New cassane diterpenoids from *Caesalpinia sappan* and their antiplasmodial activity

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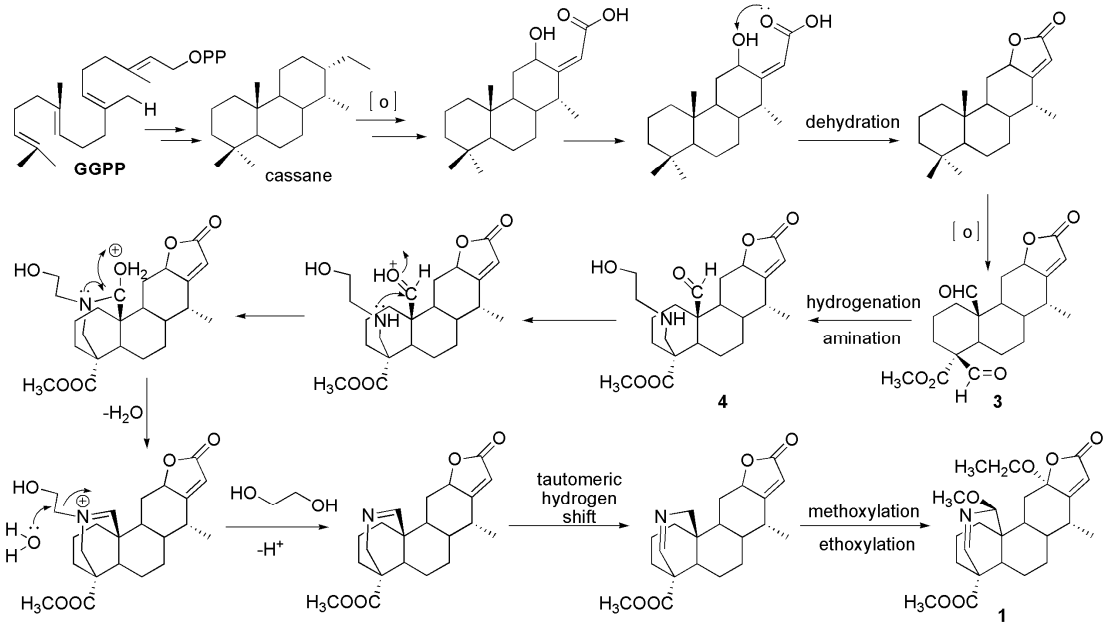
Abstract: One new cassane diterpene possessing unusual *N* bridge between C-19 and C-20 named caesalsappanin R (**1**) together with another new diterpene caesalsappanin S (**2**) were isolated from the seeds of *Caesalpinia sappan* with methanol extract. Their structures were determined by spectroscopic analysis and examined alongside existing data from prior studies. Their biological activities were profiled by the antiplasmodial.
Keywords: *Caesalpinia sappan*; cassane diterpenes; *N* bridge; antiplasmodial activity

1. The plausible biosynthetic pathway of Compound **1**

The key intermediate product **3** was produced from the precursor of geranylgeranyl pyrophosphate (GGPP) by a intramolecular cyclization, followed by oxidation, dehydration, and dehydrogenation reaction. Intermediate product **4** was proposed to be generated from 3 through the amination and hydrogenation reactions with the participation of β-aminoethanol. A plausible biosynthetic pathway to caesalpamide A (**1**) was proposed in detail (Scheme 1).



Scheme 1. Plausible biosynthesis pathway of **1**

Figure S1. ^{1}H-NMR (600 MHz, $CDCl_3$) spectrum of the new compound **1**

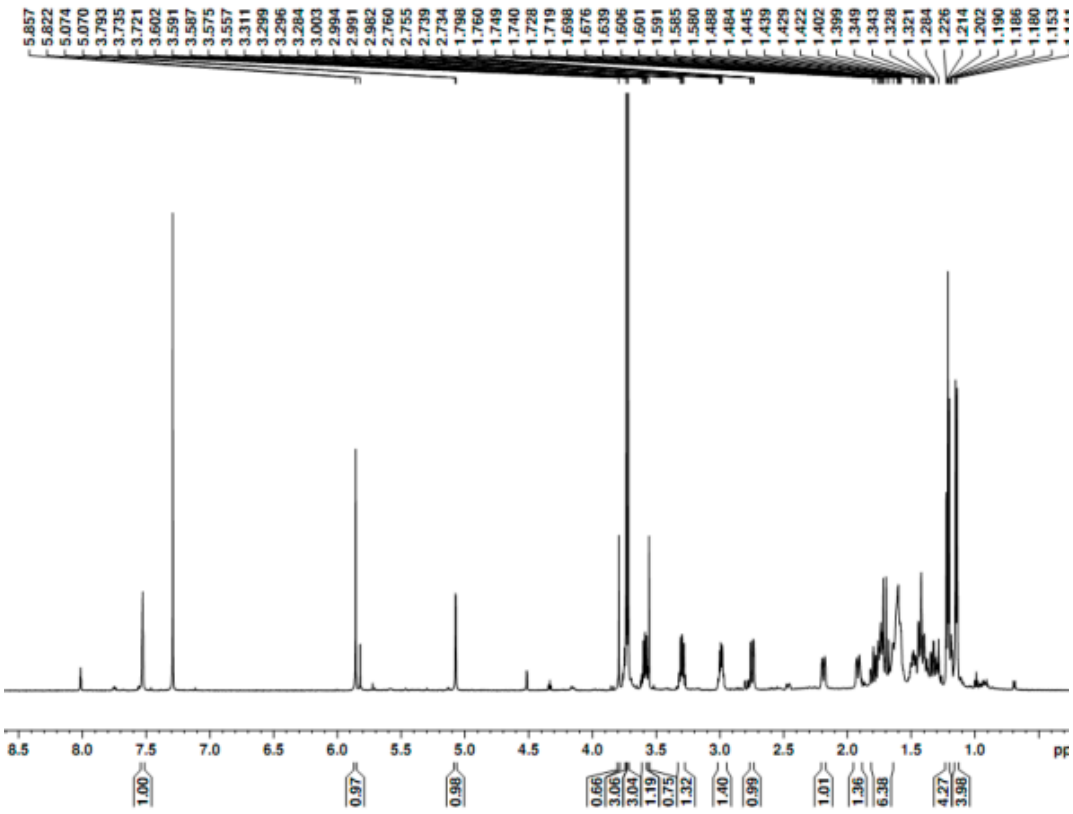


Figure S2. ^{13}C-APT (150 MHz, $CDCl_3$) spectrum of the new compound **1**

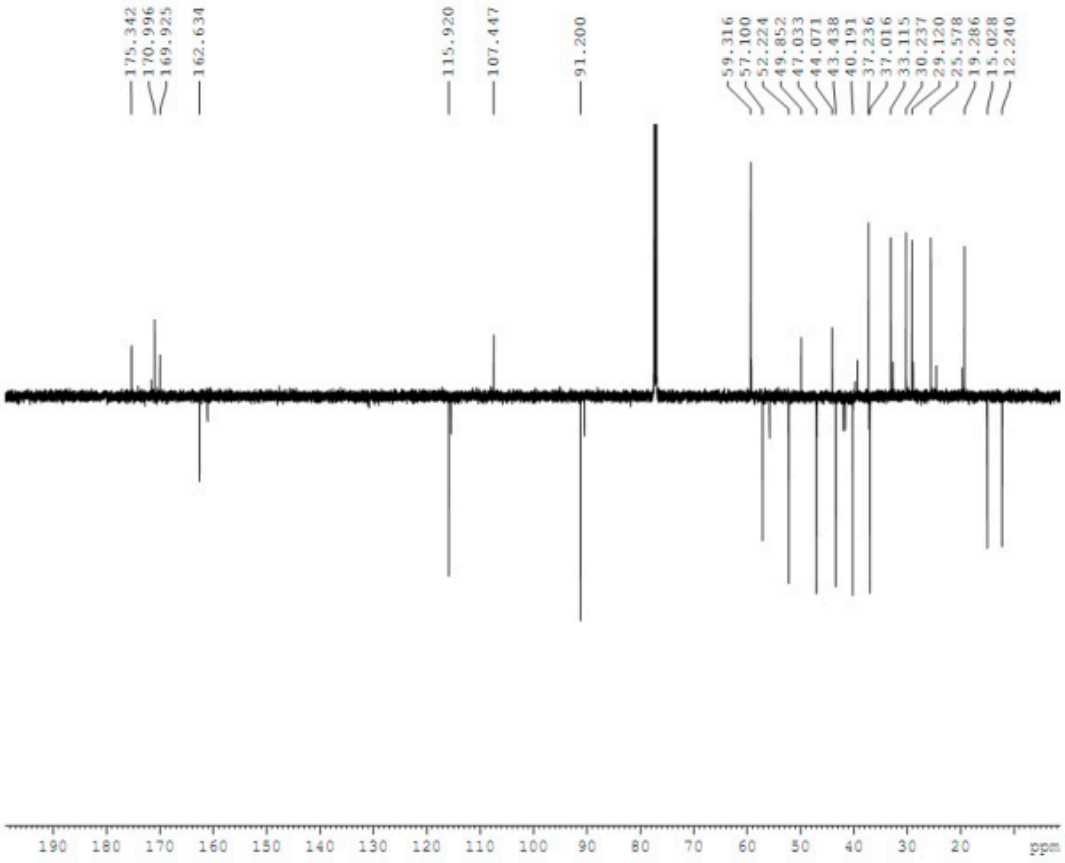


Figure S3. HSQC spectrum of the new compound **1**

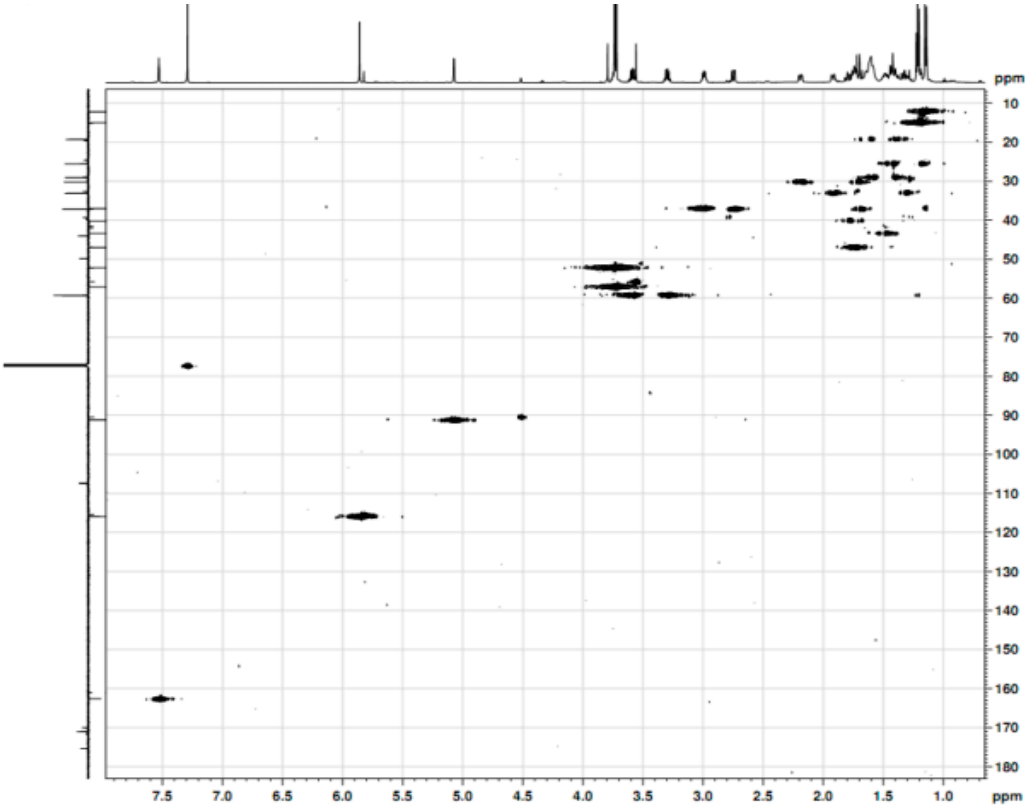


Figure S4. HMBC spectrum of the new compound **1**

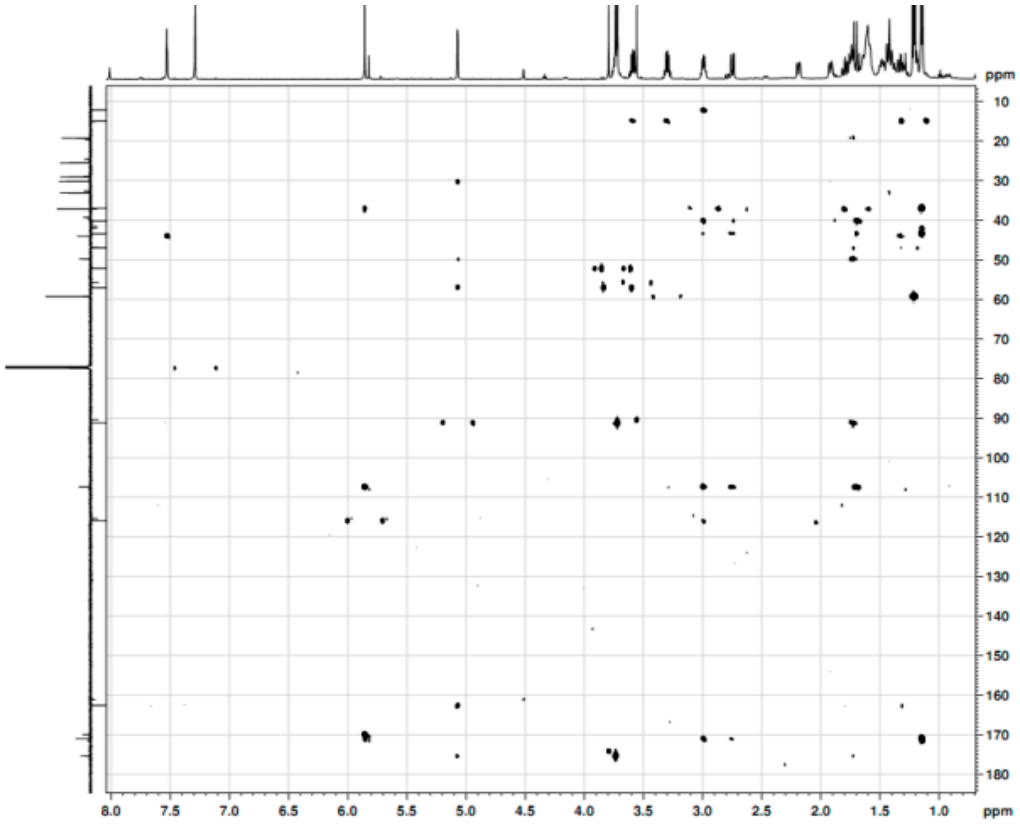


Figure S5. ^{1}H-^{1}H COSY spectrum of the new compound **1**

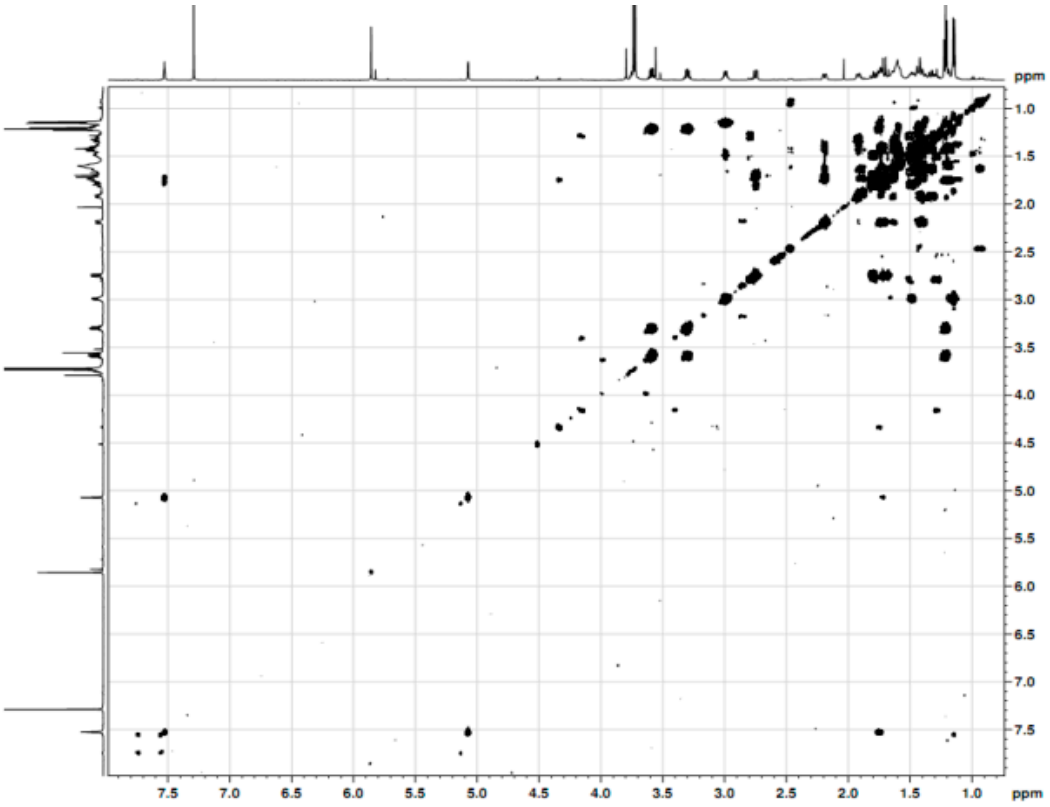


Figure S6. NOESY spectrum of the new compound **1**

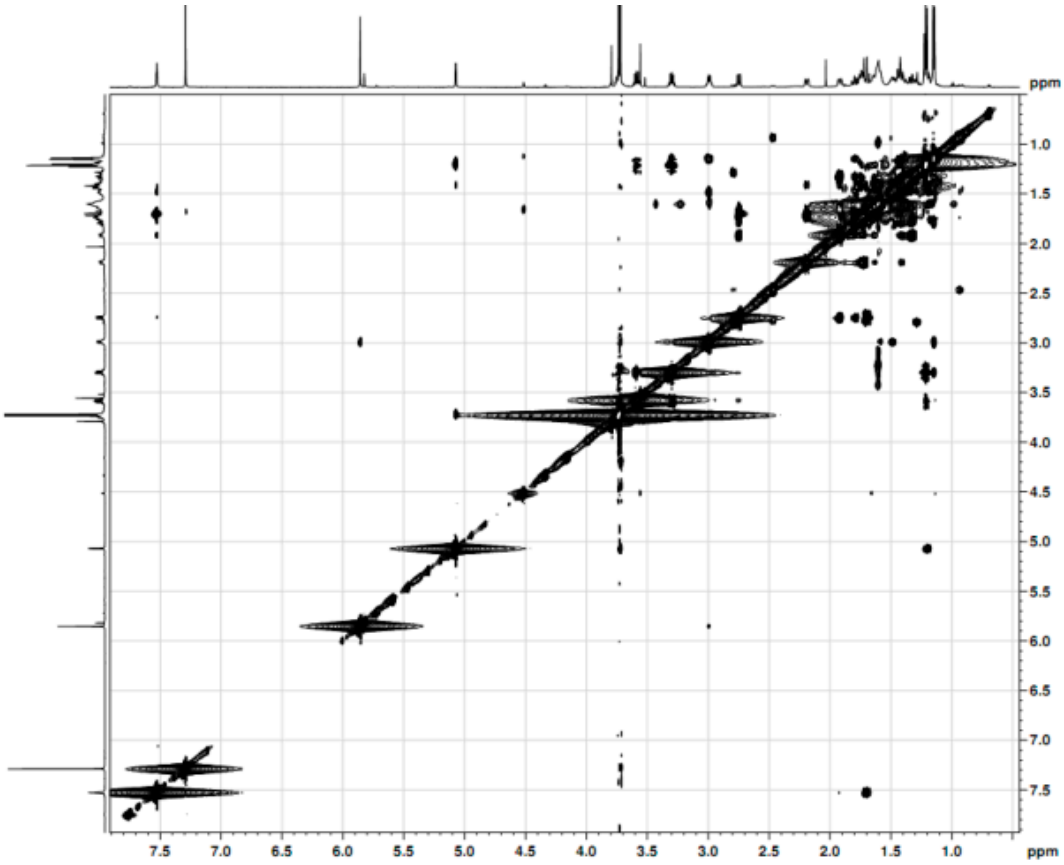


Figure S7. ^{1}H-NMR (600 MHz, $CDCl_3$) spectrum of the new compound **2**

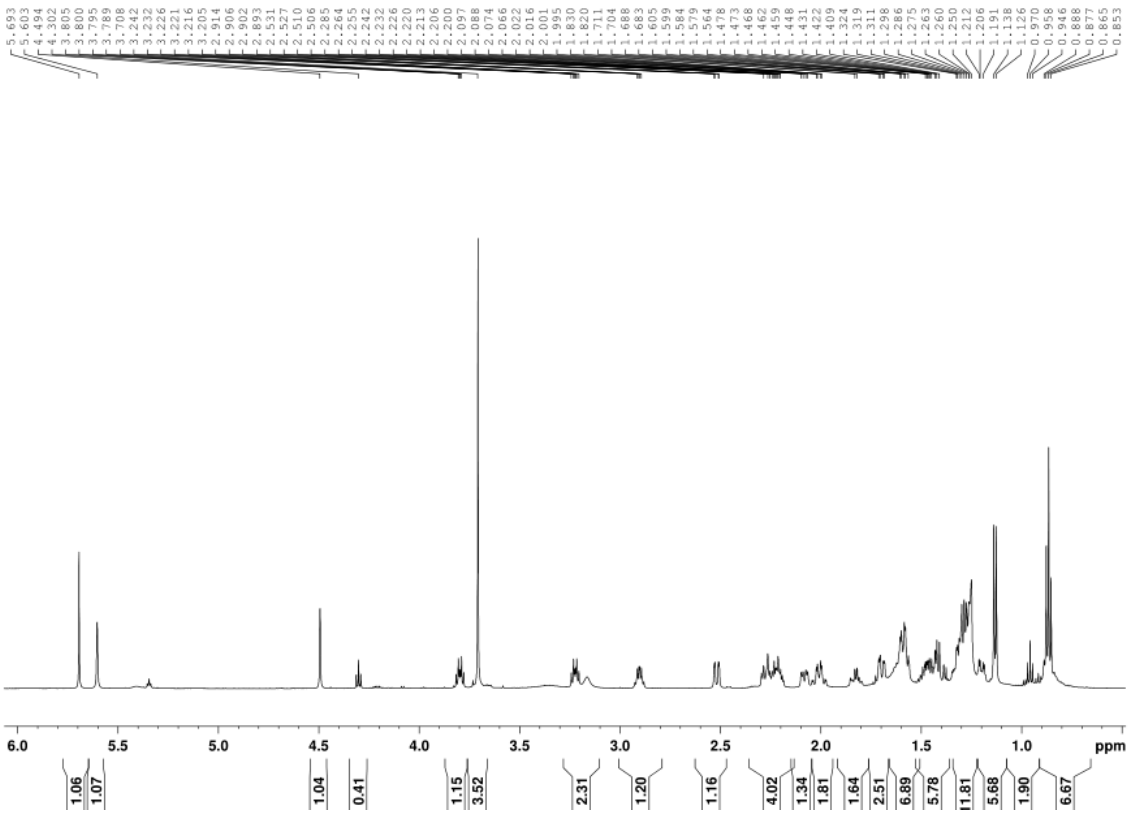


Figure S8. ^{13}C-APT (150 MHz, $CDCl_3$) spectrum of the new compound **2**

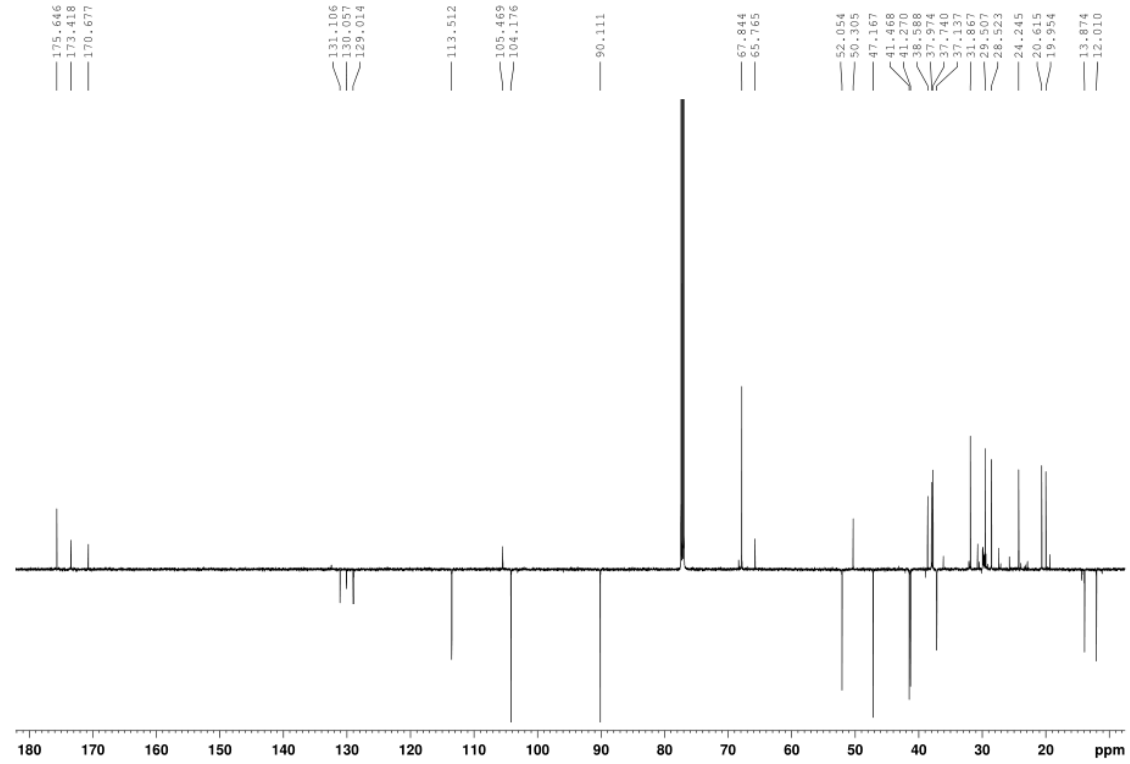


Figure S9. HSQC spectrum of the new compound **2**

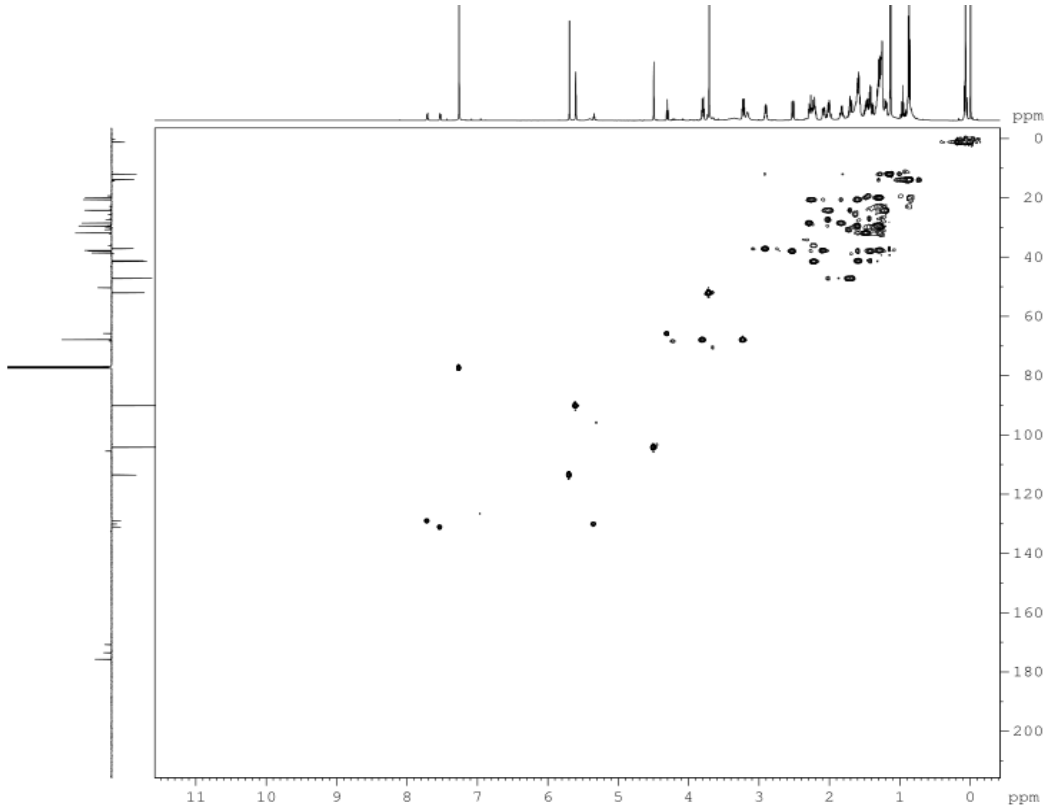


Figure S10. HMBC spectrum of the new compound **2**

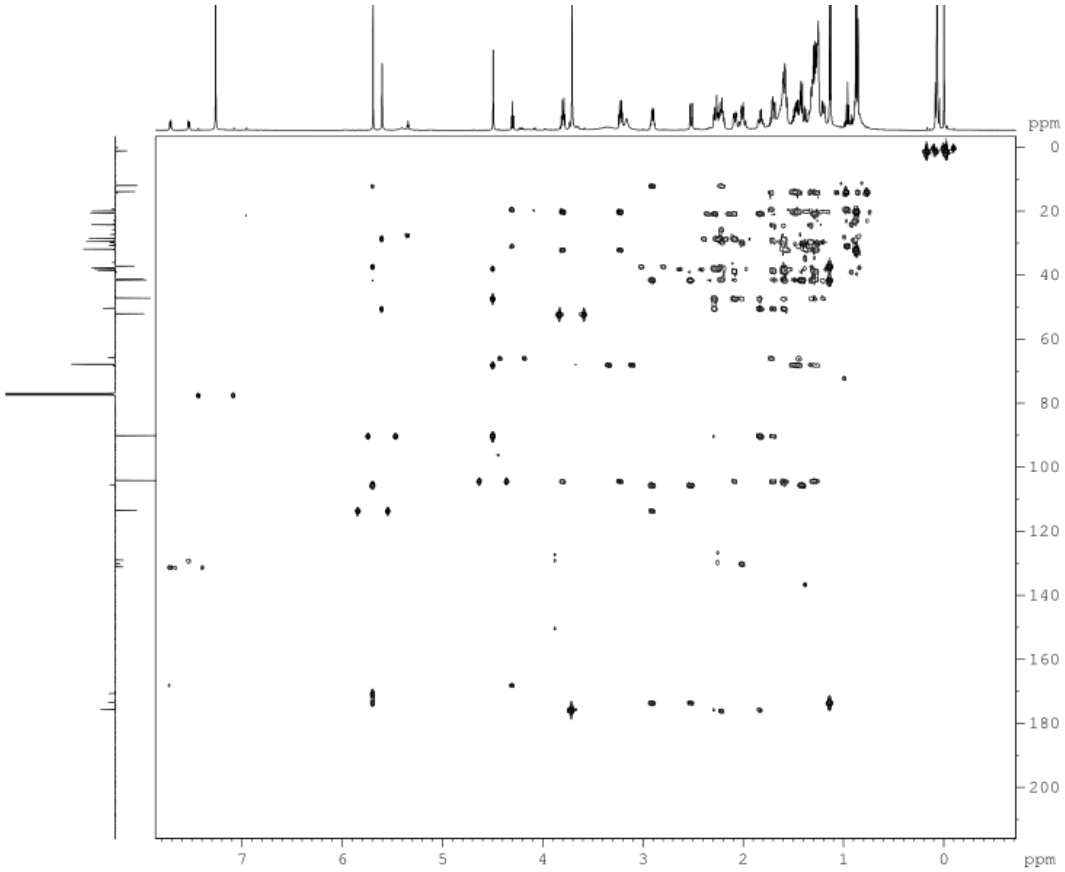


Figure S11. ^{1}H-^{1}H COSY spectrum of the new compound **2**

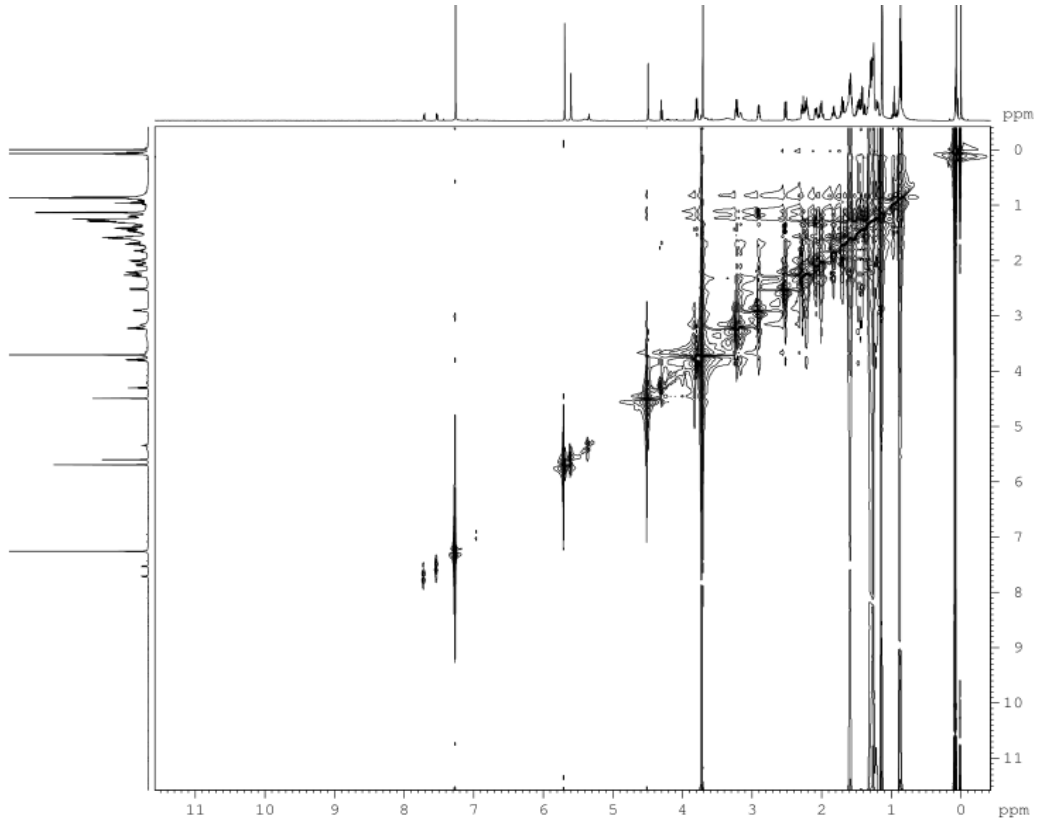


Figure S12. NOESY spectrum of the new compound **2**