

Heteropoly acid catalysts for the synthesis of fragrance compounds from biorenewables: isomerization of limonene oxide

Vinícius V. Costa,^a Kelly A. da Silva Rocha,^b Ivan V. Kozhevnikov,^c Elena F. Kozhevnikova^c
and Elena V. Gusevskaya*^a

^a Departamento de Química, Universidade Federal de Minas Gerais 31270-901, Belo Horizonte, MG, Brazil. Fax: (+)55 31 34095700; Tel:

(+)55 31 34095741. E-mail: elena@ufmg.br

^b Departamento de Química, Universidade Federal de Ouro Preto, 35400-000, Ouro Preto, MG, Brazil

^c Department of Chemistry, University of Liverpool, Liverpool L69 7ZD, UK.

Supplementary Information

Table of contents

Catalyst characterization data-----S2

Product characterization data -----S3-S7

Catalyst characterization data

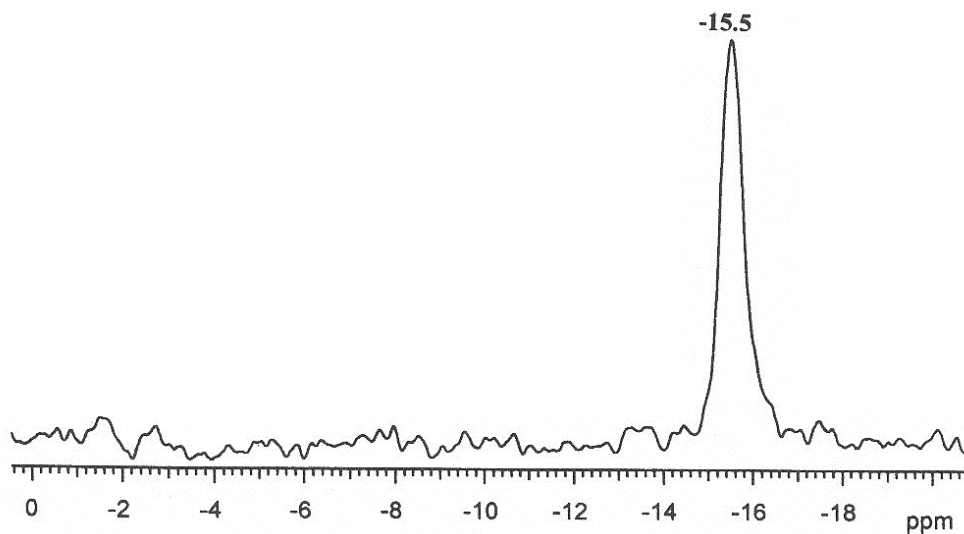


Fig. S1. ^{31}P MAS NMR spectrum for 20% $\text{H}_3\text{PW}_{12}\text{O}_{40}/\text{SiO}_2$.

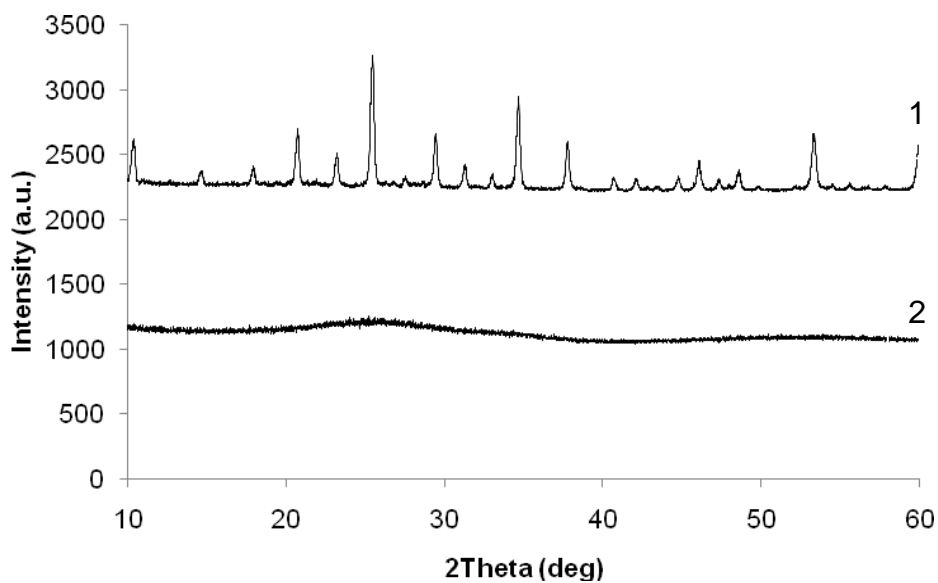


Fig. S2. XRD patterns for $\text{H}_3\text{PW}_{12}\text{O}_{40}$ (1) and 20% $\text{H}_3\text{PW}_{12}\text{O}_{40}/\text{SiO}_2$ (2).

The acid properties of the catalysts under study ($\text{H}_3\text{PW}_{12}\text{O}_{40}$, $\text{H}_3\text{PW}_{12}\text{O}_{40}/\text{SiO}_2$ and $\text{Cs}_{2.5}\text{H}_{0.5}\text{PW}_{12}\text{O}_{40}$) have been discussed in detail elsewhere,^{35,36} including the number and the nature of acid sites and their strength.

Product characterization data

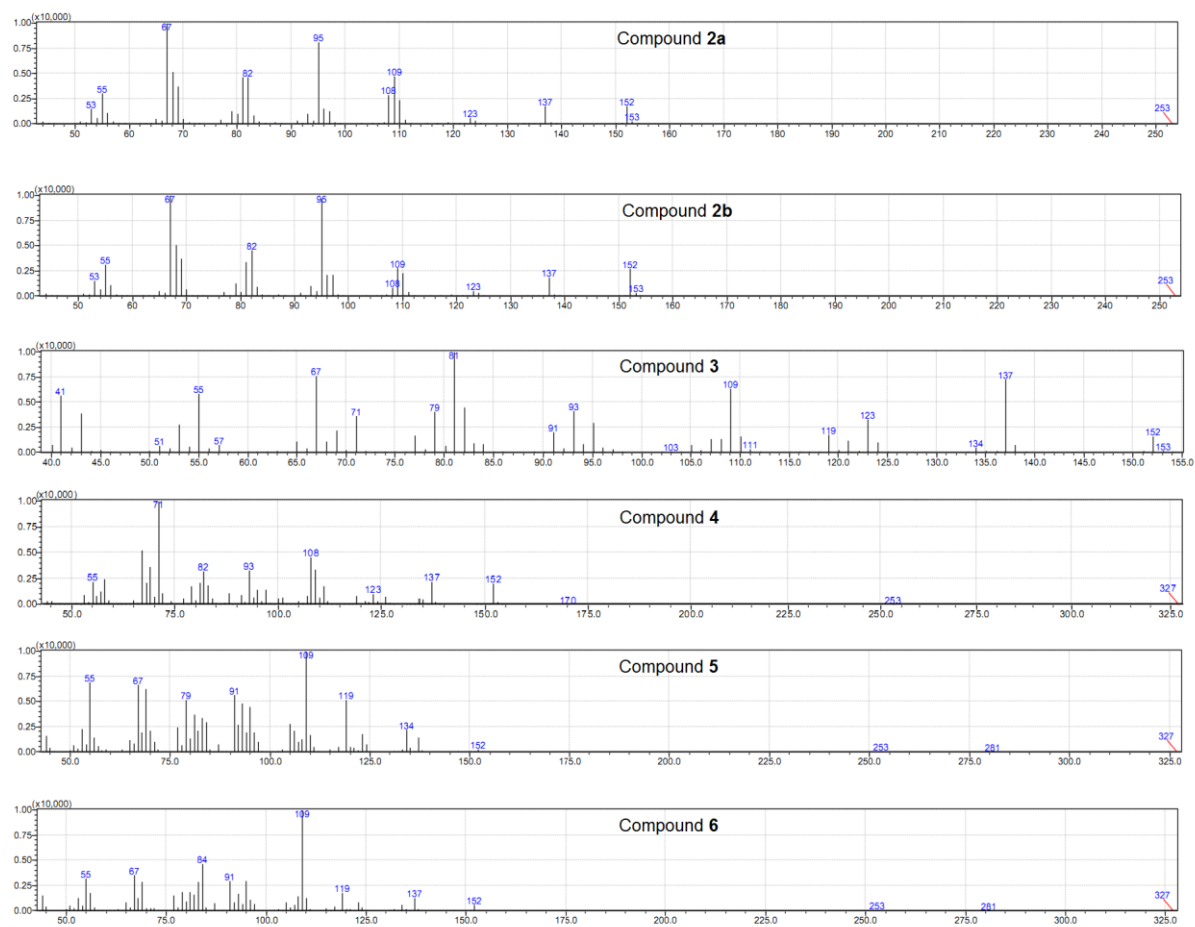


Fig. S3. Mass spectra of compounds **2a**, **2b**, **3**, **4**, **5** and **6** (the structures are shown on Scheme 1).

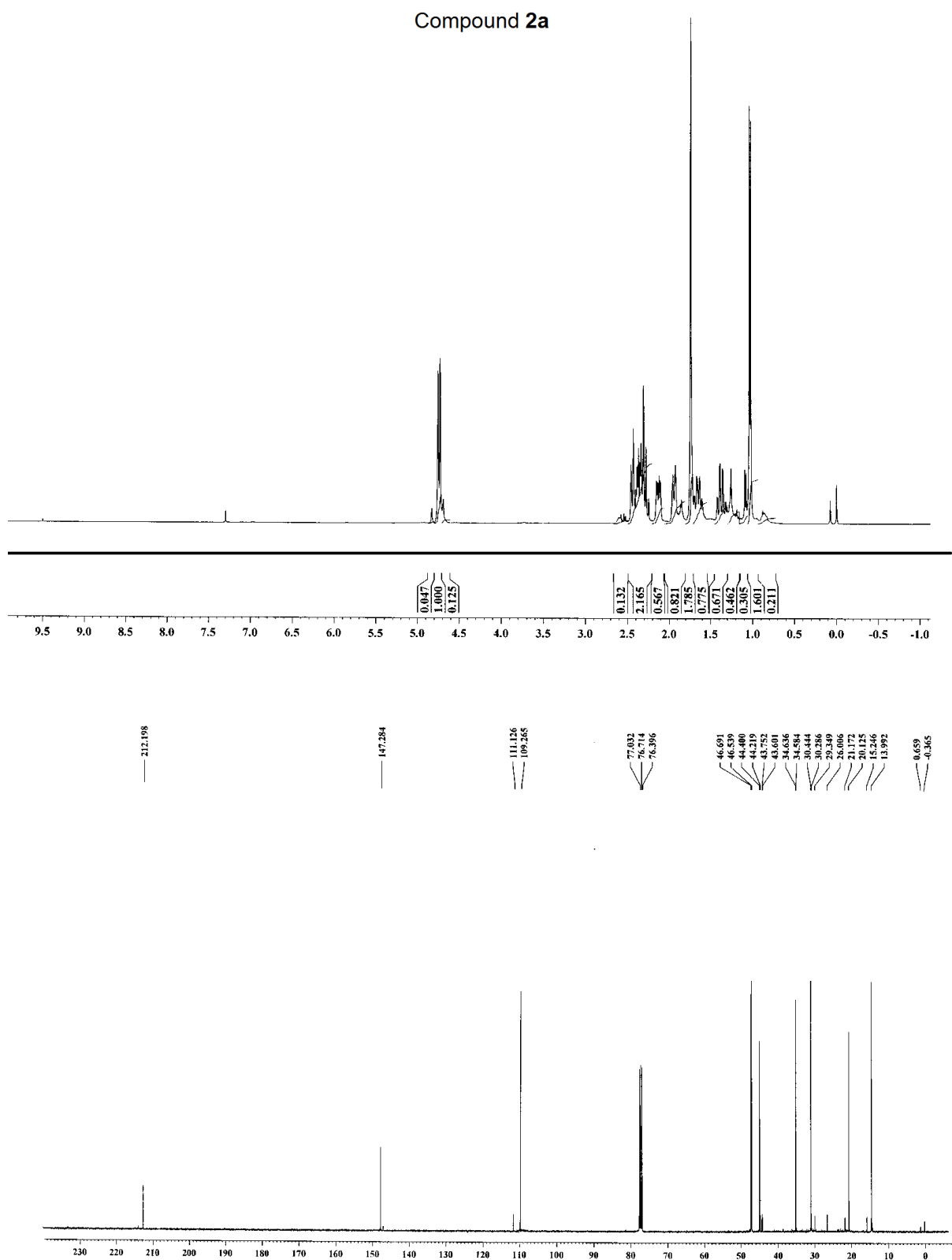


Fig. S4. ^1H and ^{13}C spectra of compound 2a.

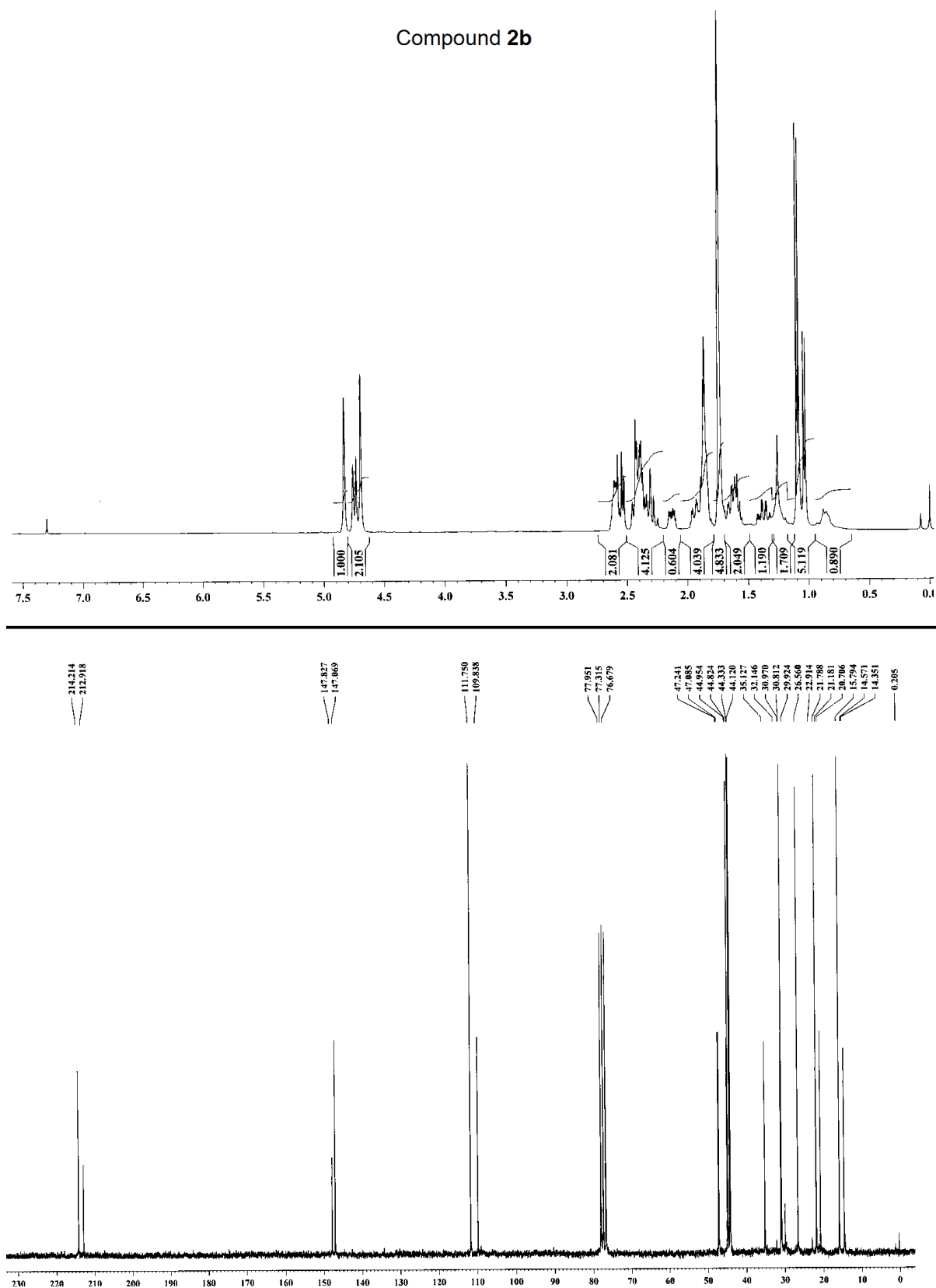


Fig. S5. ¹H and ¹³C spectra of compound **2b** (the solution also contains **2a**: **2a/2b** \approx 1/2).

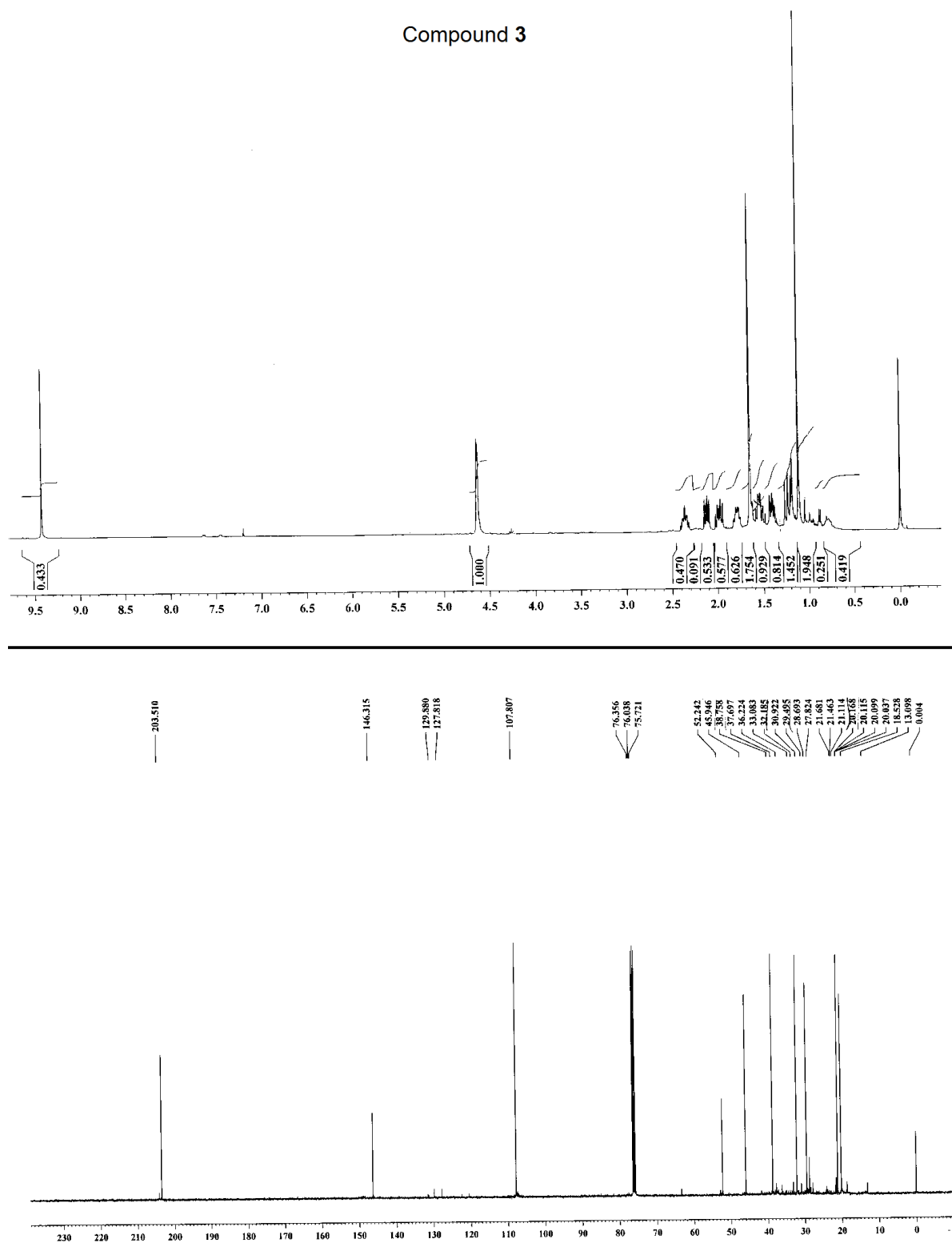


Fig. S6. ¹H and ¹³C spectra of compound 3.

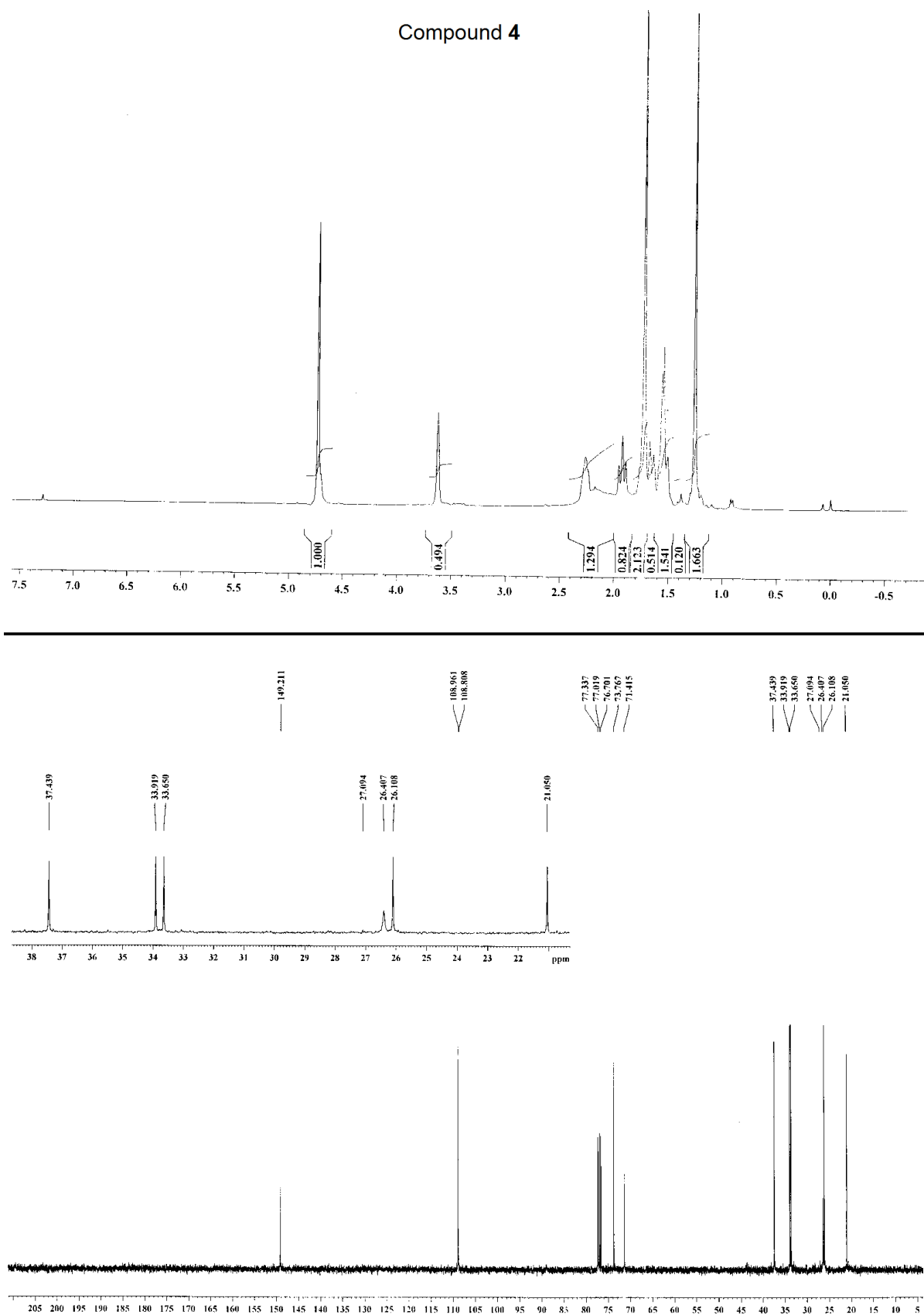


Fig. S7. ¹H and ¹³C spectra of compound 4.