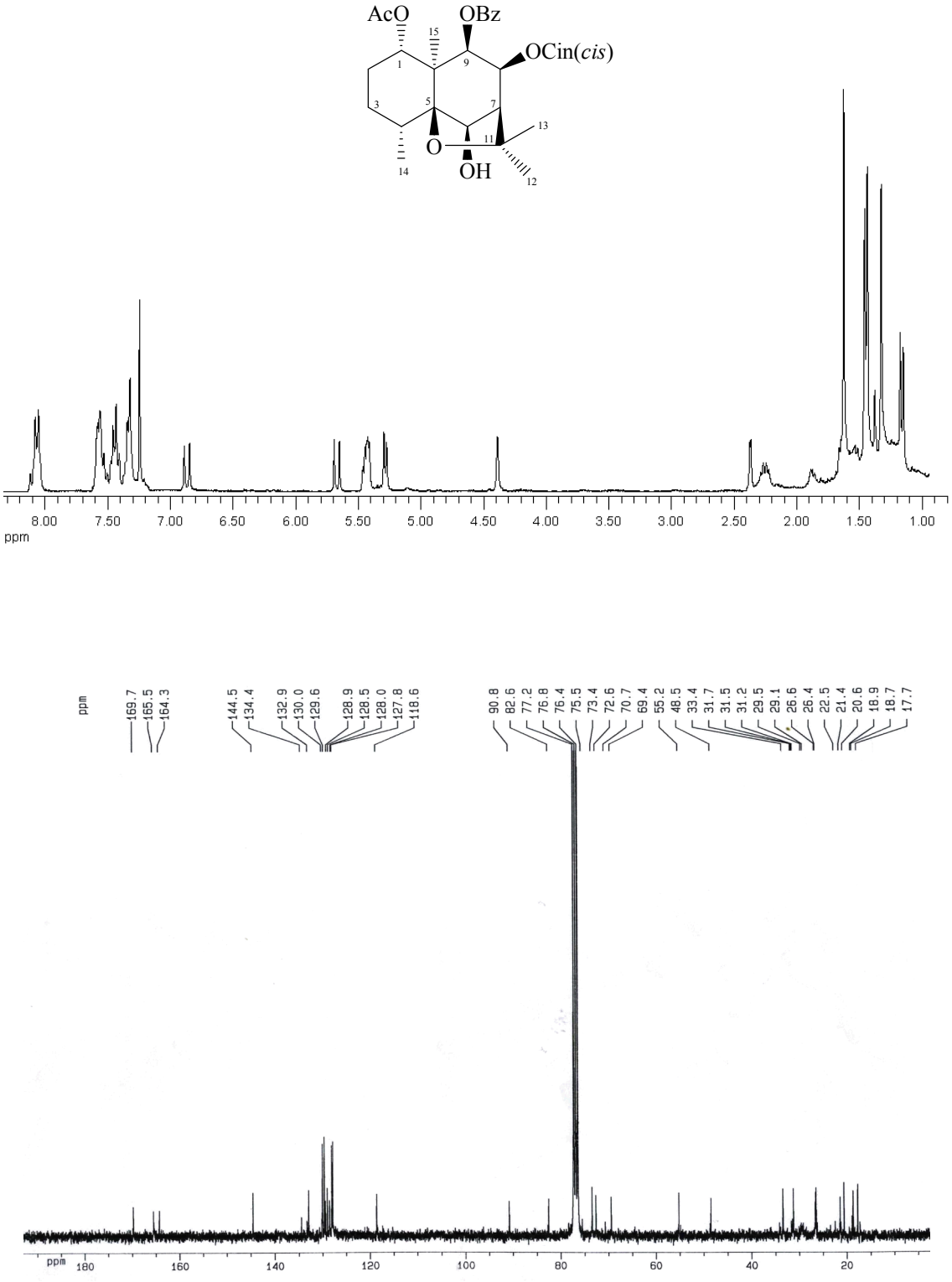


Spectra S6.
^{1}H NMR and ^{13}C NMR spectra of compound **9** (400 MHz, 100 MHz, solvent $CDCl_3$)

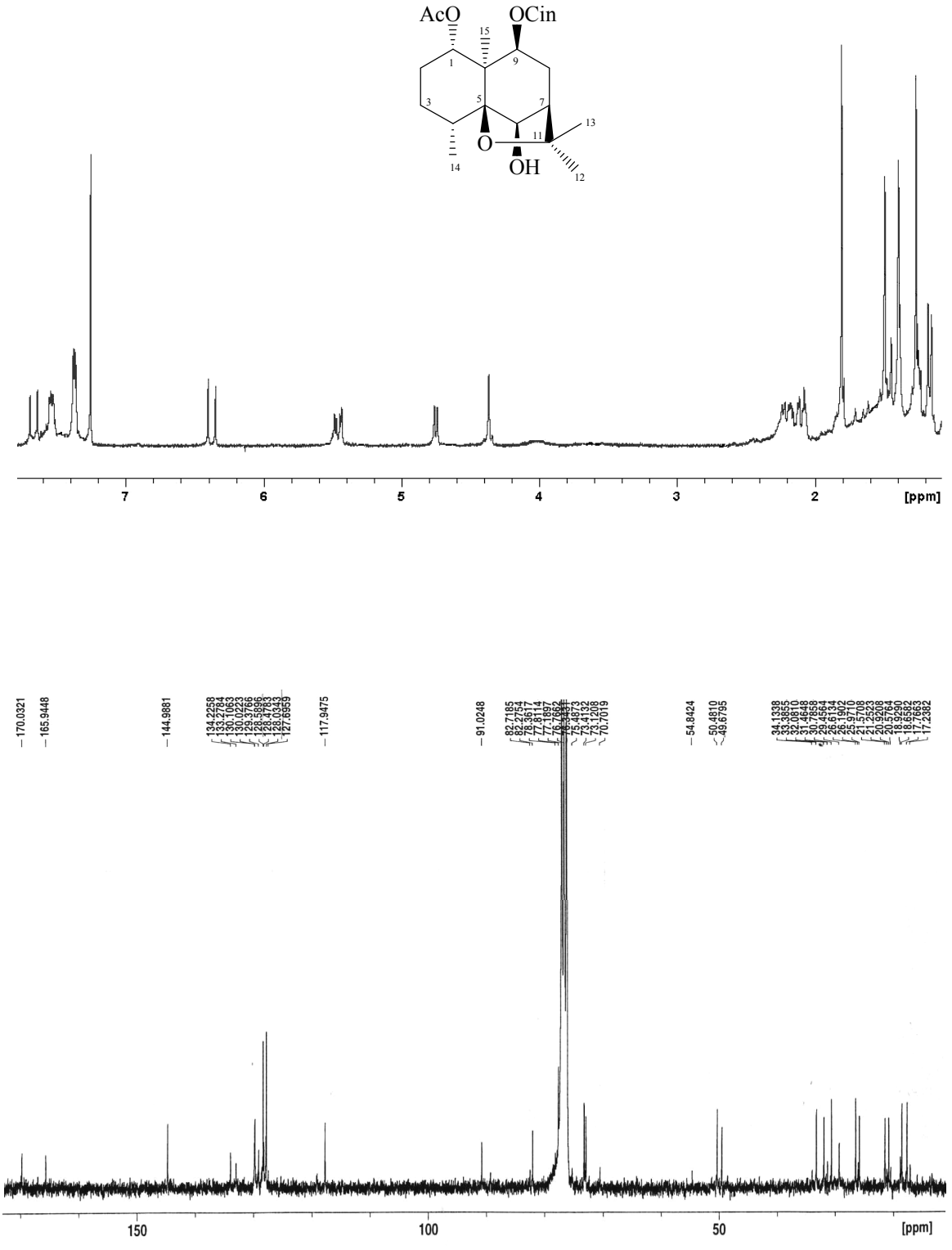




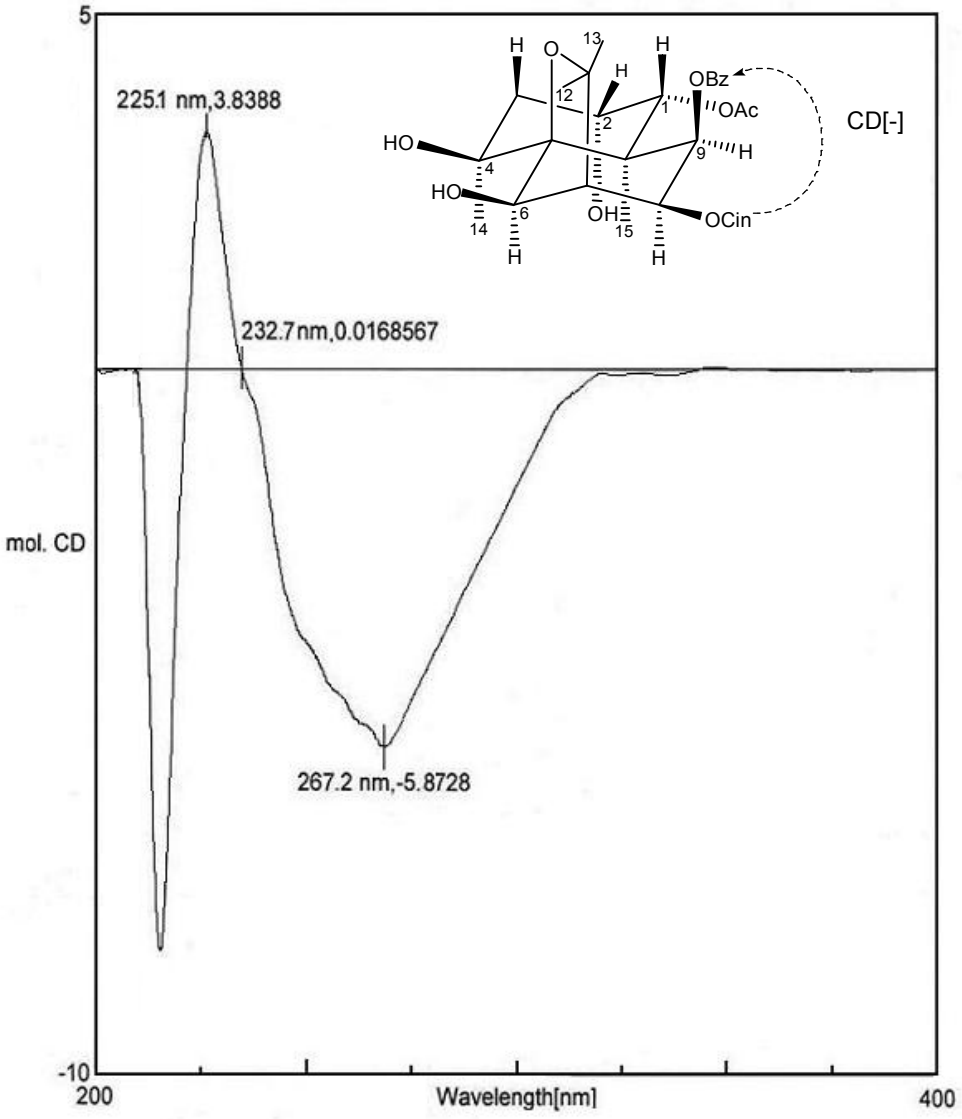
Spectra S7.
^{1}H NMR and ^{13}C NMR spectra of compound **10** (400 MHz, 100 MHz, solvent $CDCl_3$)



Spectra S8.
^{1}H NMR and ^{13}C NMR spectra of compound **11** (400 MHz, 100 MHz, solvent $CDCl_3$)



Spectra S9.
^{1}H NMR and ^{13}C NMR spectra of compound **13** (400 MHz, 100 MHz, solvent $CDCl_3$)



Spectrum S10.
Circular Dichroism curve of compound **1**

Purity criteria for target compounds. The degree of purity of the new compompouds was over 95% as indicated by the appearance of a single peak using HPLC (Varian apparatus equiped with a Prostar 335 Photodiode Array detector, using an analytical Ascetis Si colum (5 μm) with a flow rate of 0.5 mL/min).

Compound **1**: Hexane/ EtOAc 45:55 with R_t 12.23

Compound **2**: Hexane/ EtOAc 50:50 with R_t 14.46

Compound **3**: Hexane/ EtOAc 50:50 with R_t 10:35

Compound **4**: Hexane/ EtOAc 50:50 with R_t 11.57

Compound **5**: Hexane/ EtOAc 48:52 with R_t 12.19

Compound **9**: Hexane/ EtOAc 50:50 with R_t 12.56

Compound **10**: Hexane/ EtOAc 55:45 with R_t 9.46

Compound **11**: Hexane/ EtOAc 52:48 with R_t 10.37

Compound **13**: Hexane/ EtOAc 60:40 with R_t 11.38

In addition, the analytical data for determining the degree of purity for the new compounds included ^{1}H and ^{13}C NMR spectra.