

ent-KAURANE DITERPENOIDS AND OTHER CONSTITUENTS FROM THE STEM OF *Xylopia laevigata* (ANNONACEAE)

Dayanne Meneses Silva, Emmanoel Vilaca Costa*, Paulo Cesar de Lima Nogueira e Valéria Regina de Souza Moraes

Departamento de Química, Universidade Federal de Sergipe, Av. Mal. Rondon, s/n, 49100-000 São Cristóvão – SE, Brasil

Sócrates Cabral de Holanda Cavalcanti

Departamento de Farmácia, Universidade Federal de Sergipe, Av. Mal. Rondon, s/n, 49100-000 São Cristóvão – SE, Brasil

Marcos José Salvador

Curso de Farmácia, Departamento de Biologia Vegetal, Instituto de Biologia, Universidade Estadual de Campinas, CP 6109, 13083-970 Campinas – SP, Brasil

Luis Henrique Gonzaga Ribeiro e Fernanda Ramos Gadelha

Departamento de Bioquímica, Instituto de Biologia, Universidade Estadual de Campinas, CP 6109, 13083-970 Campinas – SP, Brasil

Andersson Barison

Departamento de Química, Universidade Federal do Paraná, CP 19081, 81531-990 Curitiba – PR, Brasil

Antonio Gilberto Ferreira

Departamento de Química, Universidade Federal de São Carlos, CP 676, 13565-905 São Carlos – SP, Brasil

Department of Quantum Mathematics and Physics, SISSA, Trieste, Italy and Istituto Nazionale di Fisica Nucleare, Sezione di Trieste, Italy

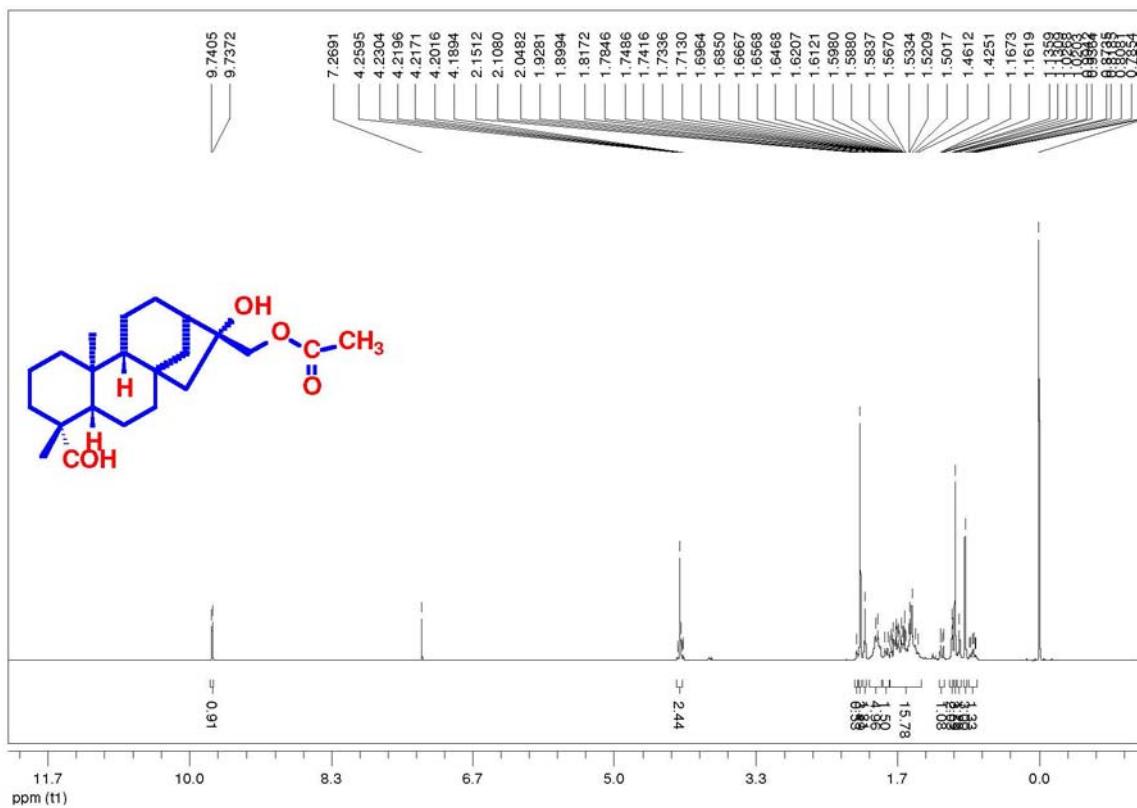


Figure 1S. ^1H NMR spectrum of *ent*-16 β -hydroxy-17-acetoxy-kauran-19-al (**7**) in CDCl_3 at 400 MHz

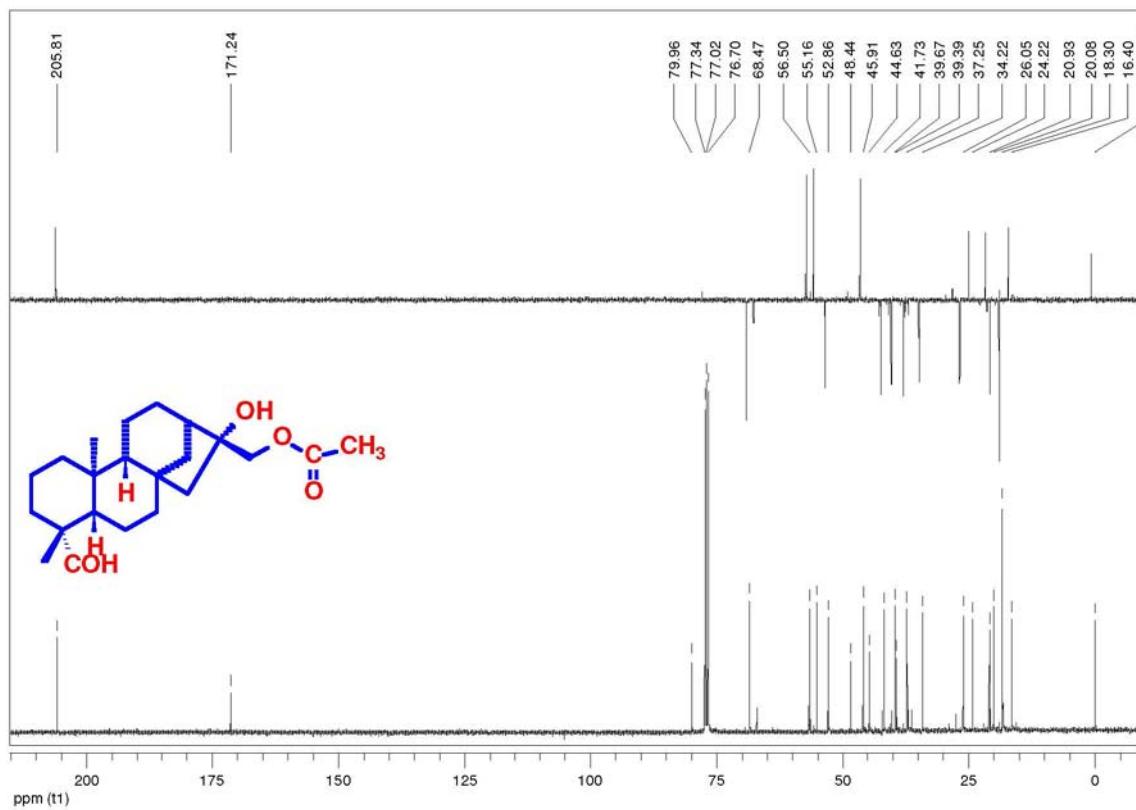


Figure 2S. $^{13}\text{C}\{^1\text{H}\}$ and DEPT 135 NMR spectra of *ent*-16 β -hydroxy-17-acetoxy-kauran-19-al (7) in CDCl_3 at 100 MHz

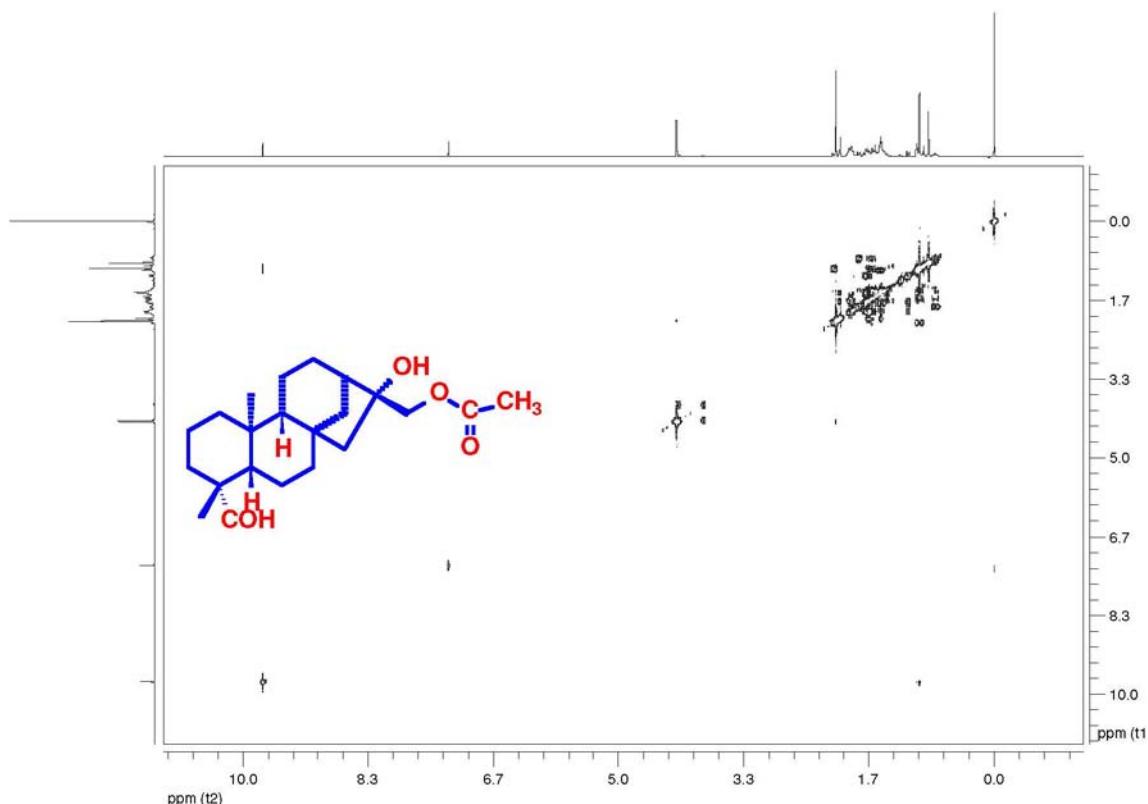
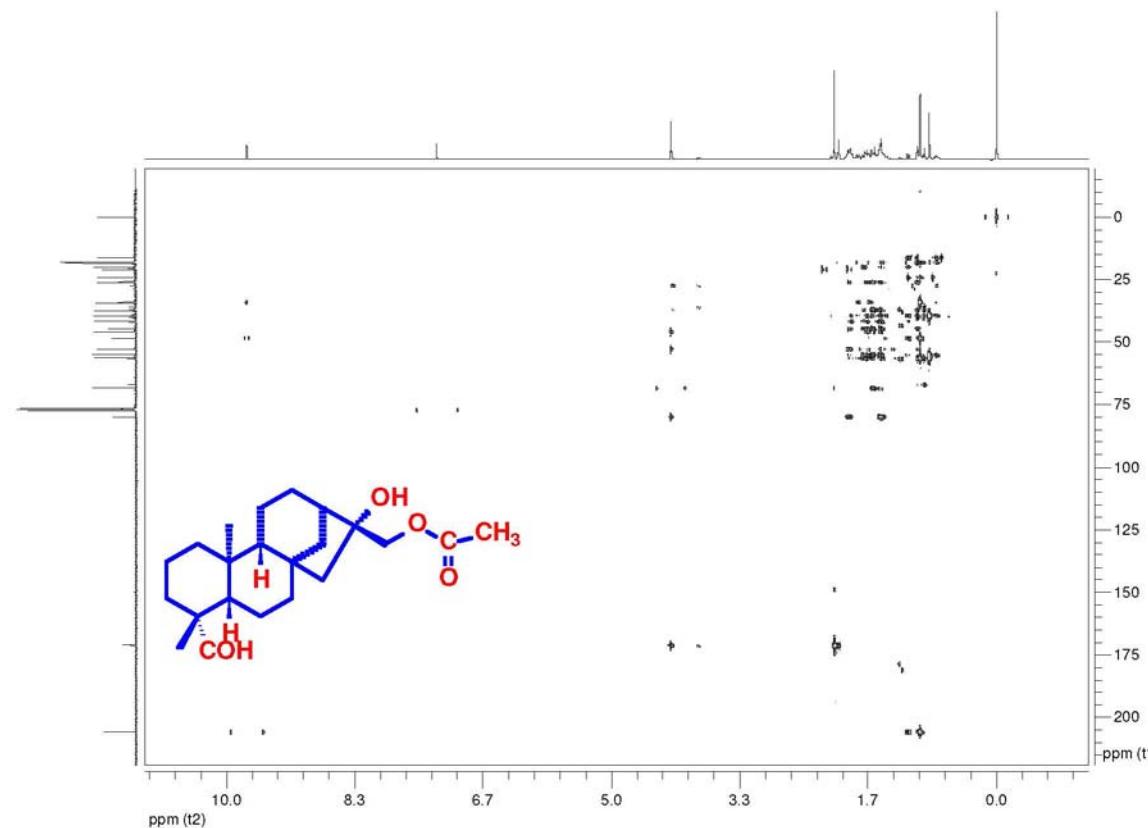
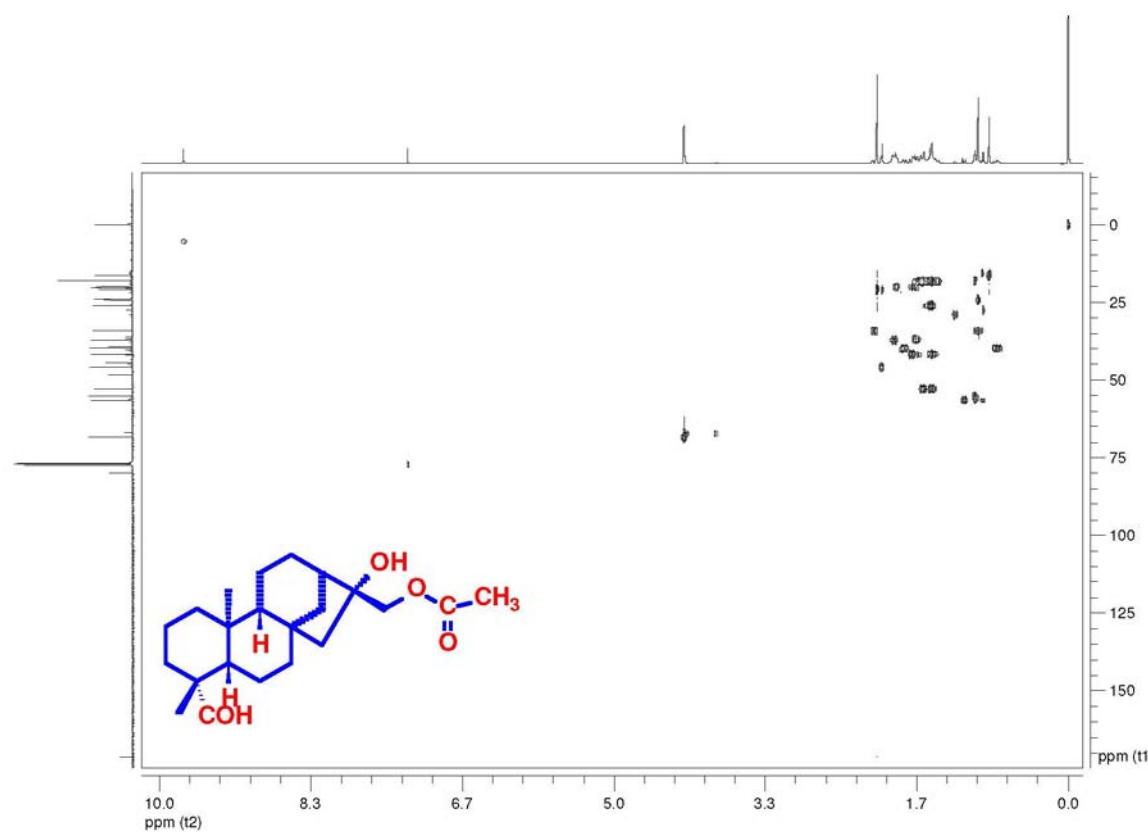


Figure 3S. ^1H - ^1H correlation map from COSY NMR experiment of *ent*-16 β -hydroxy-17-acetoxy-kauran-19-al (7) in CDCl_3 at 400 MHz



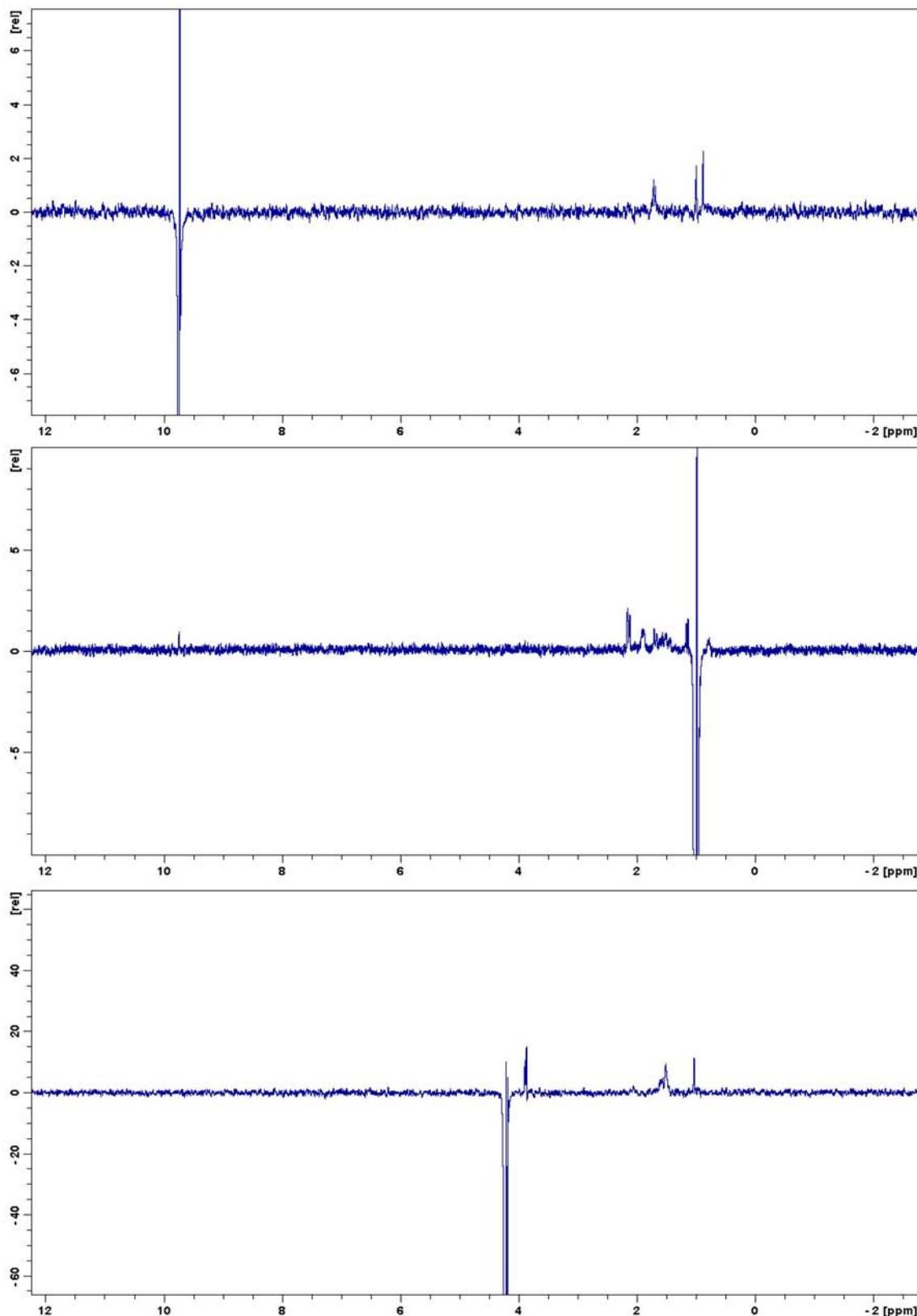


Figure 6S. 1D NOE experiments for ent- 16β -hydroxy-17-acetoxy-kauran-19-al (7) in CDCl_3 at 400 MHz

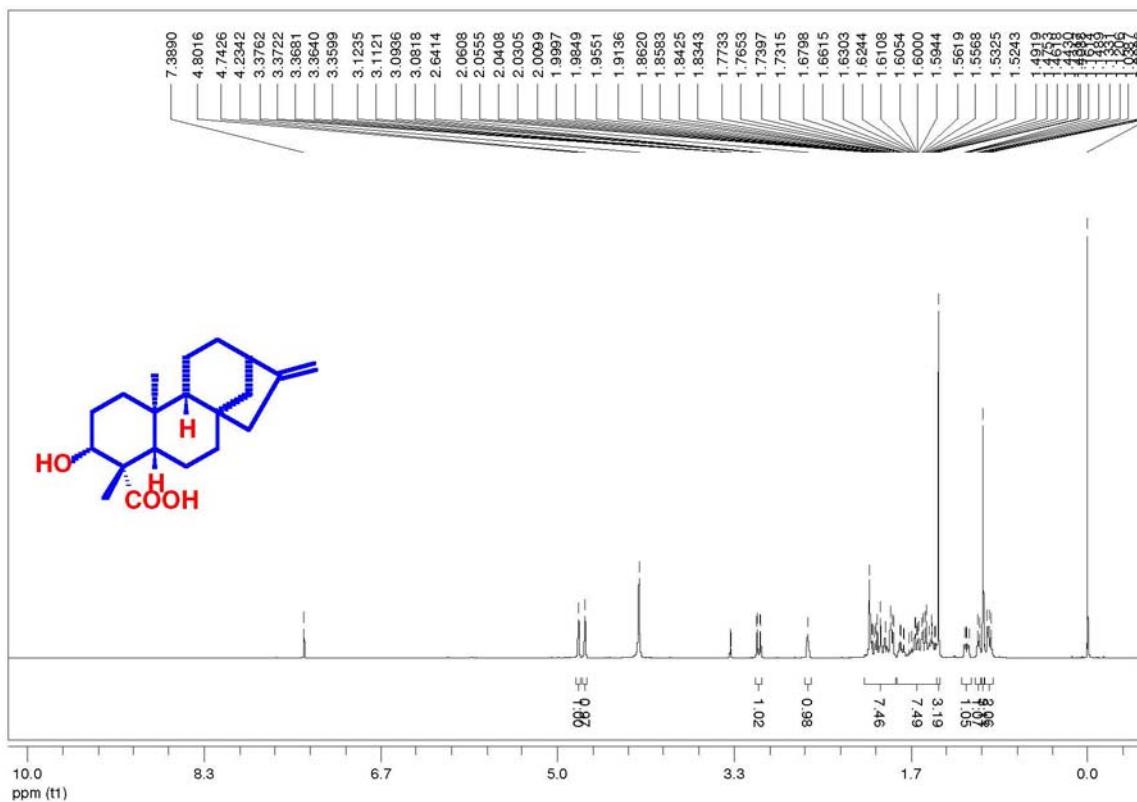


Figure 7S. ^1H NMR spectrum of *ent*-3 β -hydroxy-kaur-16-en-19-oic acid (**8**) in CDCl_3 + drops of CD_3OD at 400 MHz

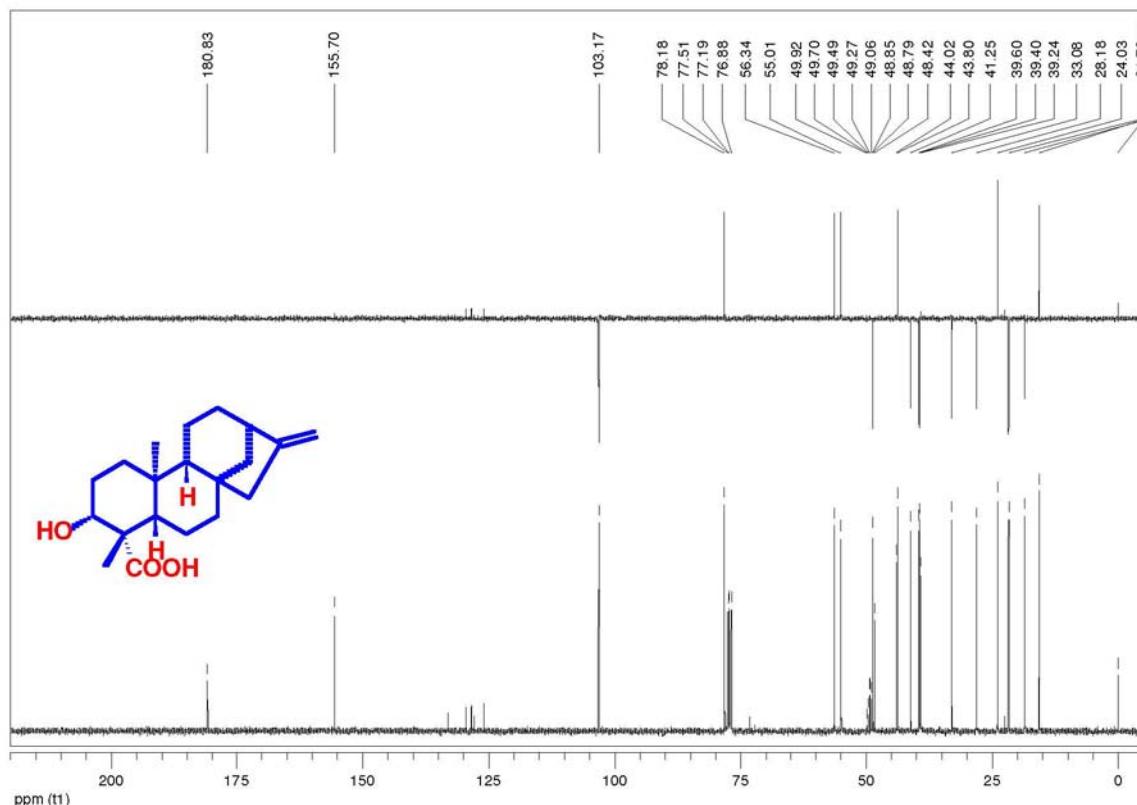


Figure 8S. ^{13}C { ^1H } and DEPT 135 NMR spectra of ent- β -hydroxy-kaur-16-en-19-oic acid (**8**) in $\text{CDCl}_3 + \text{drops of CD}_3\text{OD}$ at 100 MHz

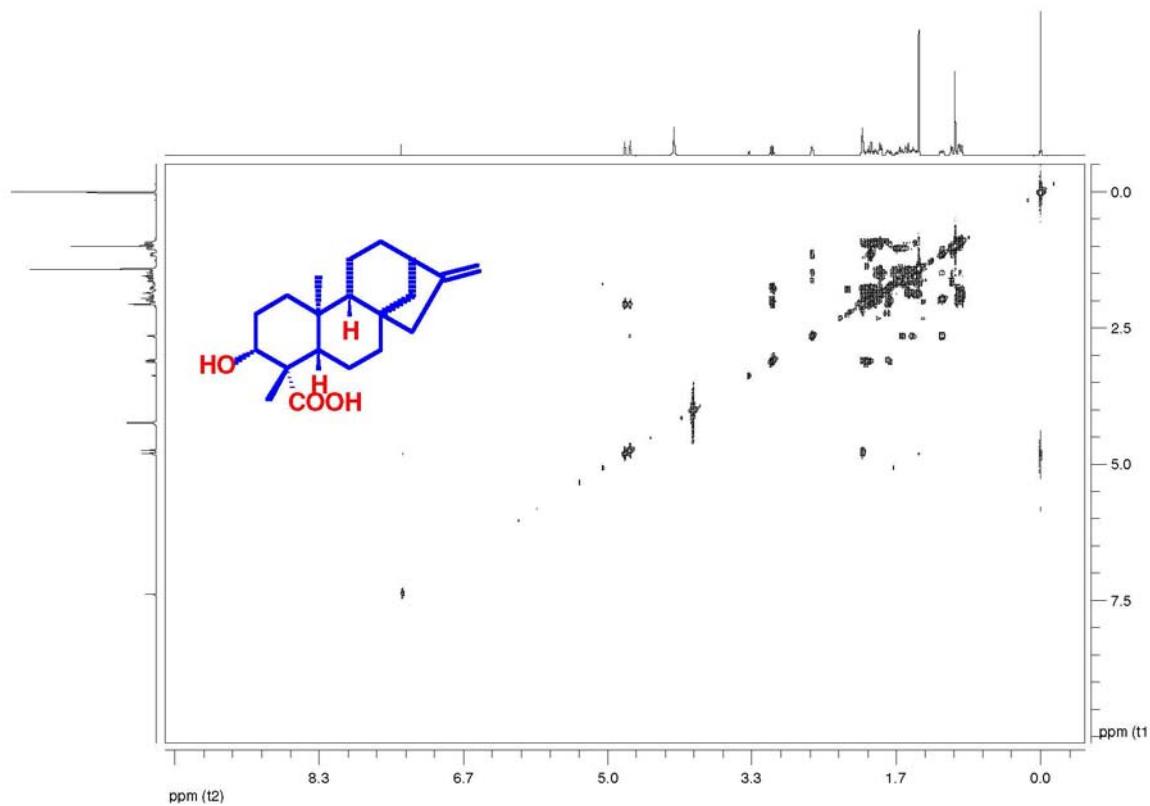


Figure 9S. ^1H - ^1H correlation map from COSY NMR experiment of ent-3 β -hydroxy-kaur-16-en-19-oic acid (8) in CDCl_3 + drops of CD_3OD at 400 MHz

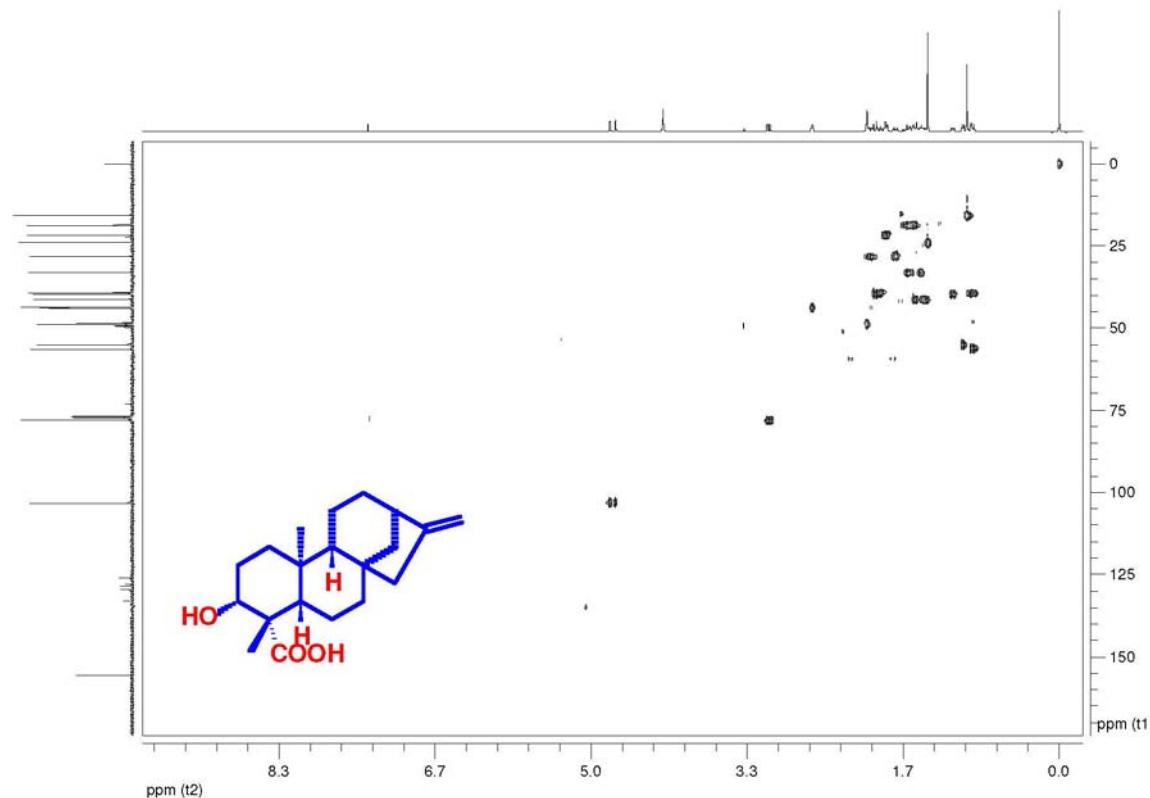


Figure 10S. ^1H - ^{13}C one-bond correlation map from HSQC NMR experiment of ent-3 β -hydroxy-kaur-16-en-19-oic acid (8) in CDCl_3 + drops of CD_3OD at 400 and 100 MHz

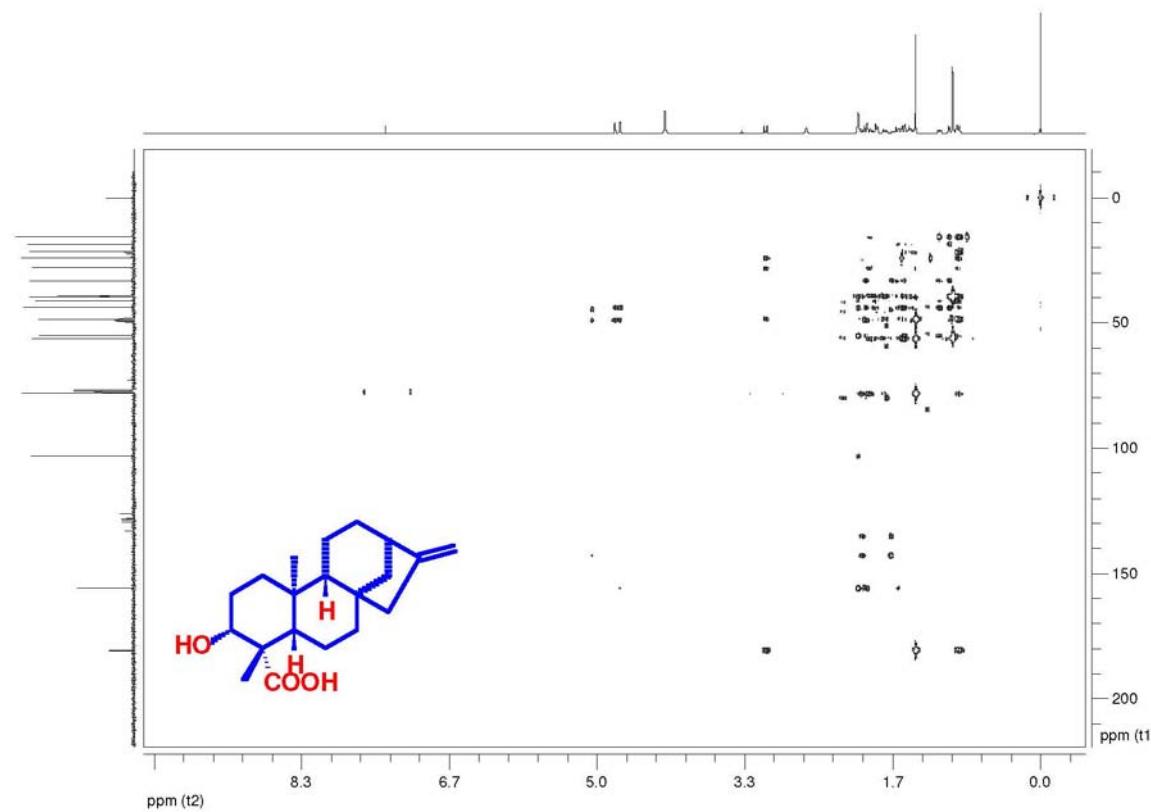


Figure 11S. ^1H - ^{13}C long-range correlation map from HMBC NMR experiment of *ent*-3 β -hydroxy-kaur-16-en-19-oic acid (8) in $\text{CDCl}_3 + \text{drops of } \text{CD}_3\text{OD}$ at 400 and 100 MHz

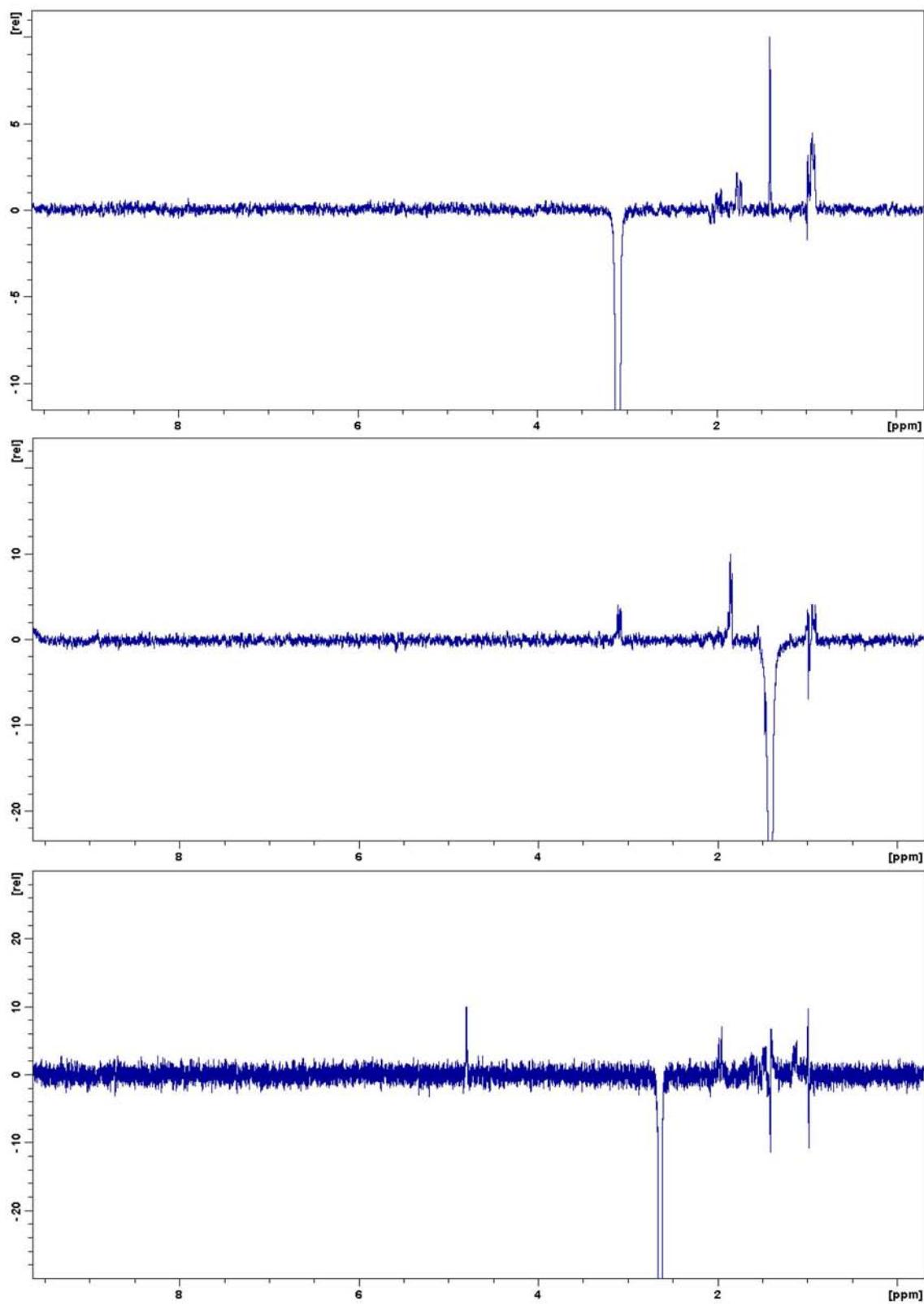


Figure 12S. 1D NOE experiments for *ent*-3 β -hydroxy-kaur-16-en-19-oic acid (8) in $CDCl_3$ + drops of CD_3OD at 400 MHz

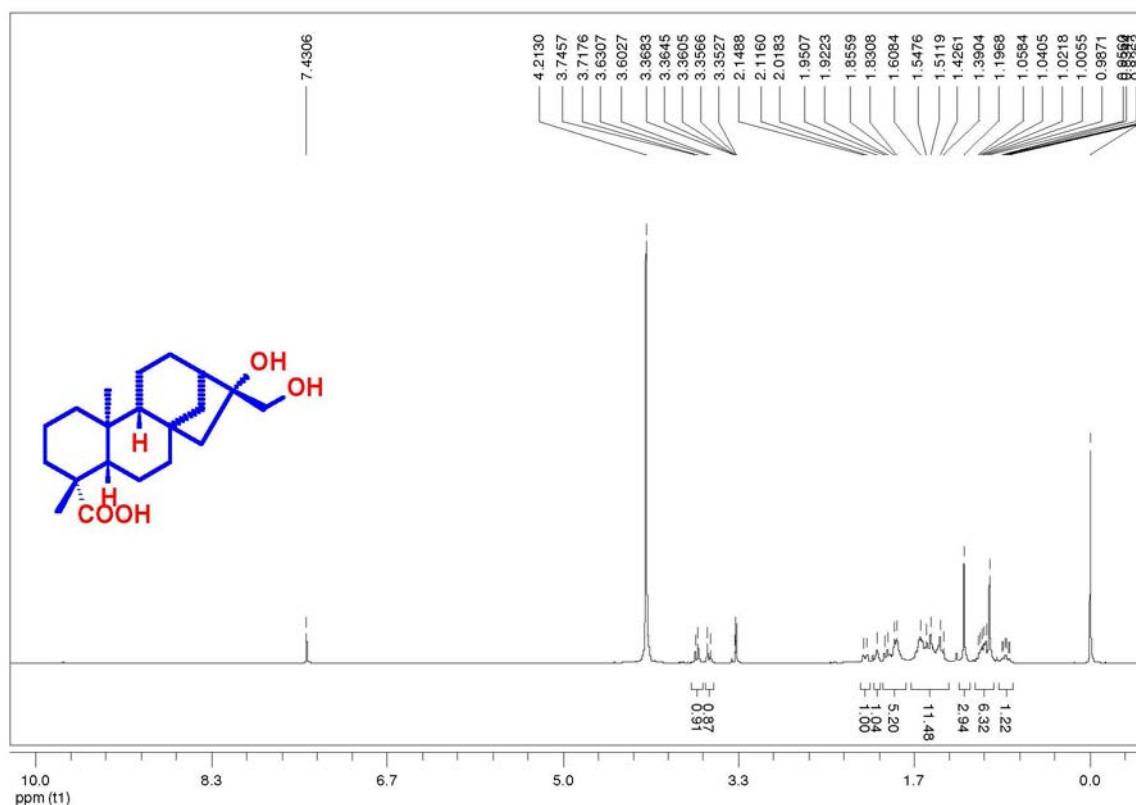


Figure 13S. ^1H NMR spectrum of *ent*-16 β ,17-dihydroxy-kauran-19-oic acid (**9**) in CDCl_3 + drops of CD_3OD at 400 MHz

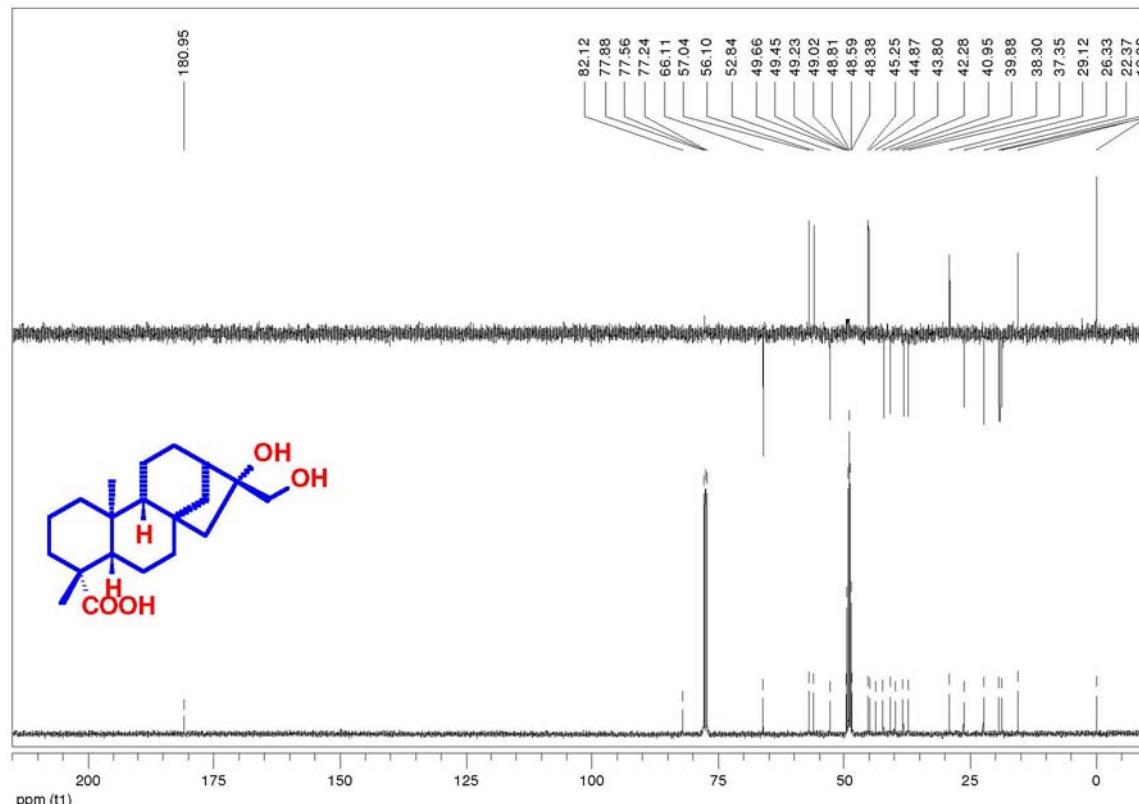


Figure 14S. $^{13}\text{C}\{^1\text{H}\}$ and DEPT 135 NMR spectra of *ent*-16 β ,17-dihydroxy-kauran-19-oic acid (**9**) in CDCl_3 + drops of CD_3OD at 100 MHz

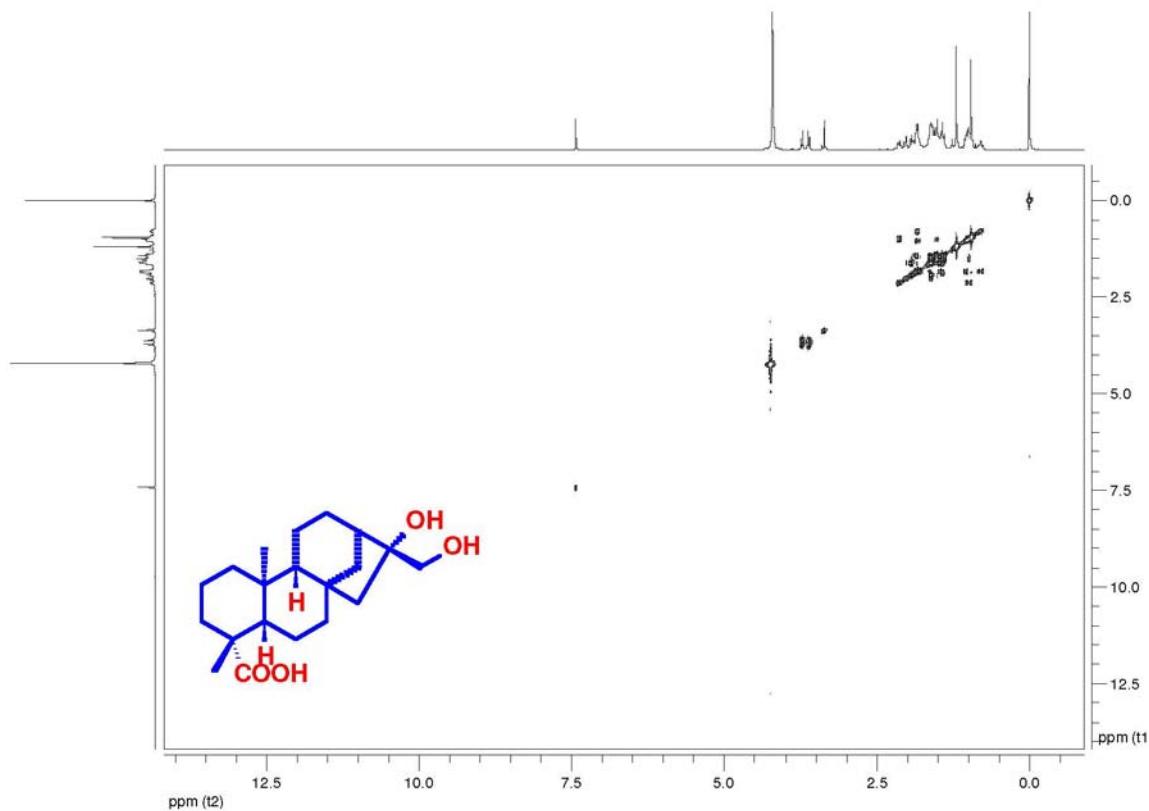


Figure 15S. ^1H - ^1H correlation map from COSY NMR experiment of *ent*-16 β ,17-dihydroxy-kauran-19-oic acid (**9**) in CDCl_3 + drops of CD_3OD at 400 MHz

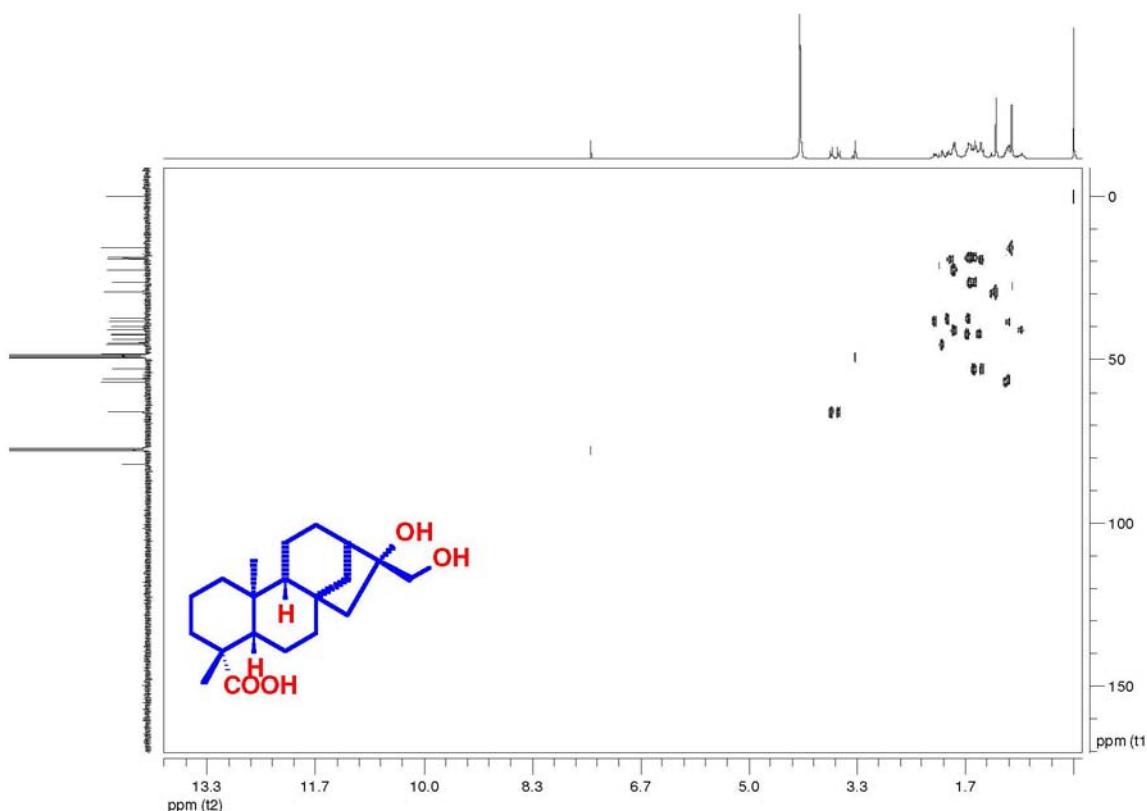


Figure 16S. ^1H - ^{13}C one-bond correlation map from HSQC NMR experiment of *ent*-16 β ,17-dihydroxy-kauran-19-oic acid (**9**) in CDCl_3 + drops of CD_3OD at 400 and 100 MHz

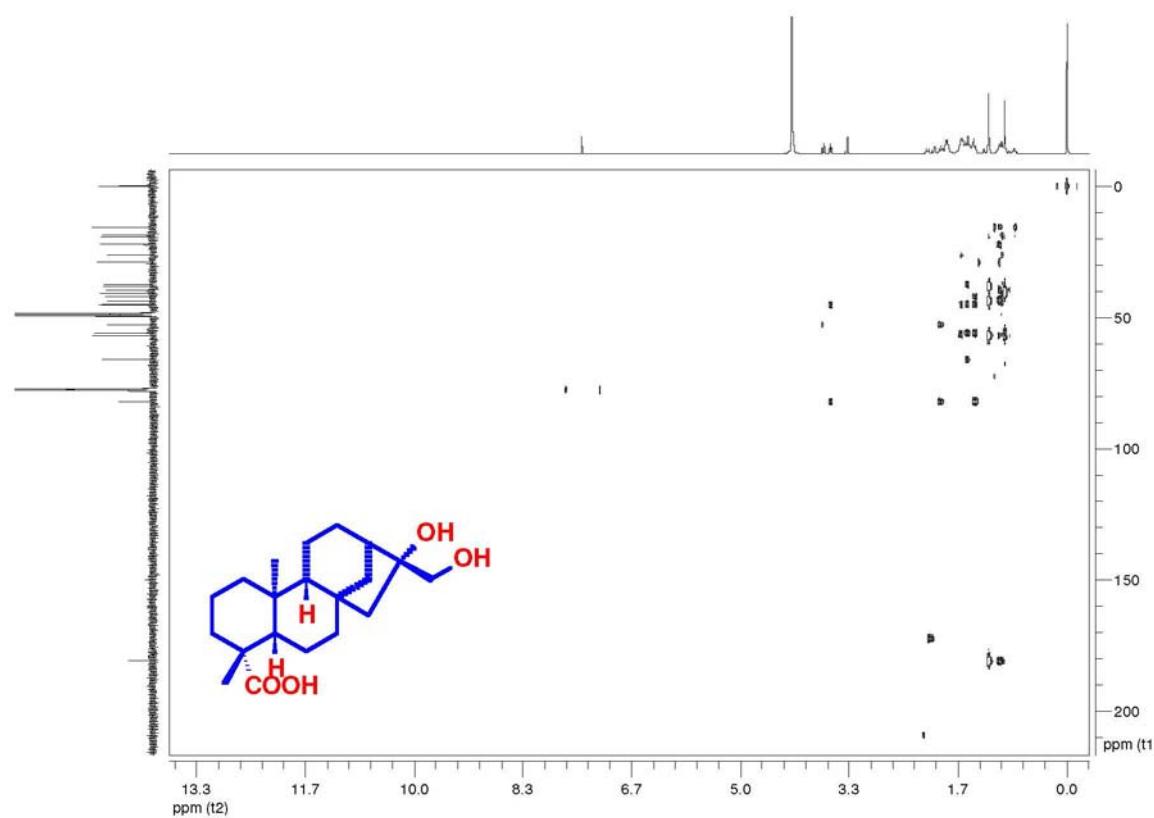


Figure 17S. ^1H - ^{13}C long-range correlation map from HMBC NMR experiment of *ent*-16 β ,17-dihydroxy-kauran-19-oic acid (**9**) in CDCl_3 + drops of CD_3OD at 400 and 100 MHz