

Supporting Information

Rec. Nat. Prod. 11:3 (2017) 304-309

Kaurane Diterpenes from the Fruits of *Zanthoxylum leprieurii* (Rutaceae)

Stephanie T. Guetchueng^{1,2}, Lutfun Nahar¹, Kenneth J. Ritchie¹, Fyaz M. D. Ismail¹, Jean D. Wansi^{1,3}, Andrew Evans¹ and Satyajit D. Sarker^{1,*}

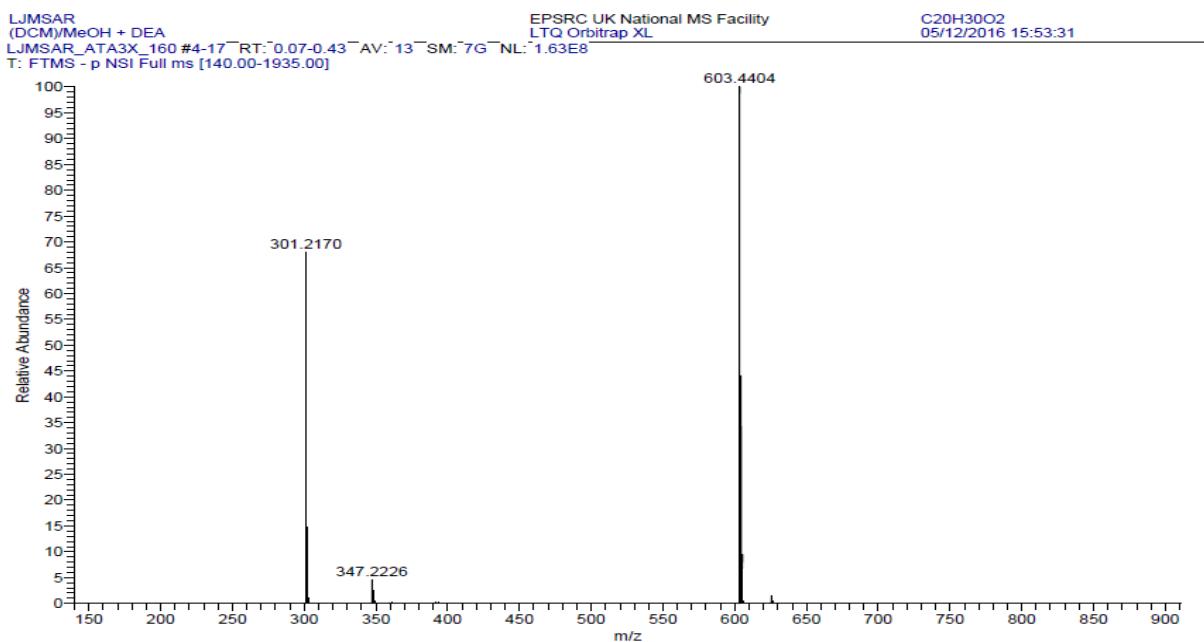
¹*Medicinal Chemistry and Natural Products Research Group, School of Pharmacy and Biomolecular Sciences, Liverpool John Moores University, Faculty of Science, James Parsons Building, Byrom Street, Liverpool L3 3AF, UK*

²*Institute of Medical Research and Medicinal Plants Studies, Ministry of Scientific Research and Innovation, PO Box 6163 Yaounde, Cameroon*

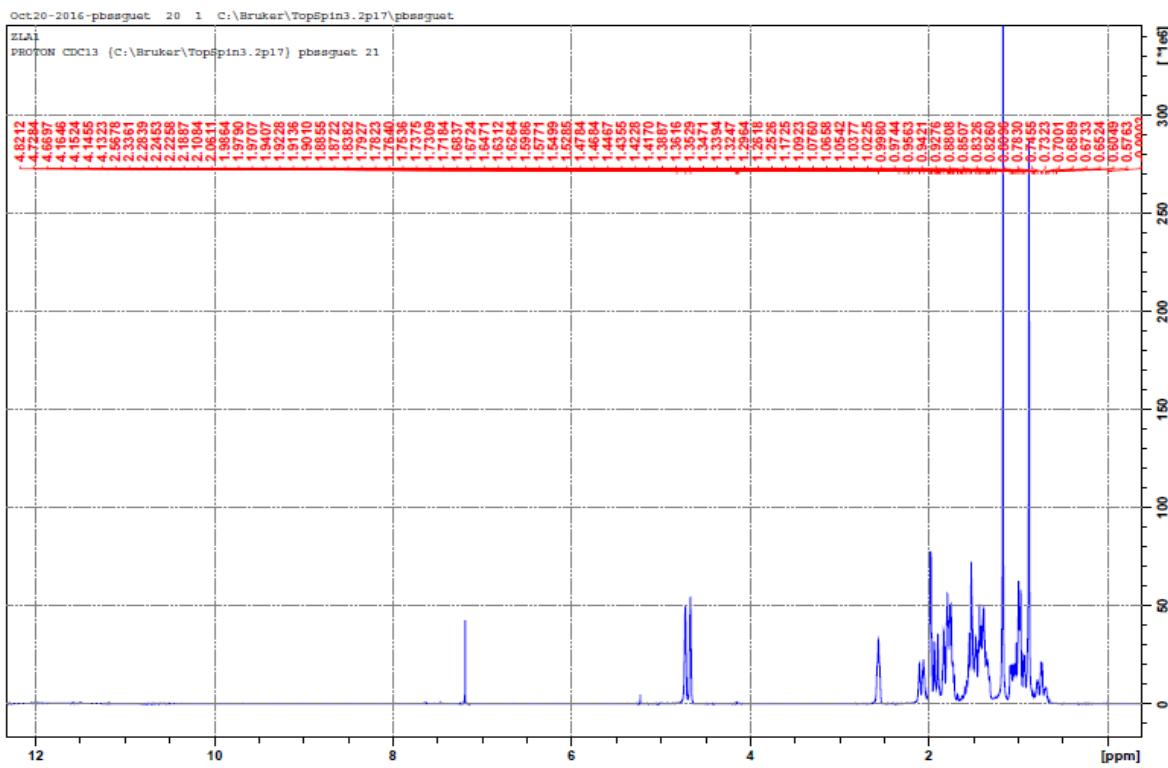
³*Department of Chemistry, University of Douala, Faculty of Science, PO Box 24157 Douala, Cameroon*

S1: HRESI-MS Spectrum of Compound 1 (kaurenoic acid)	2
S3: Expansion of the ¹ H-NMR Spectrum of Compound 1 (kaurenoic acid) (From 0 to 4.00 ppm)	3
S4: ¹³ C-NMR (75 MHz, CDCl ₃) Spectrum of Compound 1 (kaurenoic acid)	4
S6: COSY (500 MHz, CDCl ₃) Spectrum of Compound 1 (kaurenoic acid).....	5
S7: HMBC (500 MHz, CDCl ₃) Spectrum of Compound 1 (kaurenoic acid)	5
S8: HSQC (500 MHz, CDCl ₃) Spectrum of Compound 1 (kaurenoic acid).....	6
S12: HRESI-MS Spectrum Expended of Compound 2 (xylopic acid)	7
S13: ¹ H-NMR (500 MHz, CDCl ₃) Spectrum of Compound 2 (xylopic acid).....	8
S14: ¹³ C-NMR (75 MHz, CDCl ₃) Spectrum of Compound 2 (xylopic acid)	8
S15: DEPTQ (75 MHz, CDCl ₃) Spectrum of Compound 2 (xylopic acid)	9
S16: COSY (500 MHz, CDCl ₃) Spectrum of Compound 2 (xylopic acid)	9
S17: HSQC (500 MHz, CDCl ₃) Spectrum of Compound 2 (xylopic acid)	10
S19: NOESY (500 MHz, CDCl ₃) Spectrum of Compound 2 (xylopic acid).....	11
S21: ¹ H-NMR (300 MHz, CDCl ₃) Spectrum of Compound 3 (<i>ent</i> -kauran-16 β -ol)	12
S22: Expansion of the ¹ H-NMR Spectrum of Compound 3 (<i>ent</i> -kauran-16 β -ol) (from 0 to 3.6 ppm)	13
S23: ¹³ C-NMR (75 MHz, CDCl ₃) Spectrum of Compound 3 (<i>ent</i> -kauran-16 β -ol)	13
S25: HSQC (300 MHz, CDCl ₃) Spectrum of Compound 3 (<i>ent</i> -kauran-16 β -ol)	14
S26: HMBC (500 MHz, CDCl ₃) Spectrum of Compound 3 (<i>ent</i> -kauran-16 β -ol)	14

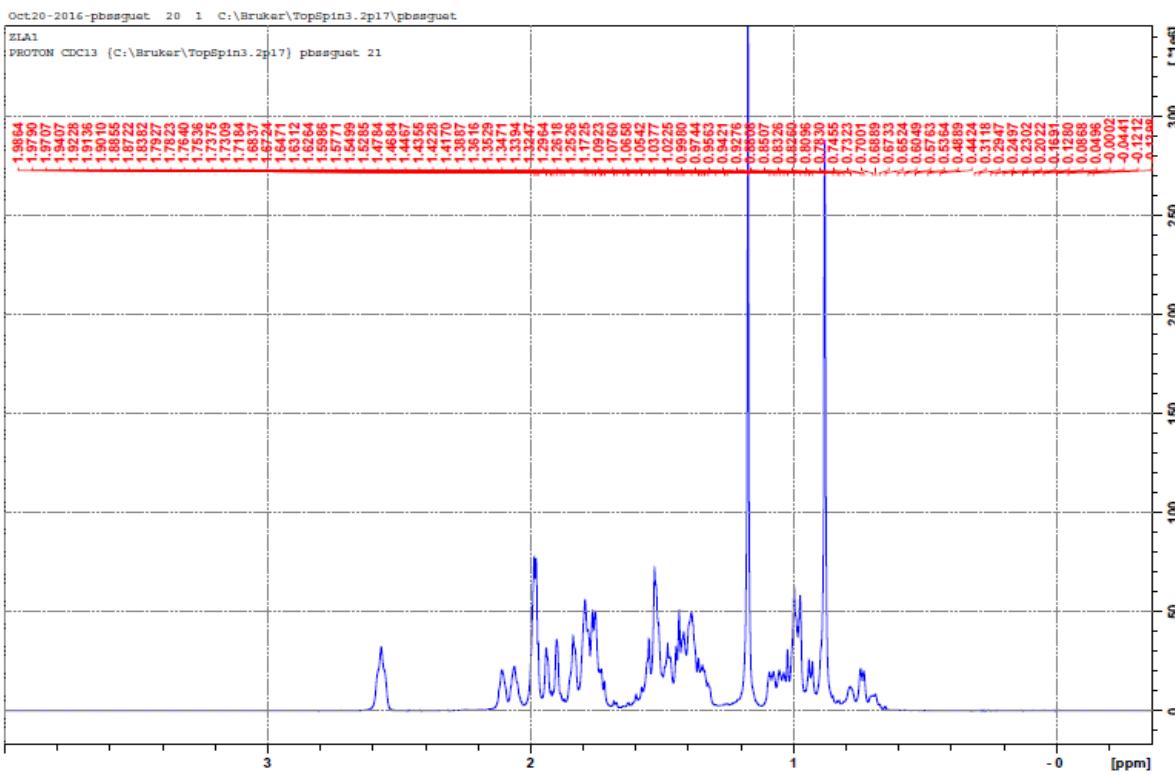
S27: Expansion of the HMBC (300 MHz, CDCl ₃) Spectrum of Compound 3 (<i>ent</i> -kauran-16 β -ol)	15
S29: ¹ H-NMR (600 MHz, CDCl ₃) Spectrum of Compound 4 (<i>ent</i> -kauran-16 β -ol-19-al).....	16
(from 0 to 4.0 ppm)	17
S31: ¹³ C-NMR (75 MHz, CDCl ₃) Spectrum of Compound 4 (<i>ent</i> -kauran-16 β -ol-19-al)	17
S32: COSY (600 MHz, CDCl ₃) Spectrum of Compound 4 (<i>ent</i> -kauran-16 β -ol-19-al).....	17
S34: HMBC (600 MHz, CDCl ₃) Spectrum of Compound 4 (<i>ent</i> -kauran-16 β -ol-19-al)	19
S38: ¹ H-NMR (600 MHz, CDCl ₃) Spectrum of Compound 5 (<i>ent</i> -kauran-16 β -ol-19oic acid)	
.....	20
S40: COSY (300 MHz, CDCl ₃ + drops of MeOH) Spectrum Spectrum of Compound 5 (<i>ent</i> -kauran-16 β -ol-19oic acid)	21
S41: HSQC (300 MHz, CDCl ₃ + drops of MeOH) Spectrum of Compound 5 (<i>ent</i> -kauran-16 β -ol-19oic acid).....	22
S42: HMBC (300 MHz, CDCl ₃ + drops of MeOH) Spectrum of Compound 5 (<i>ent</i> -kauran-16 β -ol-19oic acid).....	22
S43: NOESY (300 MHz, CDCl ₃ + drops of MeOH) Spectrum of Compound 5 (<i>ent</i> -kauran-16 β -ol-19oic acid)	23
S44: Expansion of the NOESY Spectrum of Compound 5 (<i>ent</i> -kauran-16 β -ol-19oic acid) ...	23



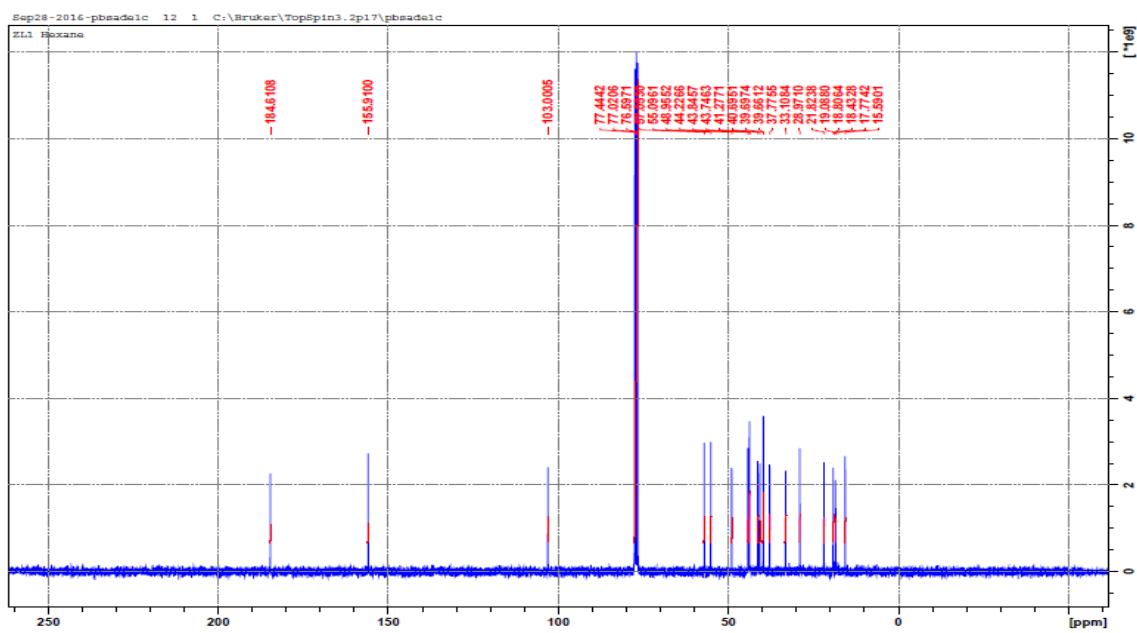
S1: HRESI-MS Spectrum of Compound 1 (kaurenoic acid)



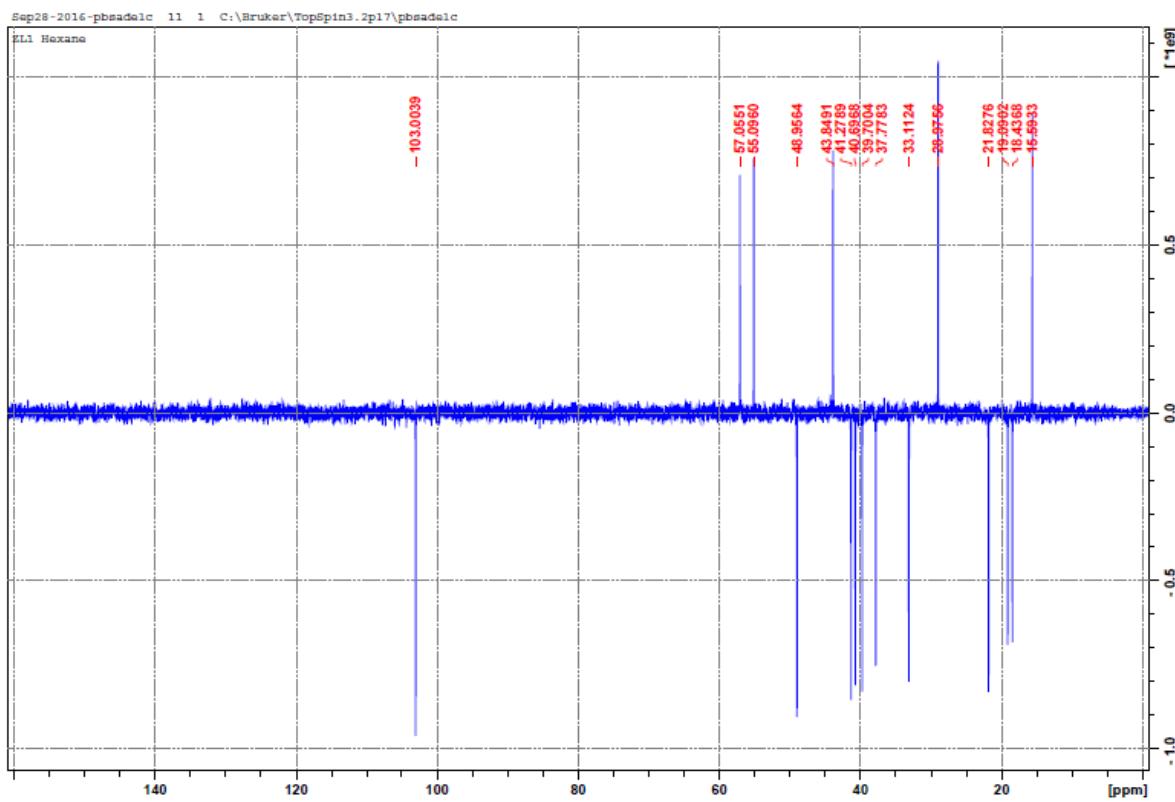
S2: ^1H -NMR (300 MHz, CDCl₃) Spectrum of Compound **1** (kaurenoic acid)



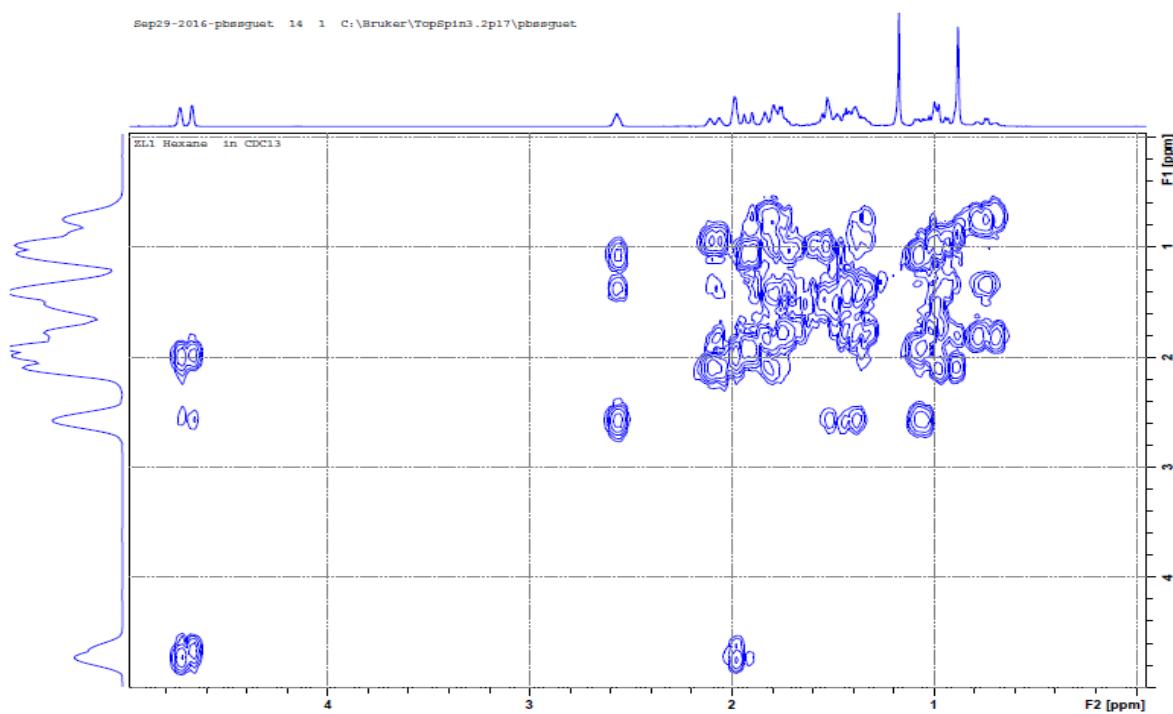
S3: Expansion of the ^1H -NMR Spectrum of Compound **1** (kaurenoic acid) (From 0 to 4.00 ppm)



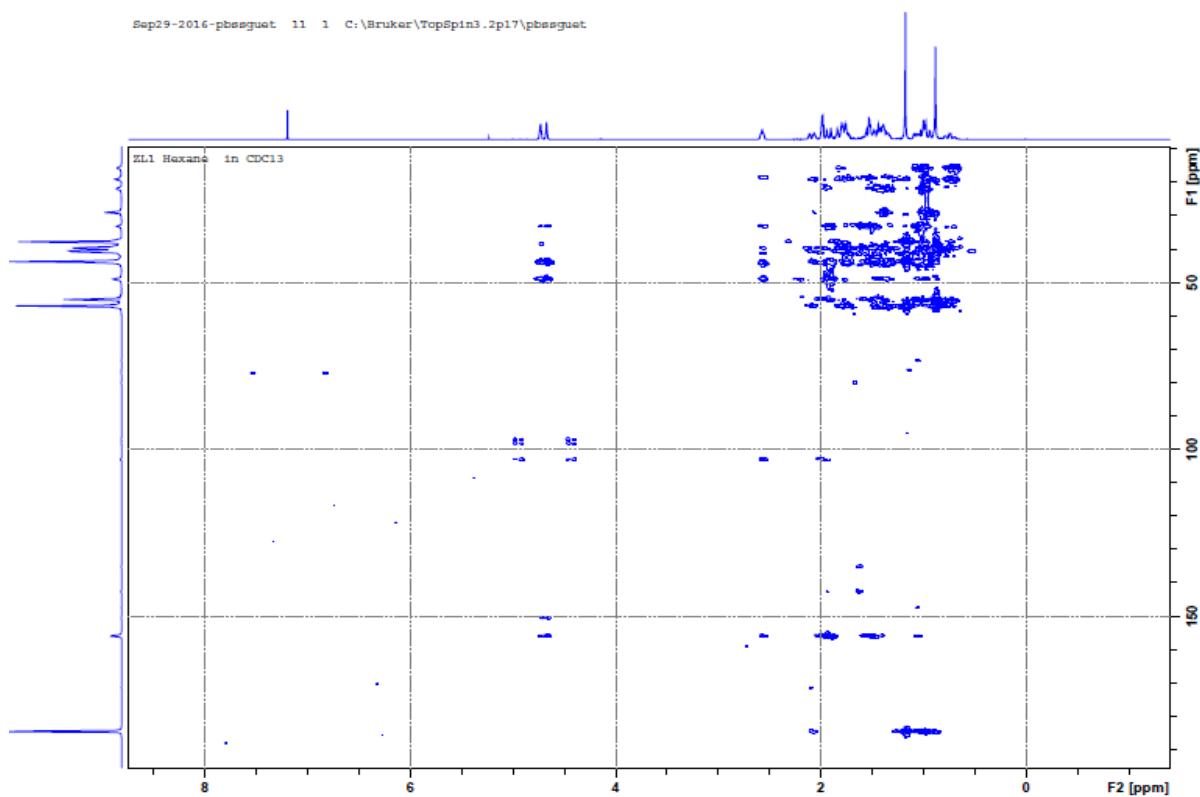
S4: ^{13}C -NMR (75 MHz, CDCl_3) Spectrum of Compound **1** (kaurenoic acid)



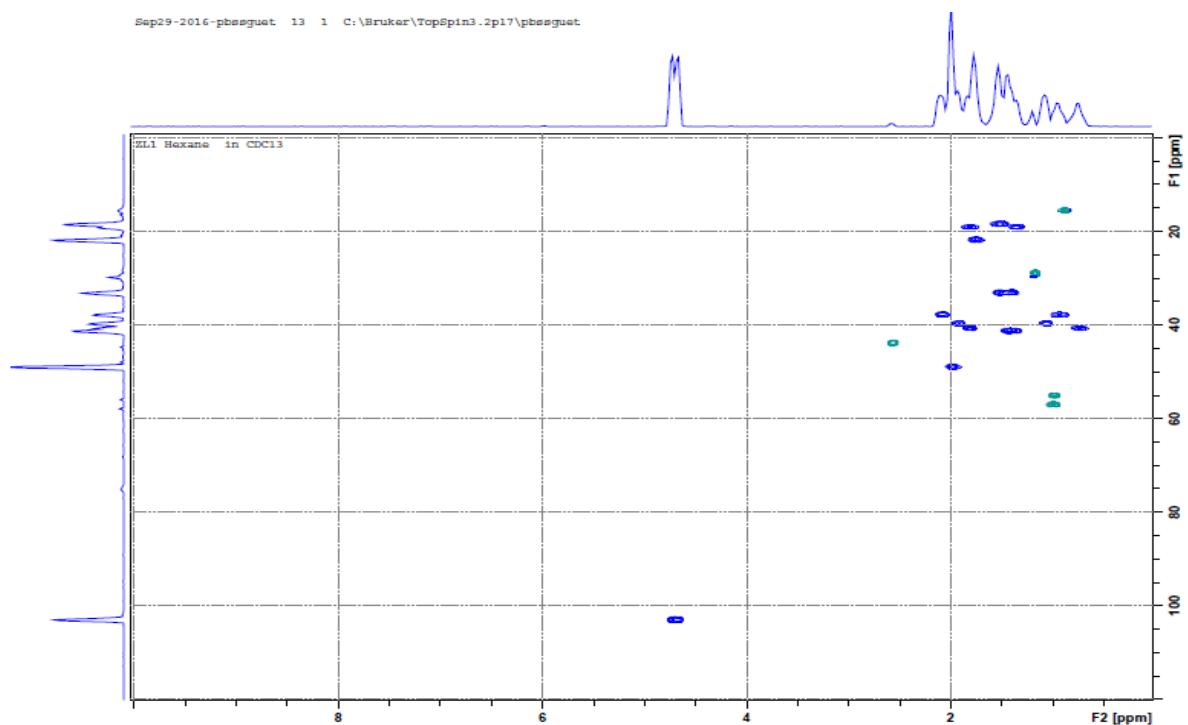
S5: DEPTQ (75 MHz, CDCl_3) Spectrum of Compound **1** (kaurenoic acid)



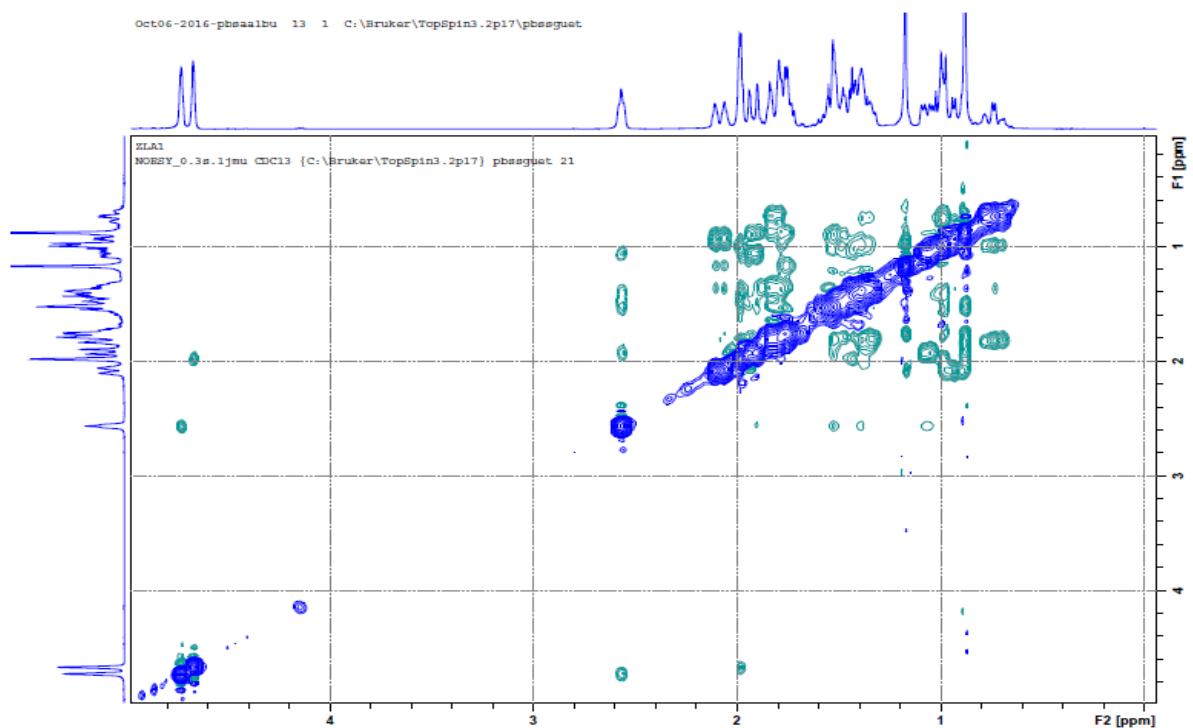
S6: COSY (500 MHz, CDCl₃) Spectrum of Compound **1** (kaurenoic acid)



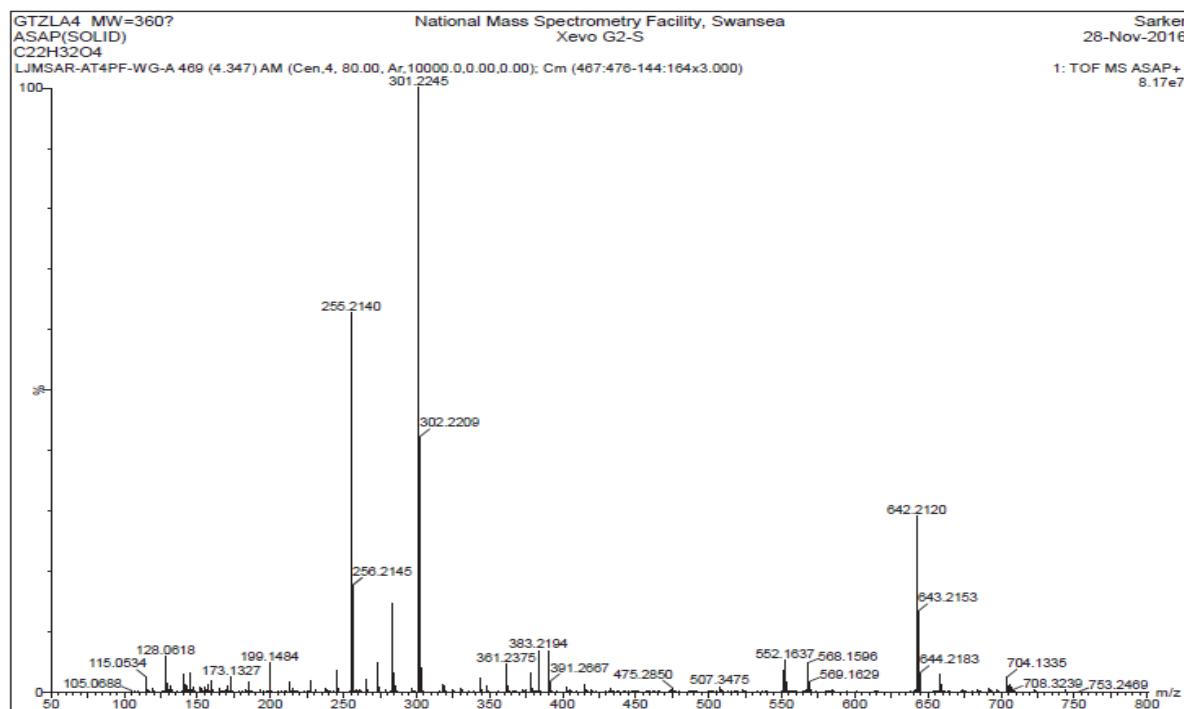
S7: HMBC (500 MHz, CDCl₃) Spectrum of Compound **1** (kaurenoic acid)



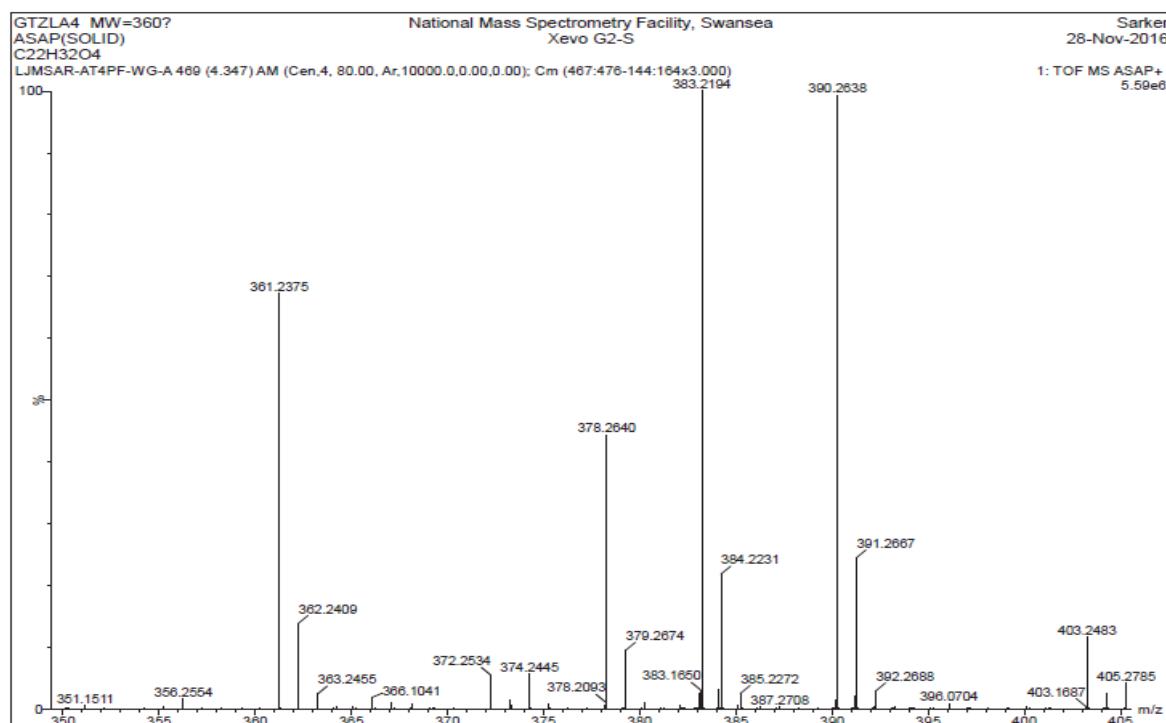
S8: HSQC (500 MHz, CDCl₃) Spectrum of Compound **1** (kaurenoic acid)



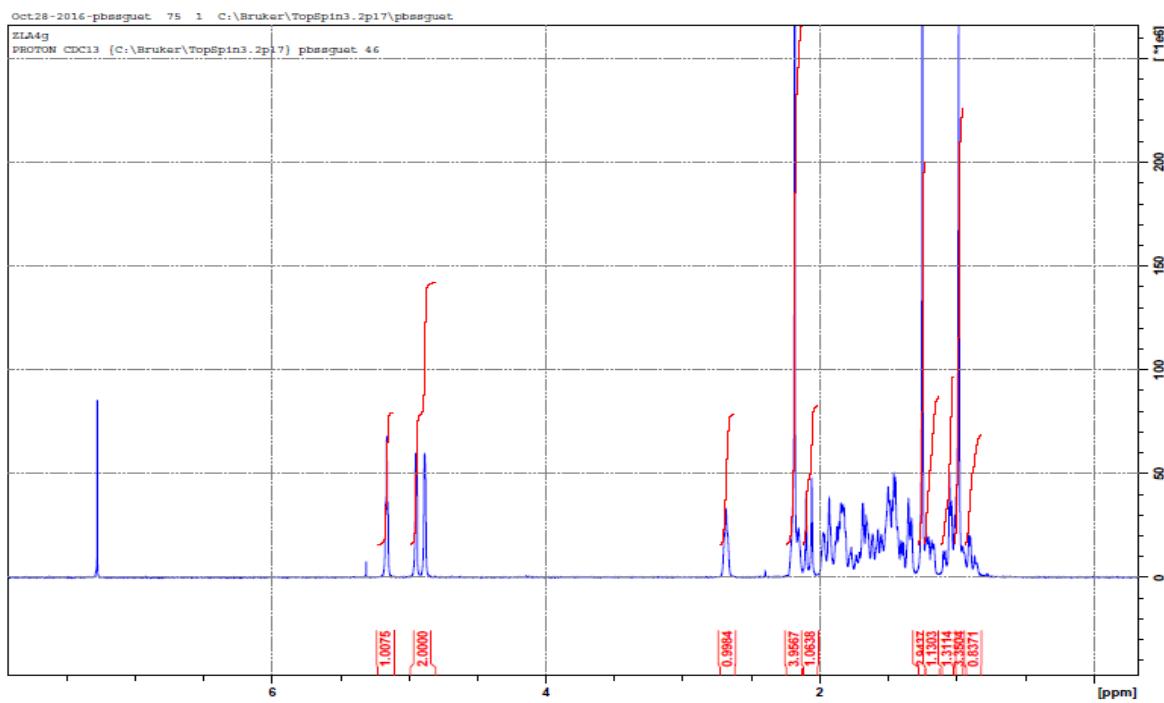
S10: NOESY (500 MHz, CDCl₃) Spectrum of Compound **1** (kaurenoic acid)



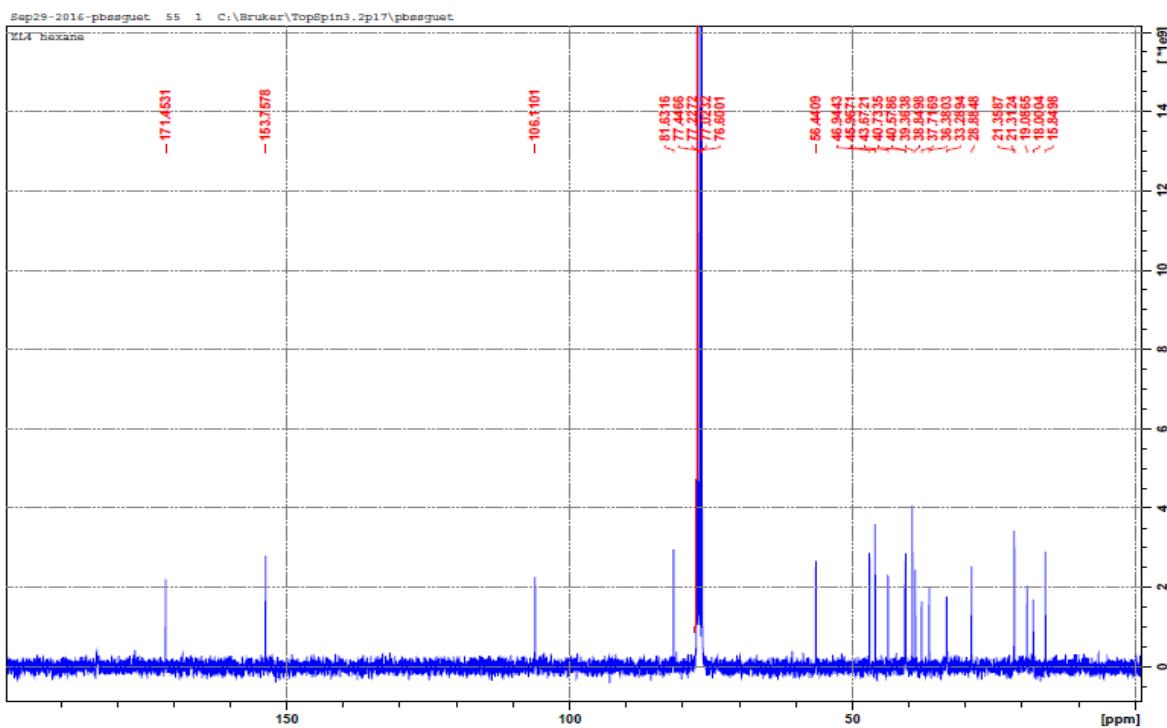
S11: HRESI-MS Spectrum of Compound 2 (xylopic acid)



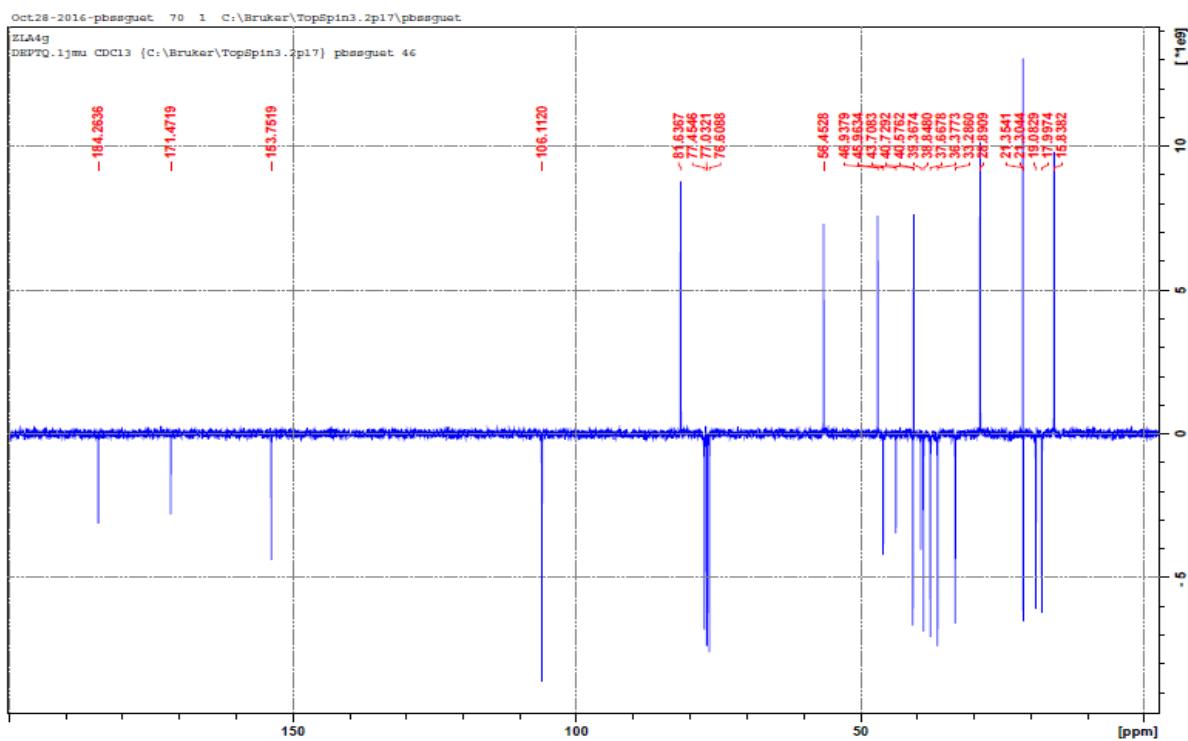
S12: HRESI-MS Spectrum Expended of Compound 2 (xylopic acid)



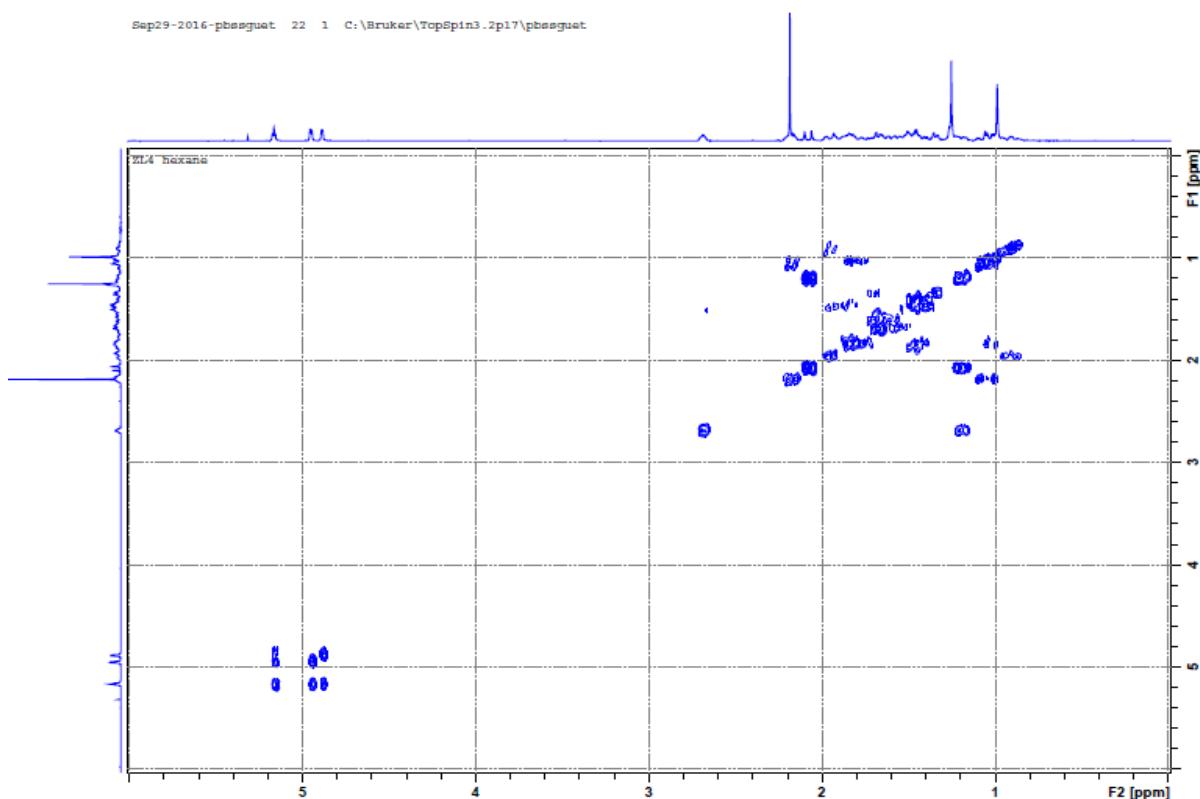
S13: ¹H-NMR (500 MHz, CDCl₃) Spectrum of Compound 2 (xylopic acid)



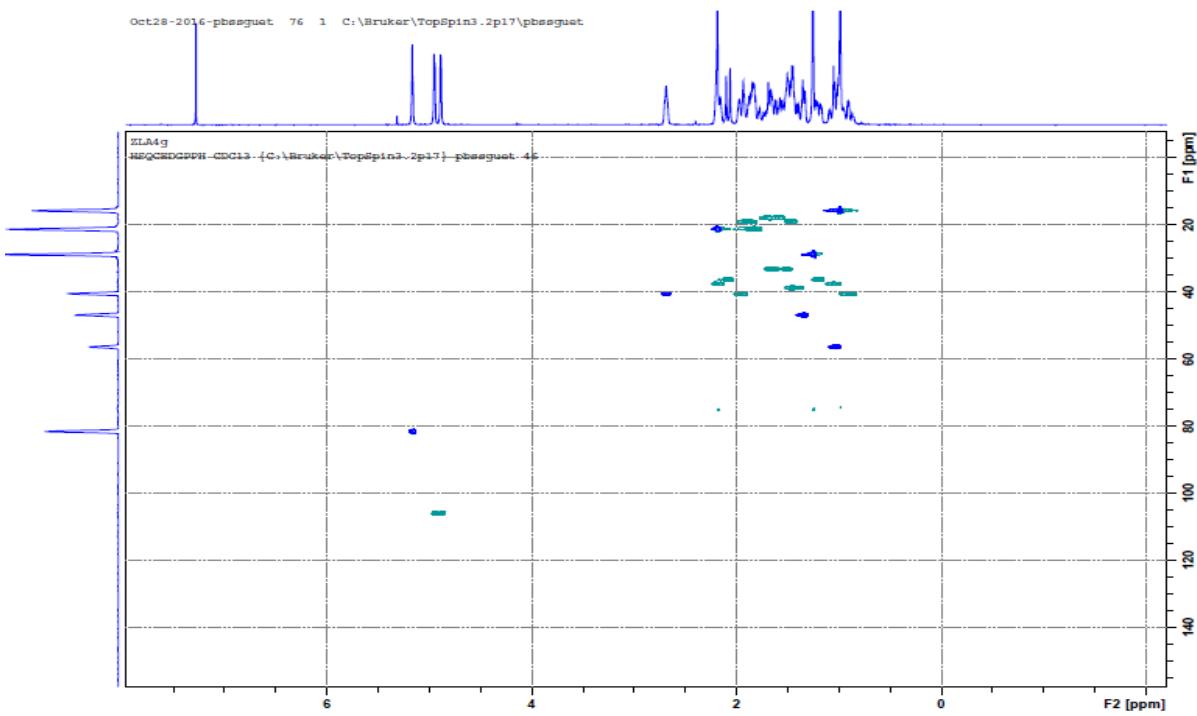
S14: ¹³C-NMR (75 MHz, CDCl₃) Spectrum of Compound 2 (xylopic acid)



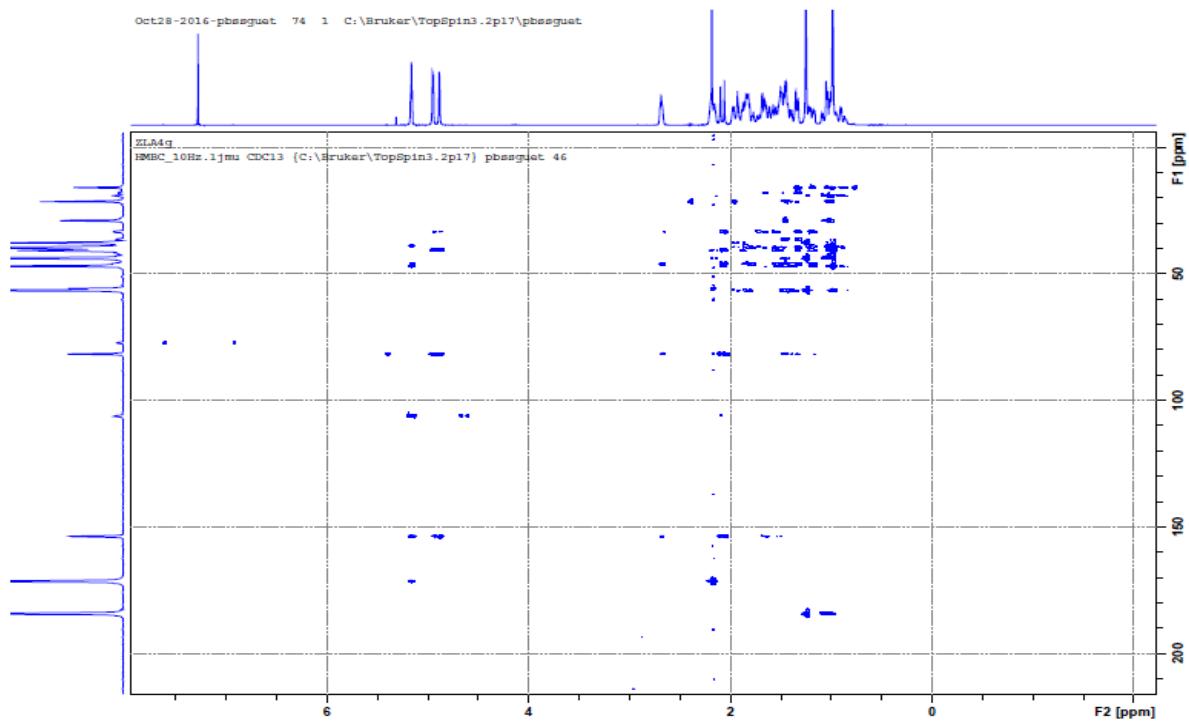
S15: DEPTQ (75 MHz, CDCl₃) Spectrum of Compound 2 (xylopic acid)



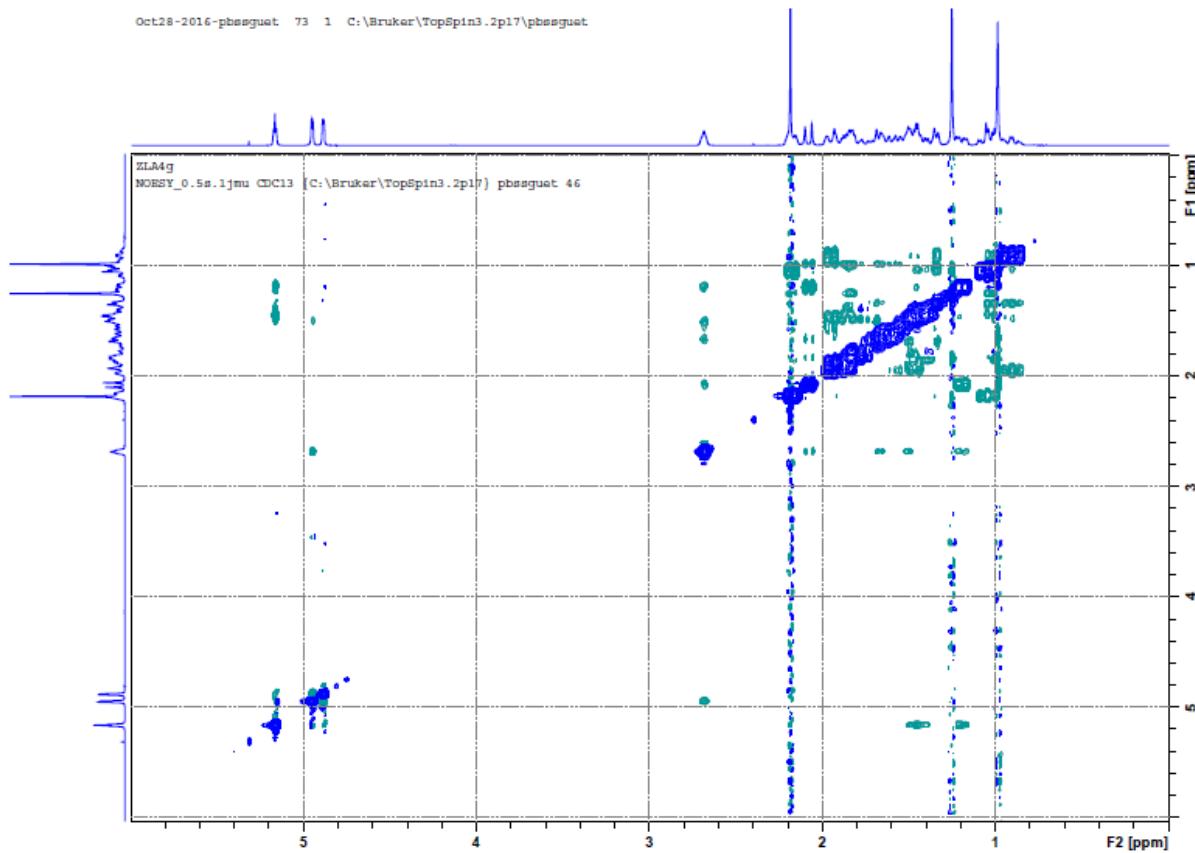
S16: COSY (500 MHz, CDCl₃) Spectrum of Compound 2 (xylopic acid)



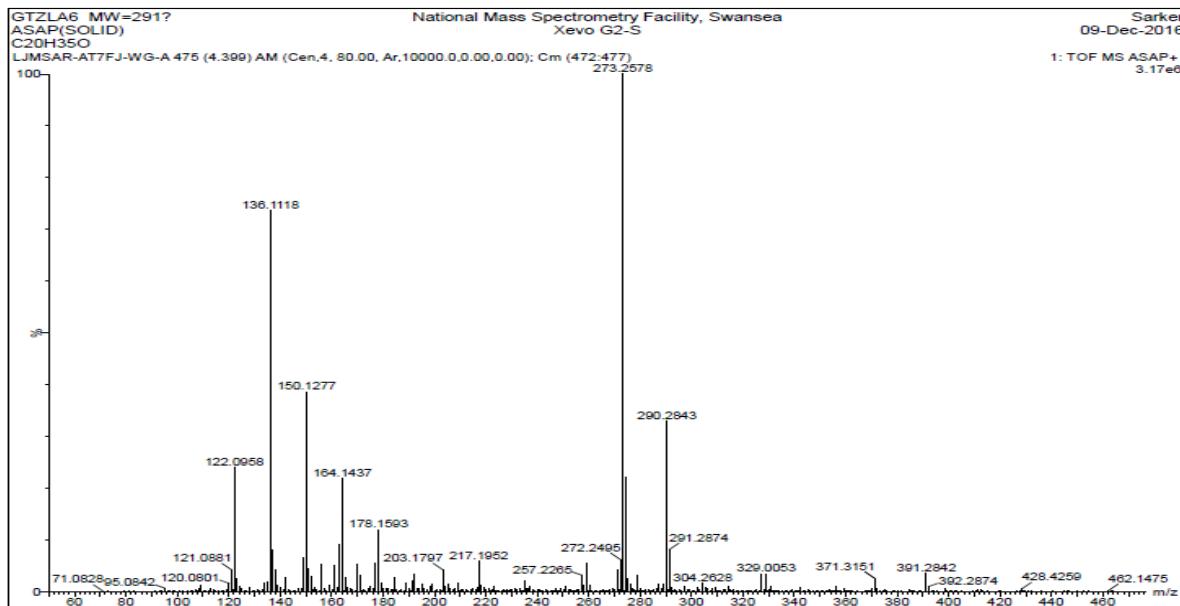
S17: HSQC (500 MHz, CDCl₃) Spectrum of Compound **2** (xylopic acid)



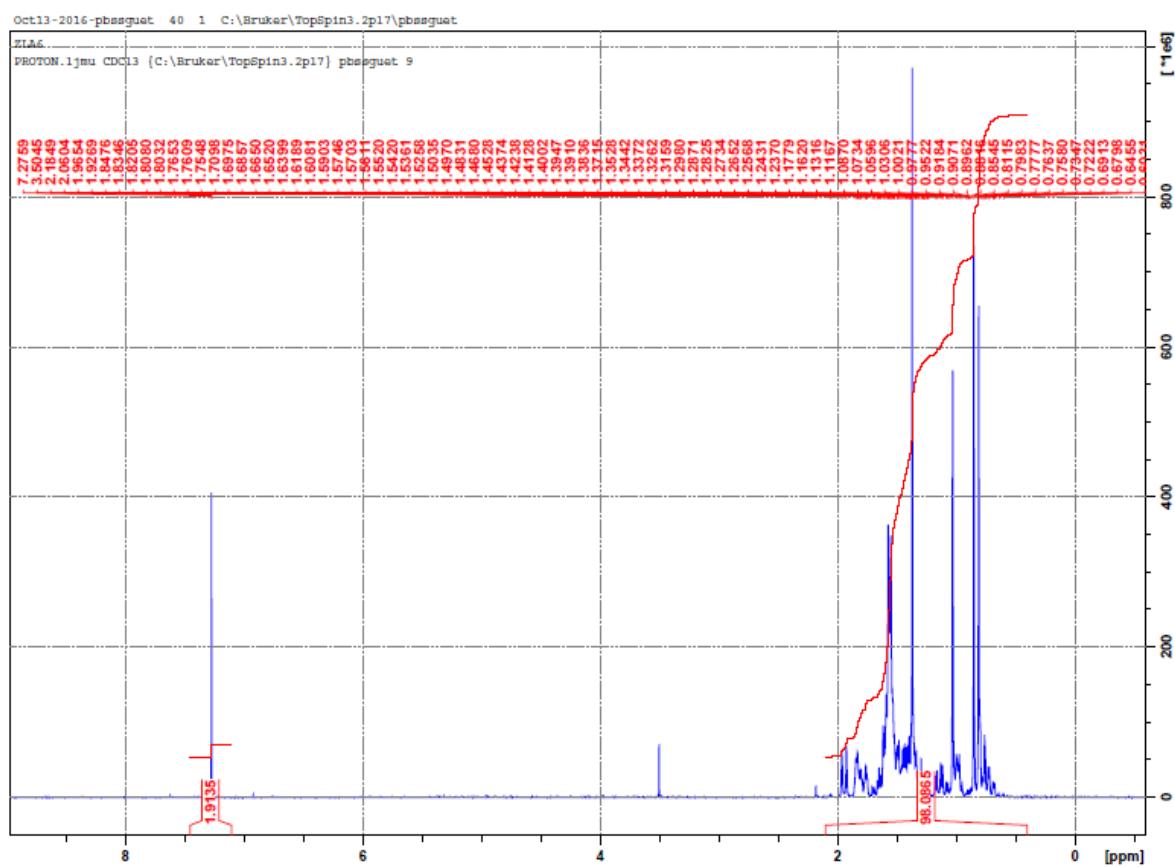
S18: HMBC (500 MHz, CDCl₃) Spectrum of Compound **2** (xylopic acid)



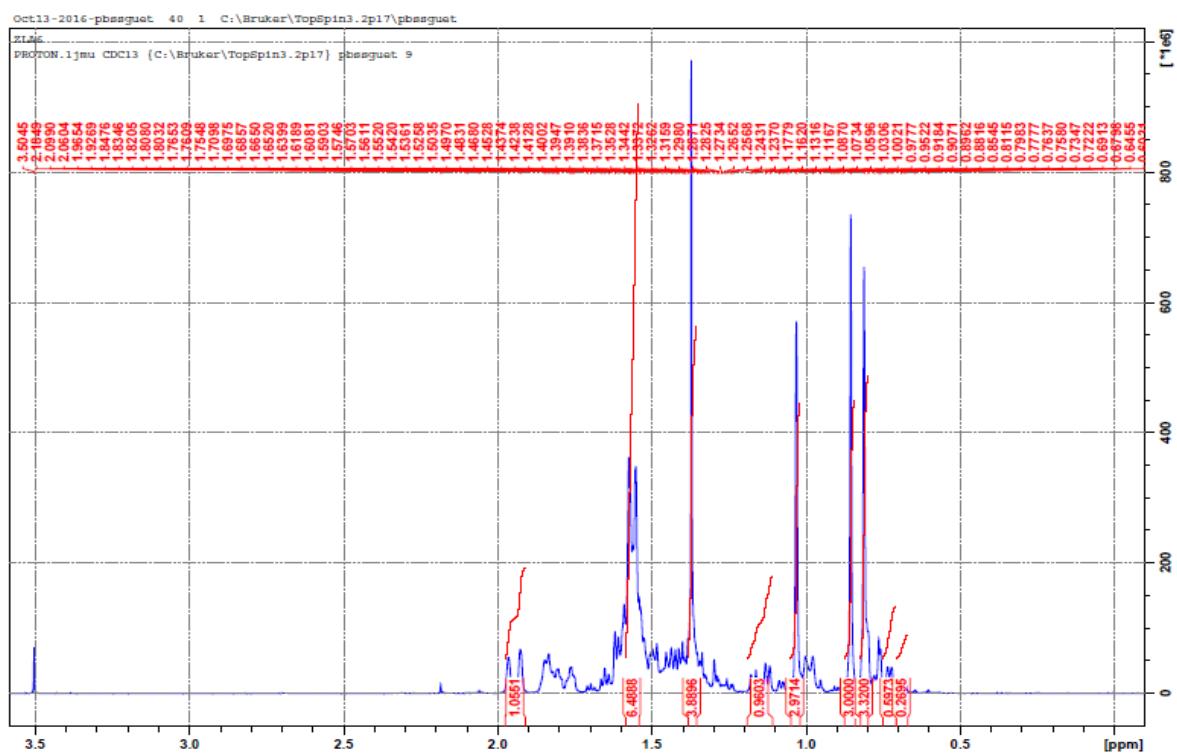
S19: NOESY (500 MHz, CDCl₃) Spectrum of Compound **2** (xylopic acid)



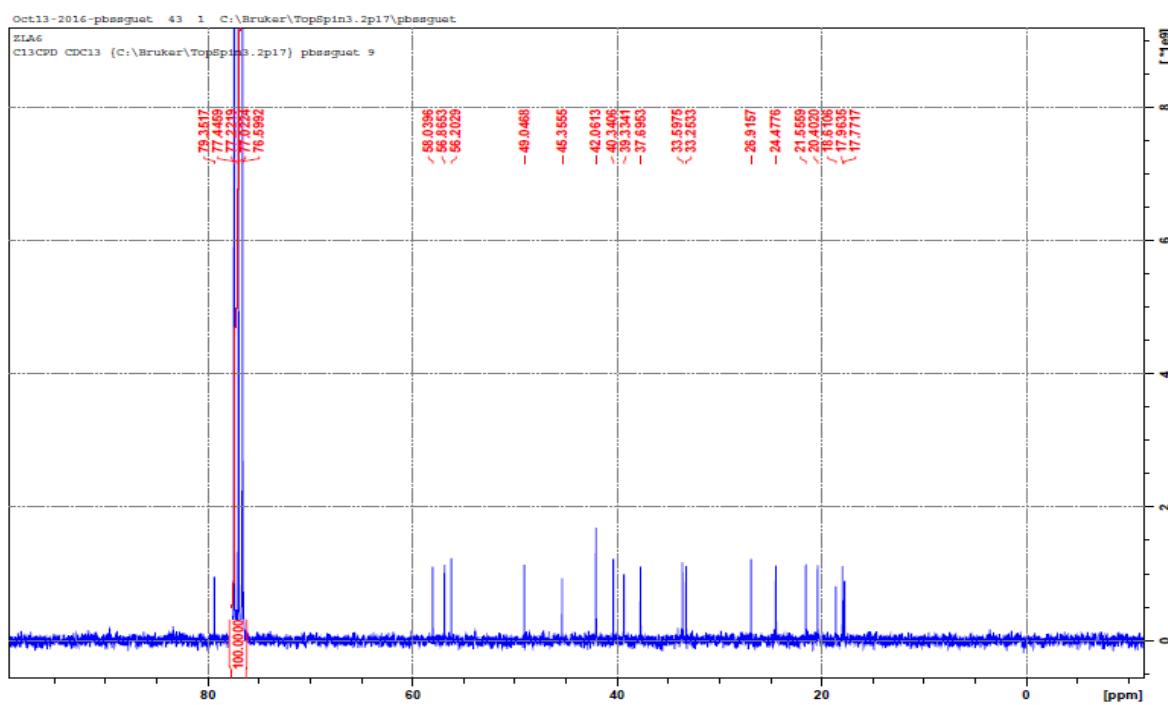
S20: HRESI-MS Spectrum of Compound **3** (ent-kauran-16β-ol)



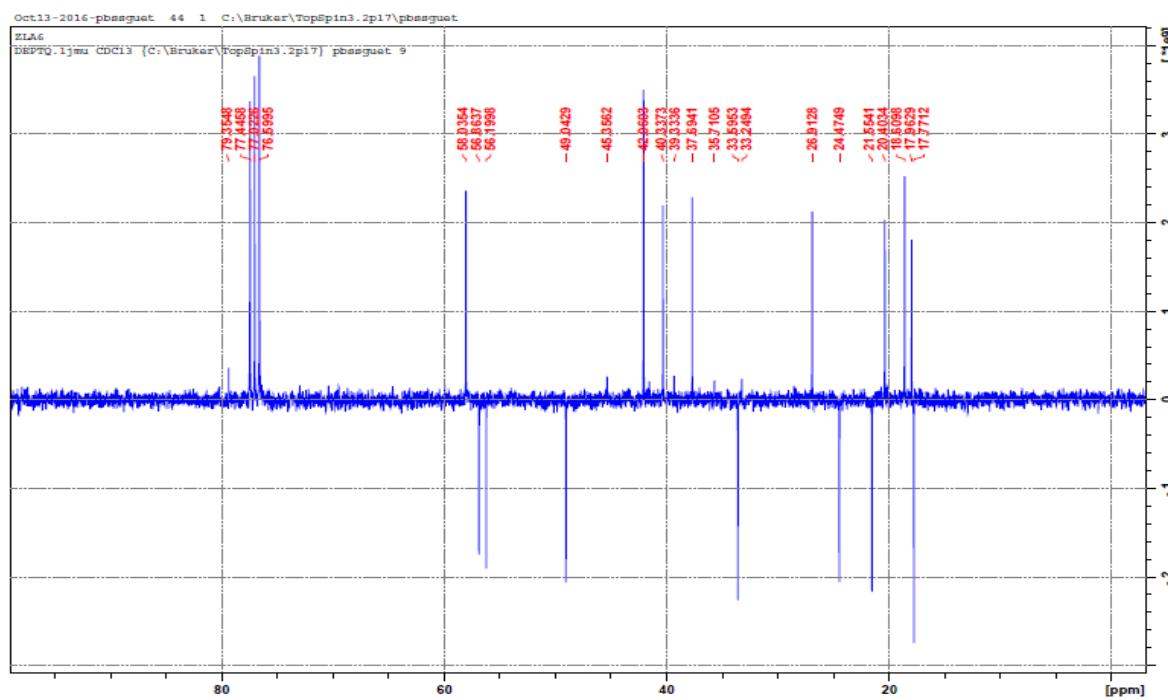
S21: ¹H-NMR (300 MHz, CDCl₃) Spectrum of Compound 3 (*ent*-kauran-16 β -ol)



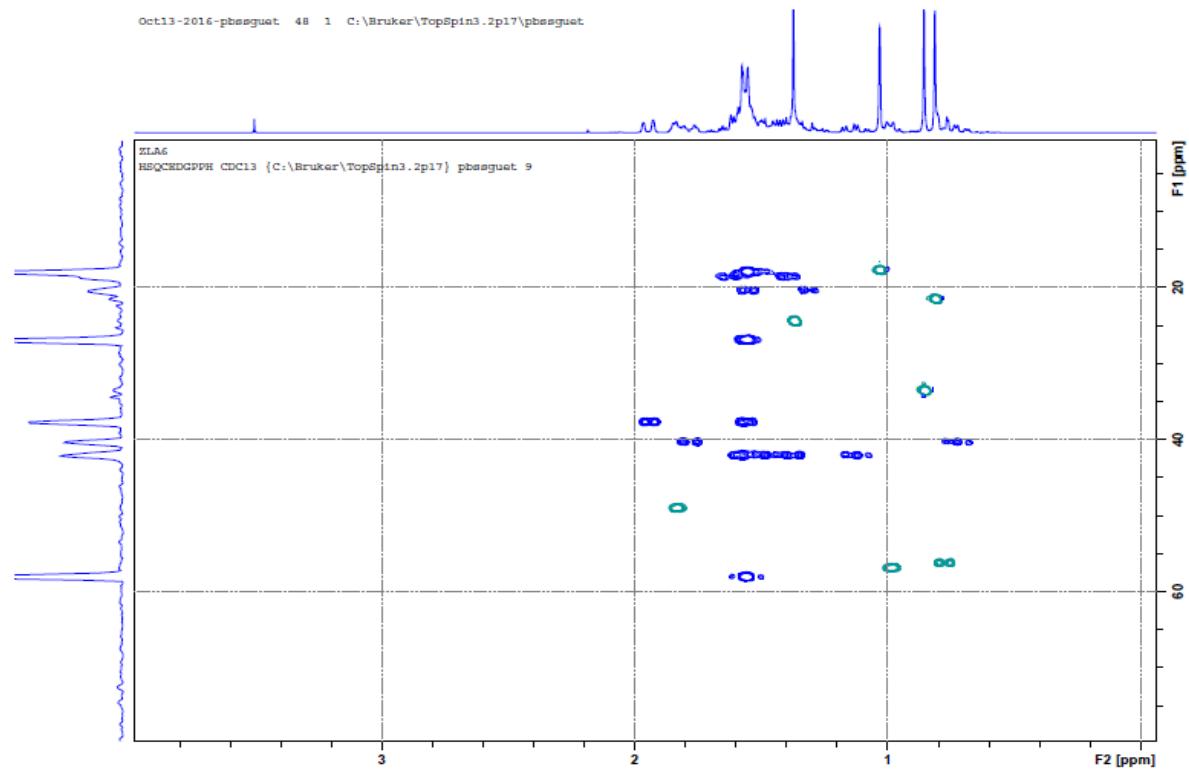
S22: Expansion of the ^1H -NMR Spectrum of Compound **3** (*ent*-kauran-16 β -ol) (from 0 to 3.6 ppm)



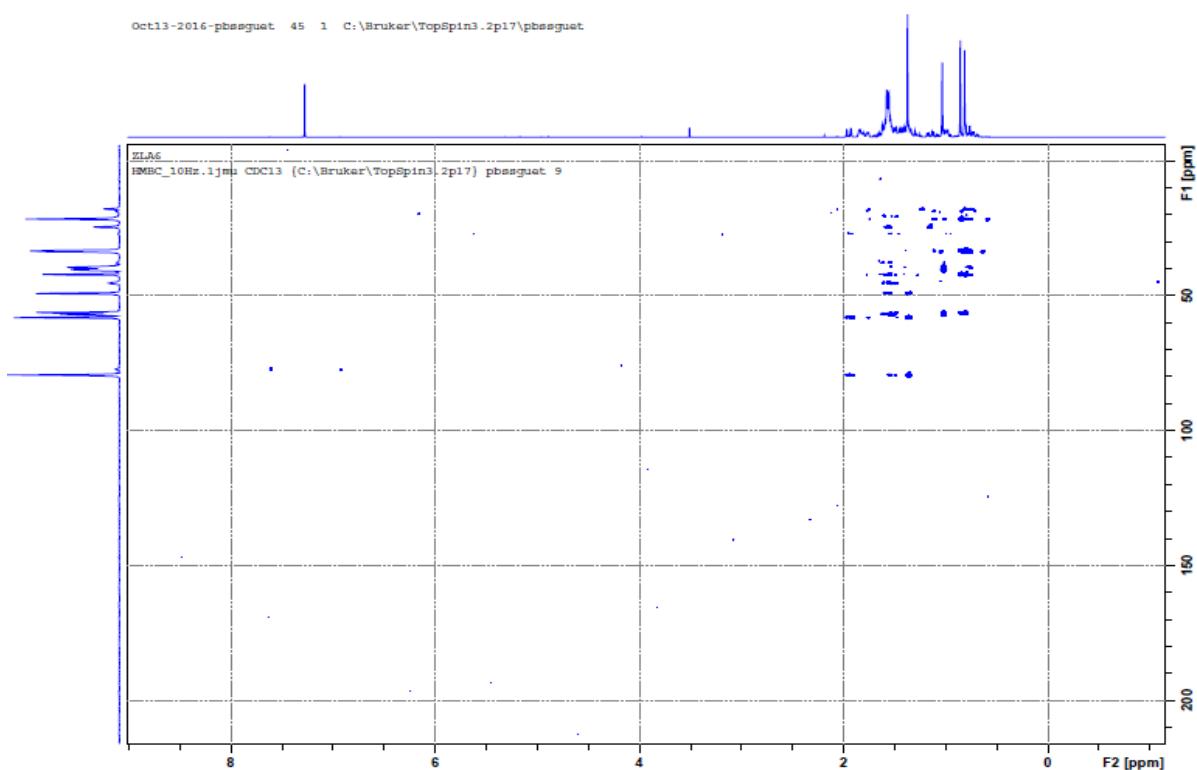
S23: ^{13}C -NMR (75 MHz, CDCl_3) Spectrum of Compound **3** (*ent*-kauran-16 β -ol)



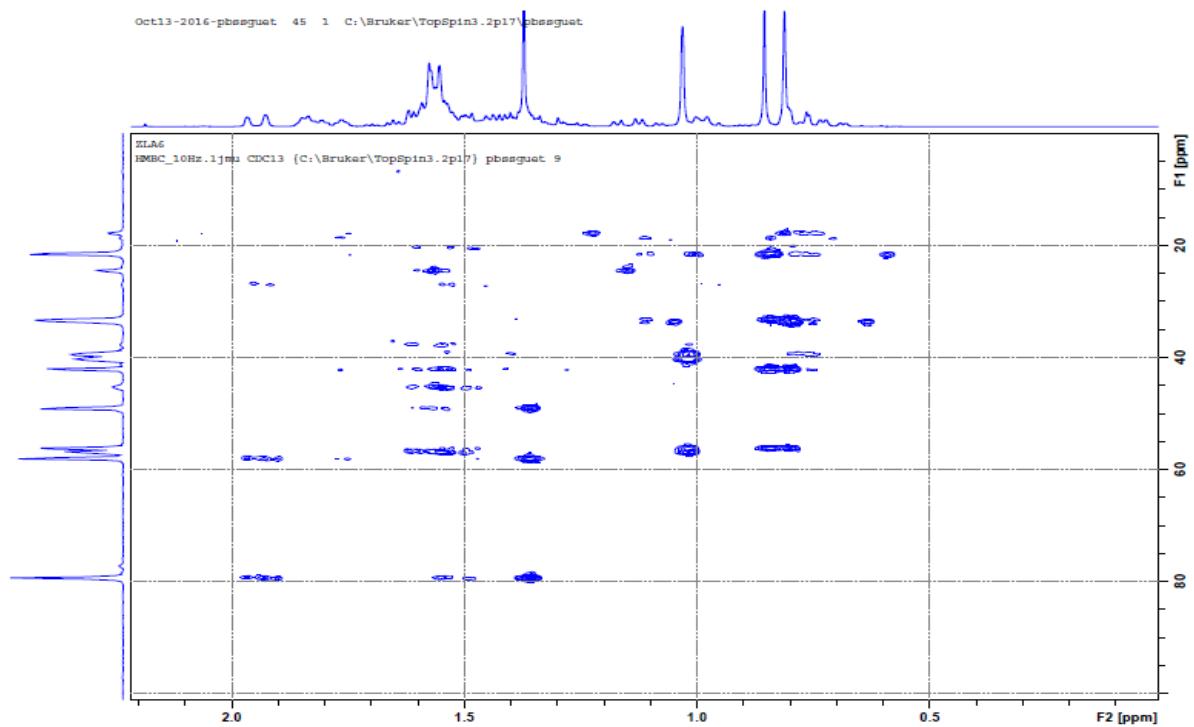
S24: DEPTQ (75 MHz, CDCl_3) Spectrum of Compound **3** (*ent*-kauran-16 β -ol)



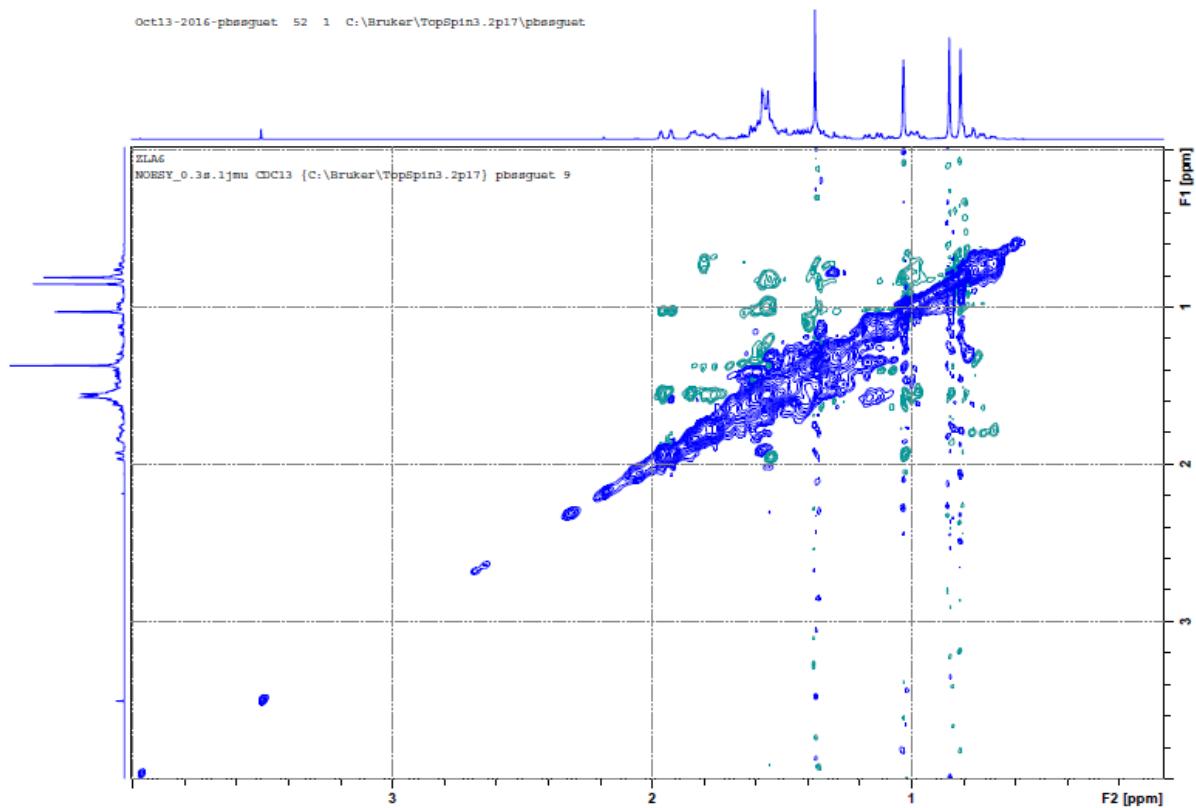
S25: HSQC (300 MHz, CDCl_3) Spectrum of Compound **3** (*ent*-kauran-16 β -ol)



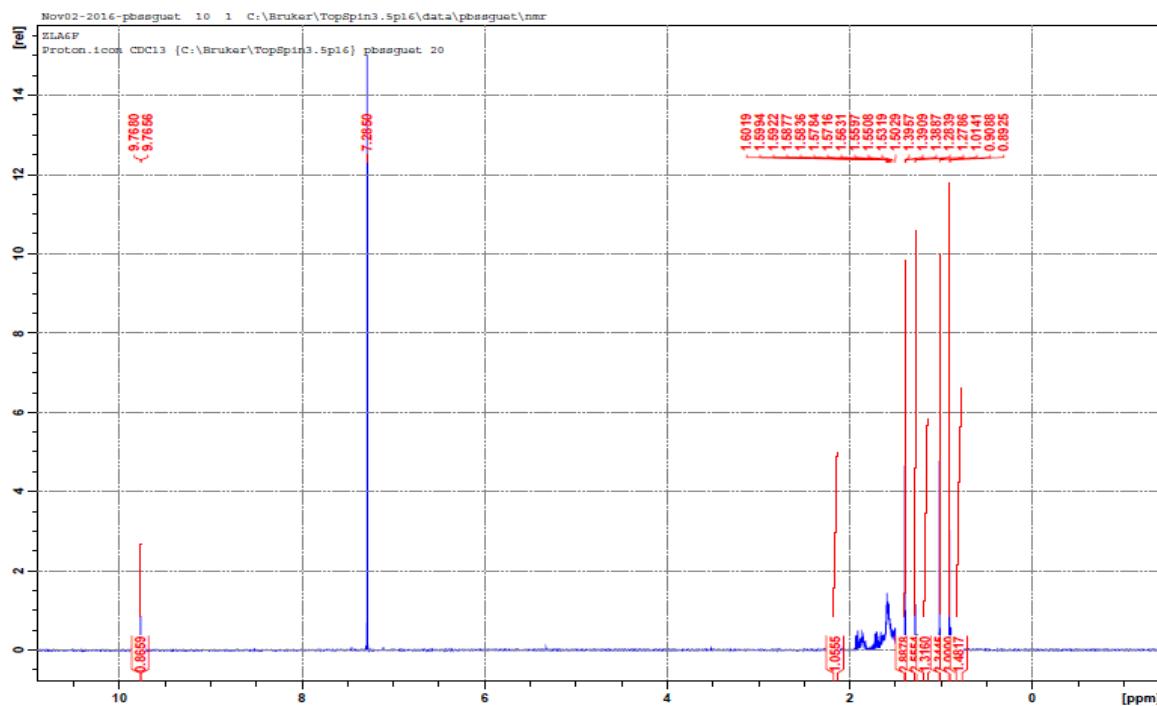
S26: HMBC (500 MHz, CDCl_3) Spectrum of Compound **3** (*ent*-kauran-16 β -ol)



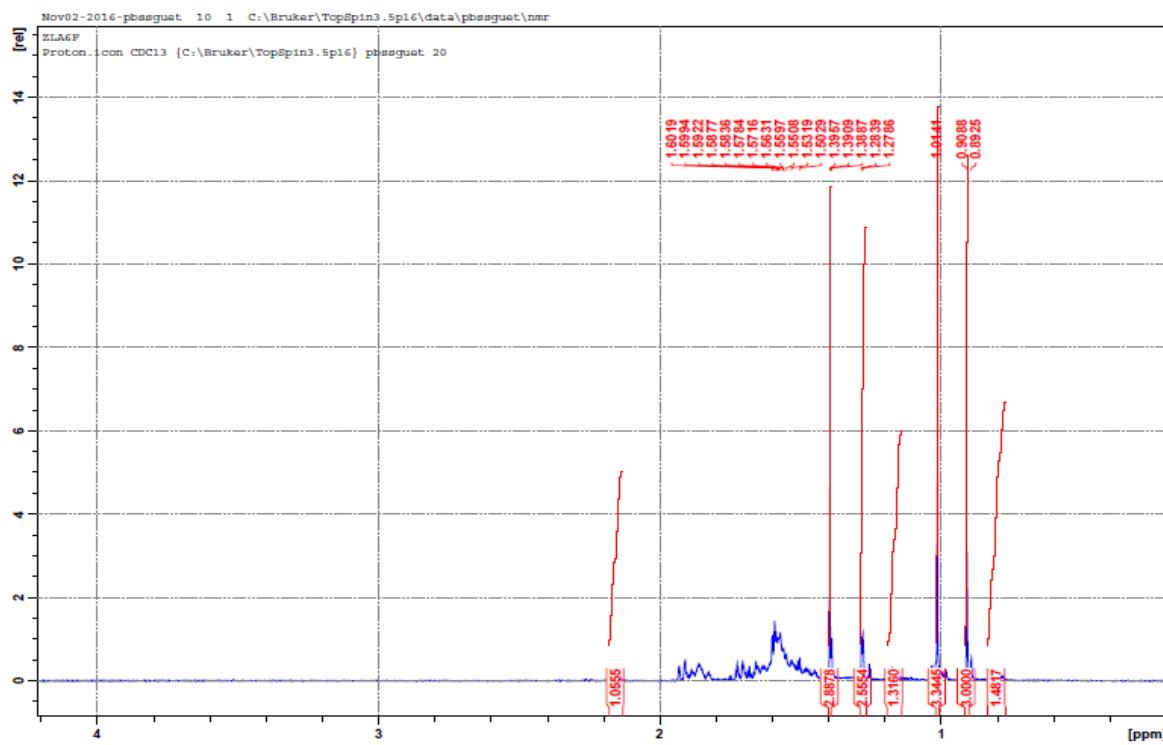
S27: Expansion of the HMBC (300 MHz, CDCl_3) Spectrum of Compound 3 (*ent*-kauran-16 β -ol)



S28: NOESY (500 MHz, CDCl_3) Spectrum of Compound 3 (*ent*-kauran-16 β -ol)

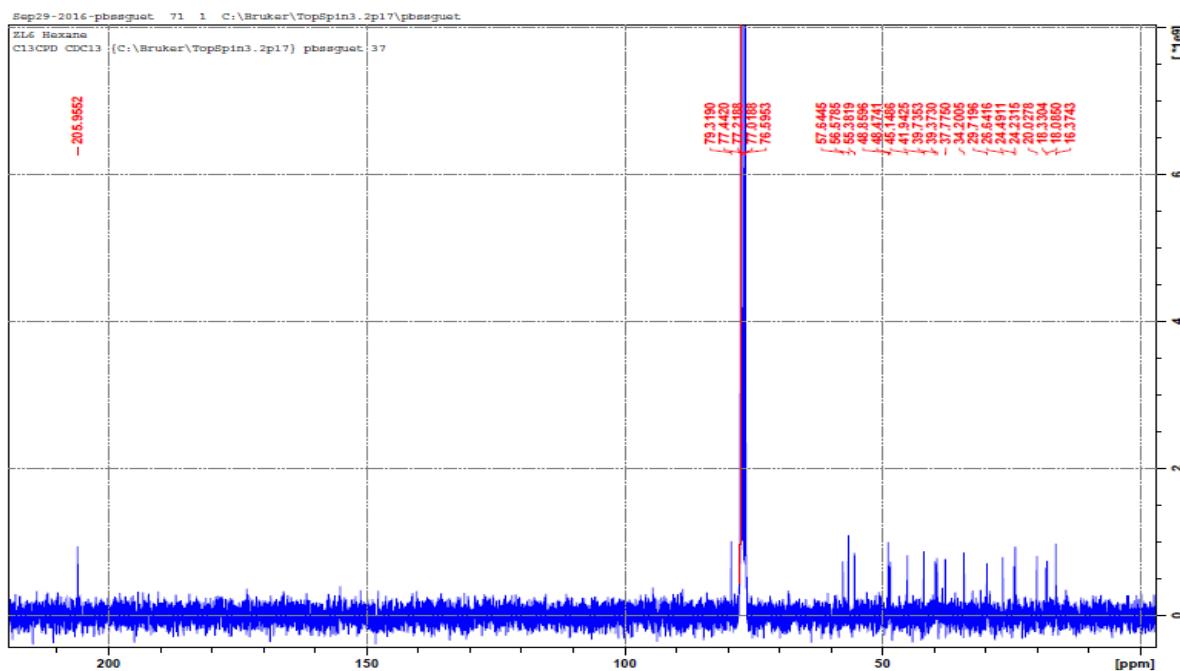


S29: ^1H -NMR (600 MHz, CDCl_3) Spectrum of Compound 4 (*ent*-kauran-16 β -ol-19-al)

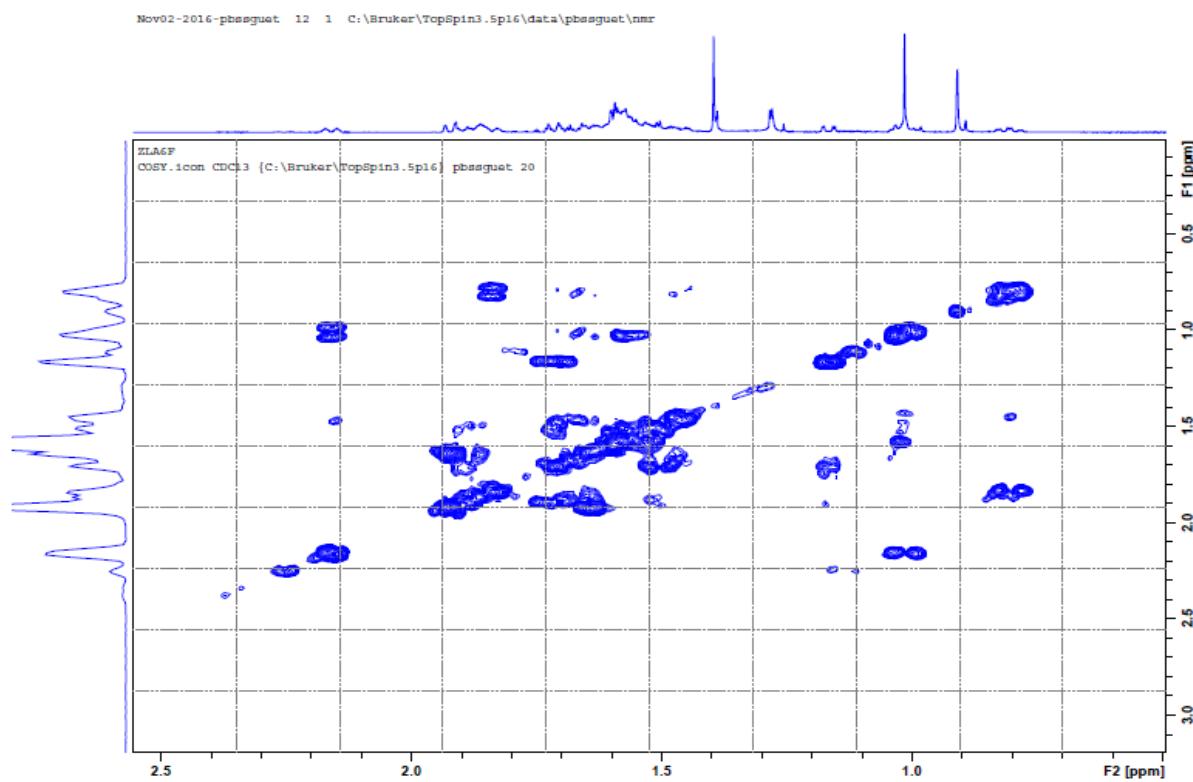


S30: Expansion of the ^1H -NMR Spectrum of Compound 4 (*ent*-kauran-16 β -ol-19-al)

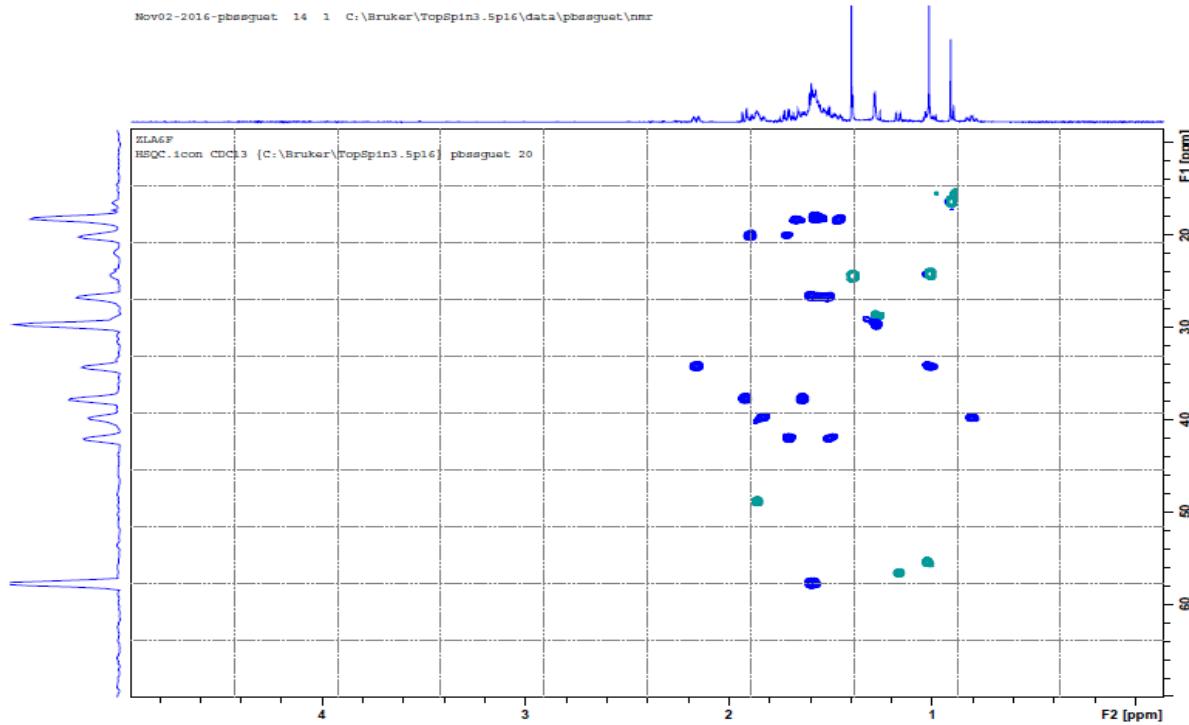
(from 0 to 4.0 ppm)



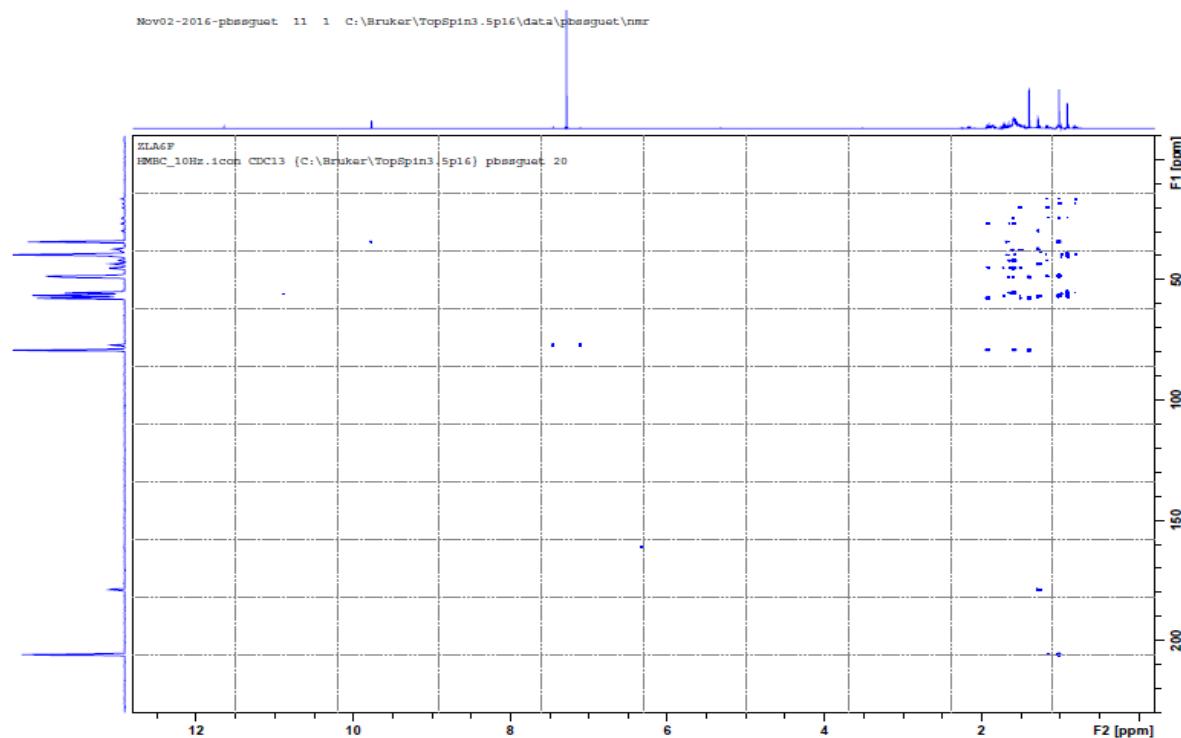
S31: ¹³C-NMR (75 MHz, CDCl₃) Spectrum of Compound 4 (*ent*-kauran-16 β -ol-19-al)



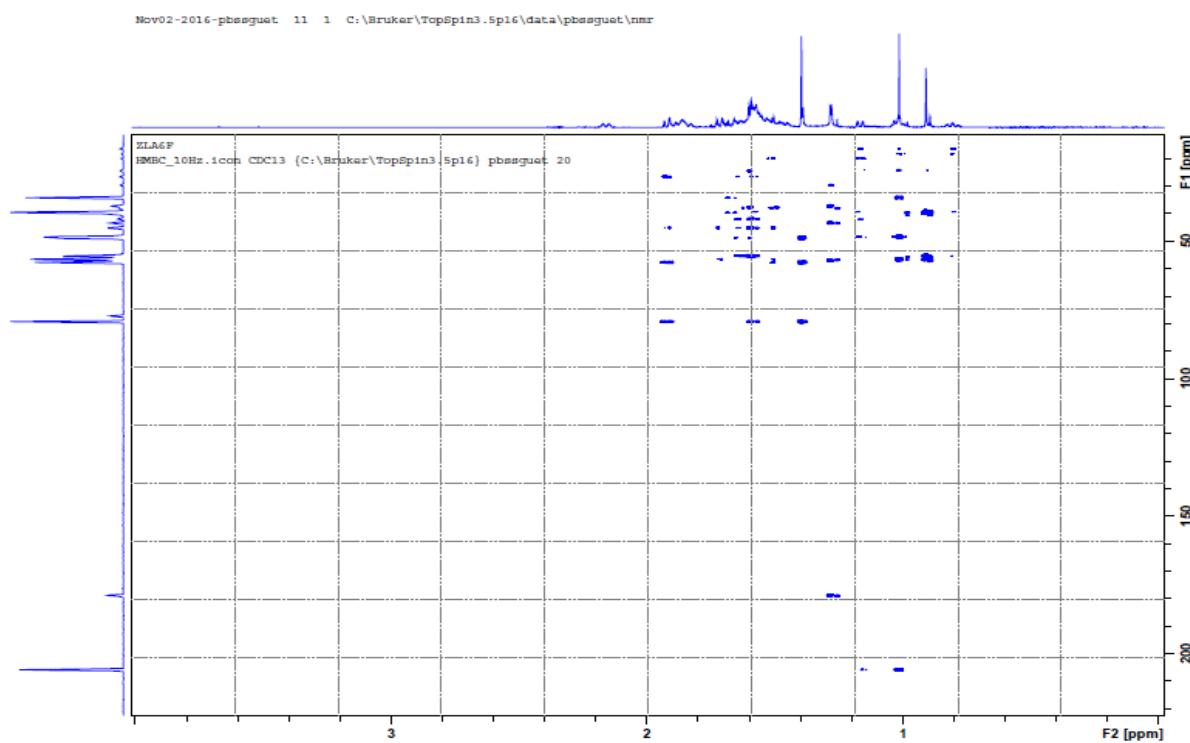
S32: COSY (600 MHz, CDCl₃) Spectrum of Compound 4 (*ent*-kauran-16 β -ol-19-al)



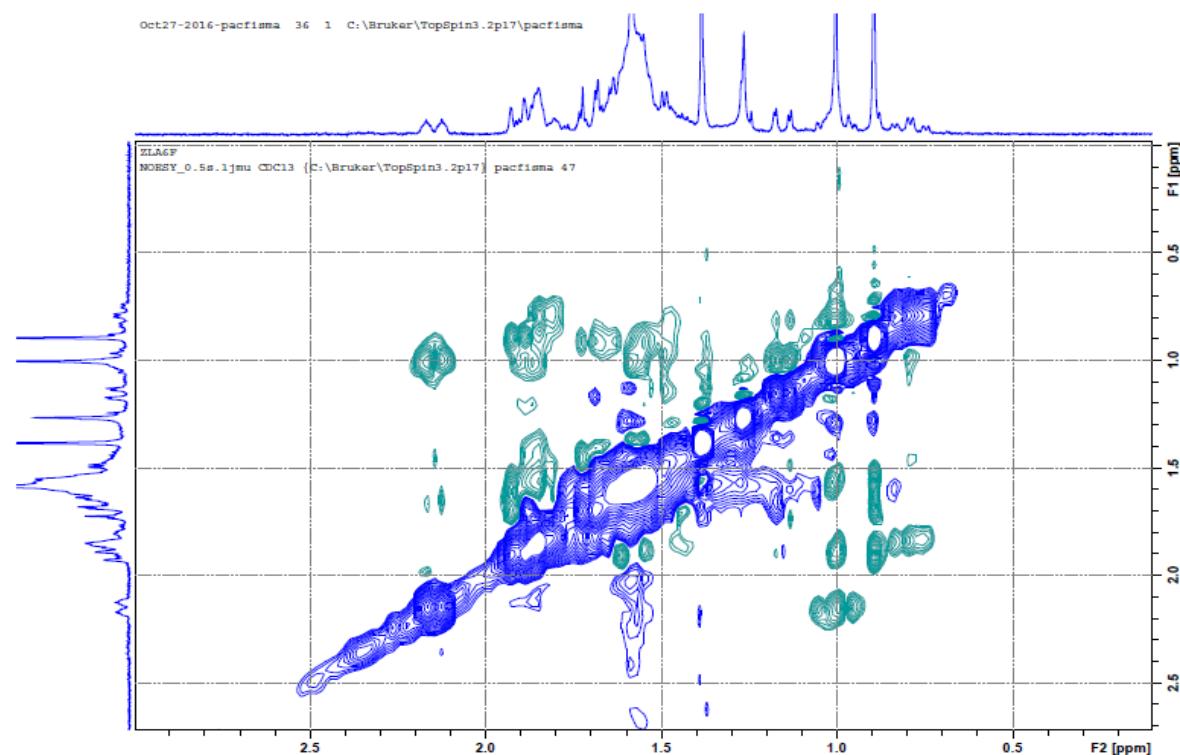
S33: HSQC (600 MHz, CDCl₃) Spectrum of Compound **4** (*ent*-kauran-16 β -ol-19-al)



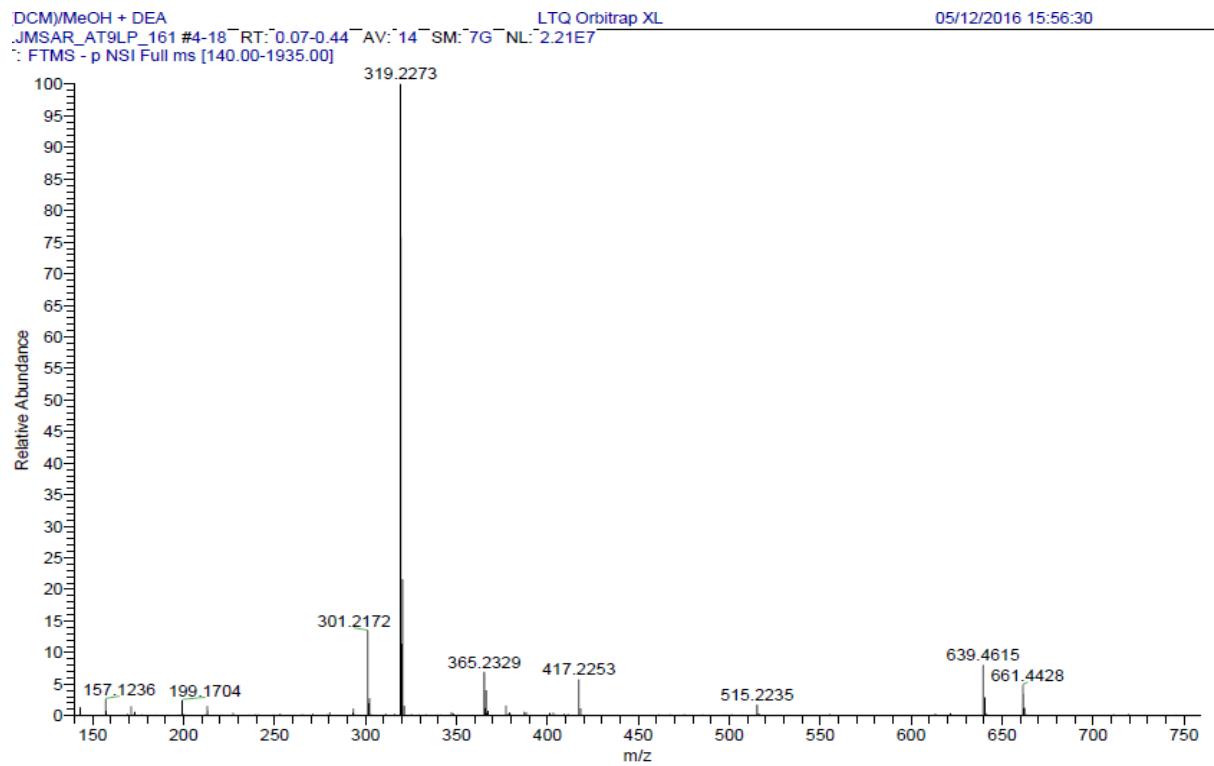
S34: HMBC (600 MHz, CDCl₃) Spectrum of Compound 4 (ent-kauran-16 β -ol-19-al)



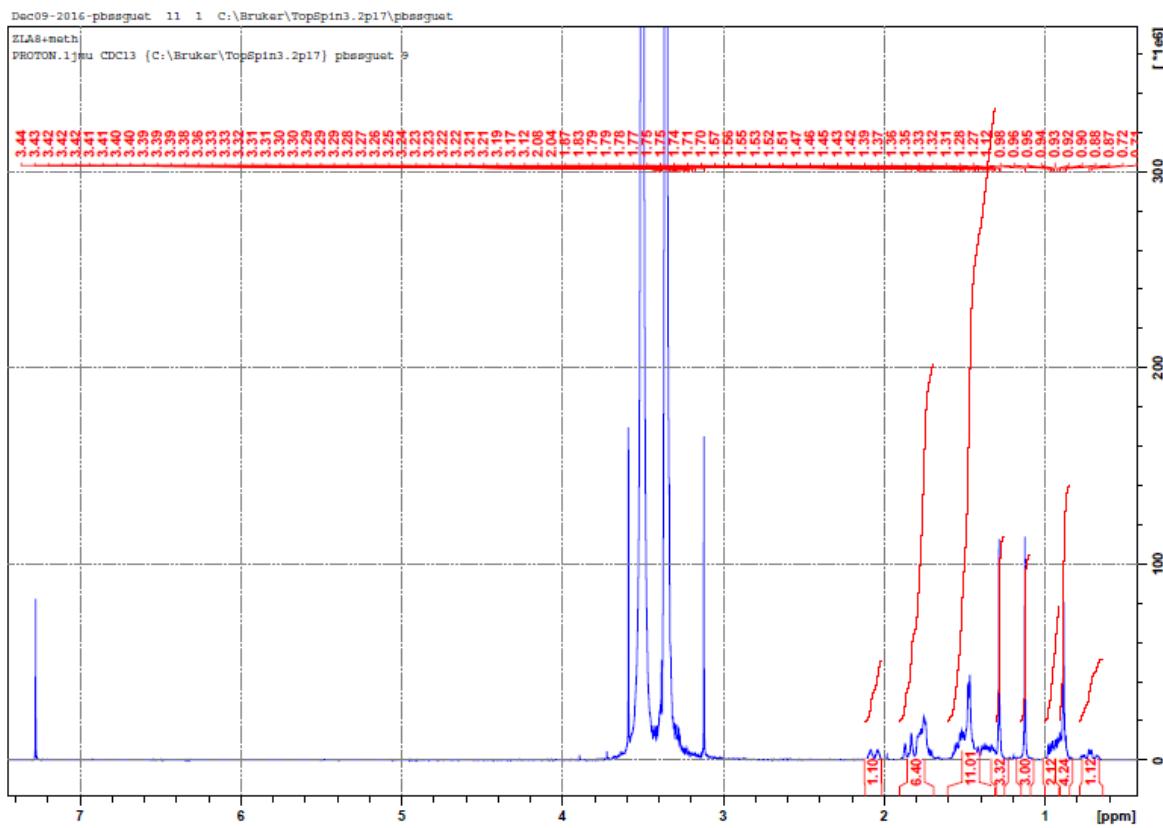
S35: Expansion of the HMBC (600 MHz, CDCl₃) Spectrum of Compound 4 (ent-kauran-16 β -ol-19-al)

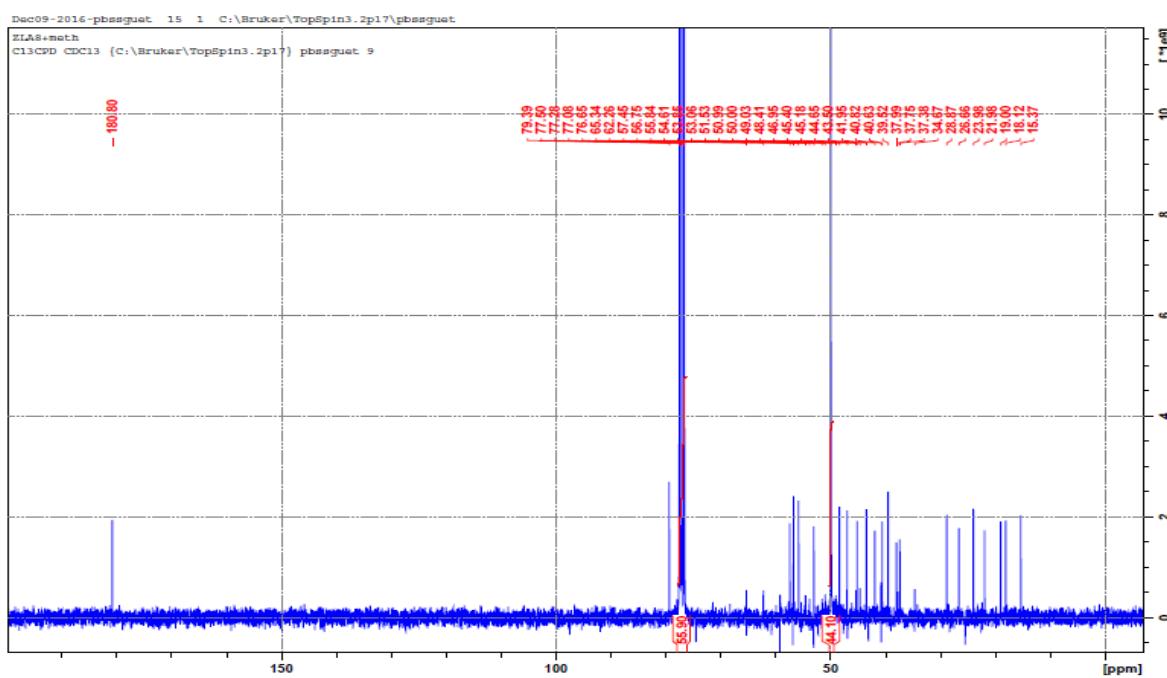


S36: NOESY (300 MHz, CDCl₃) Spectrum of Compound 4 (ent-kauran-16 β -ol-19-al)

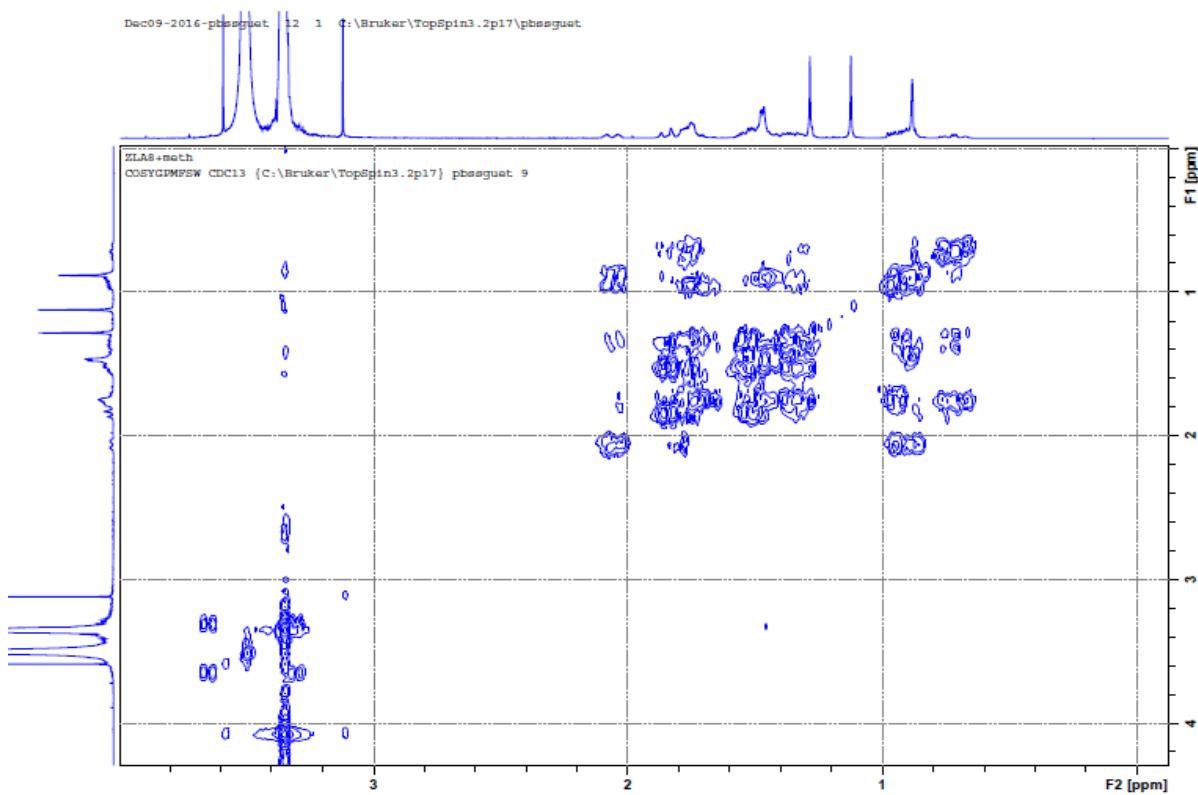


S37: HRESI-MS Spectrum of Compound 5 (*ent*-kauran-16 β -ol-19oic acid)

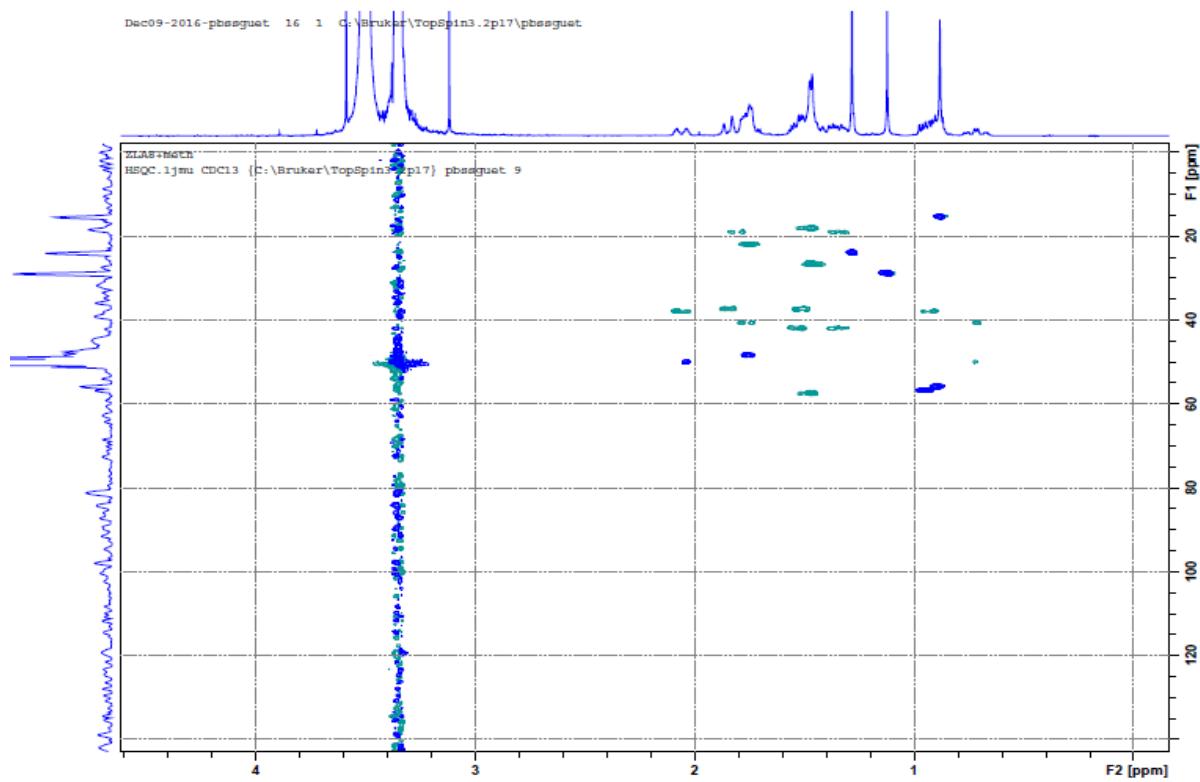




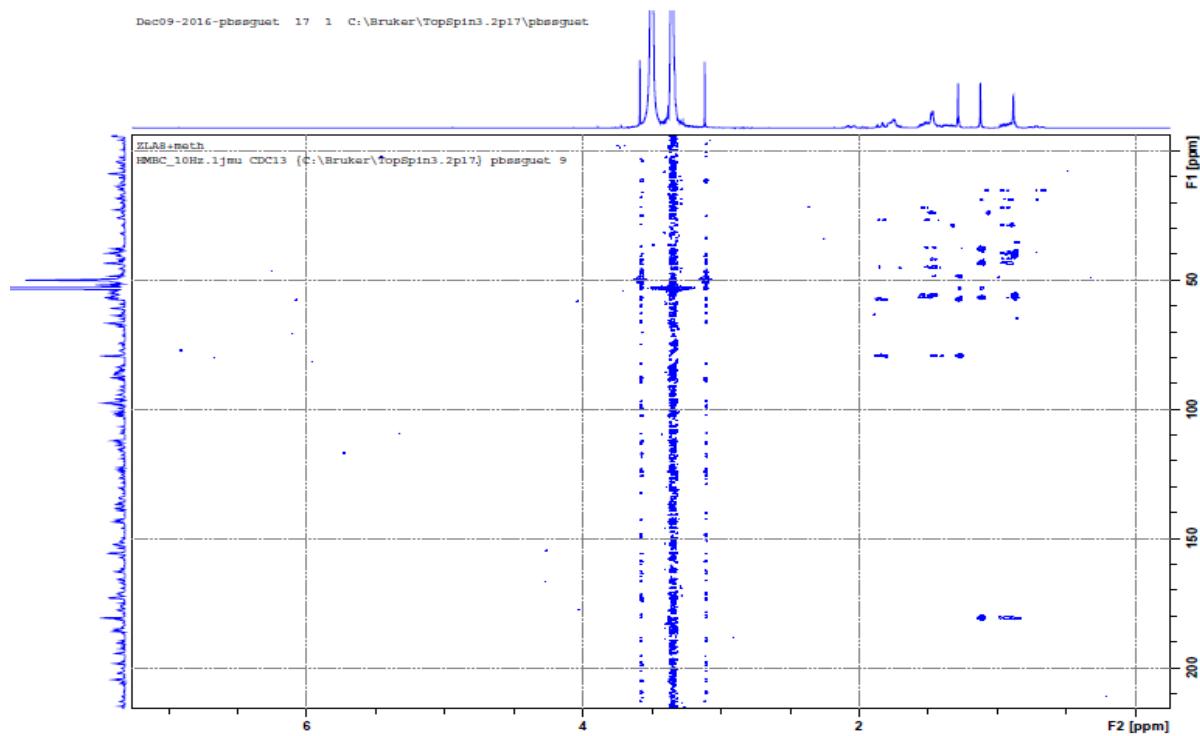
S39: ¹³C-NMR (75 MHz, CDCl₃+ drops of MeOH) Spectrum of Compound 5 (ent-kauran-16 β -ol-19oic acid)



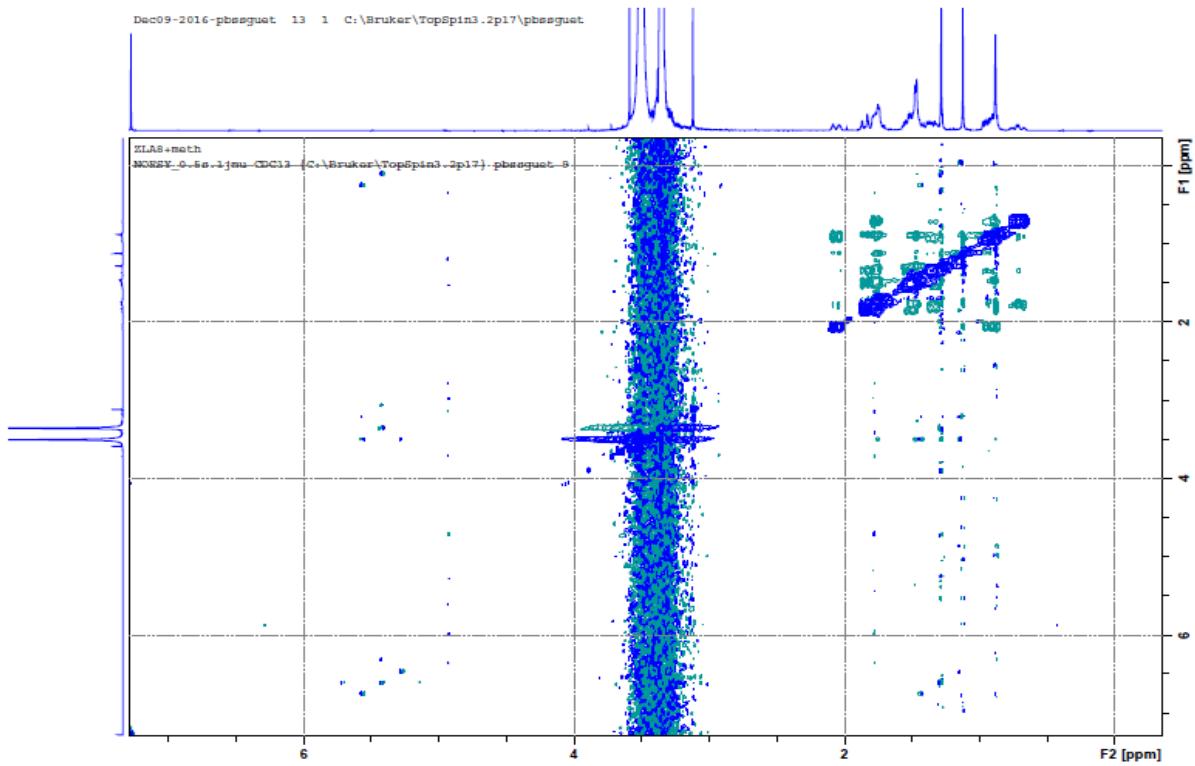
S40: COSY (300 MHz, CDCl₃+ drops of MeOH) Spectrum Spectrum of Compound 5 (ent-kauran-16 β -ol-19oic acid)



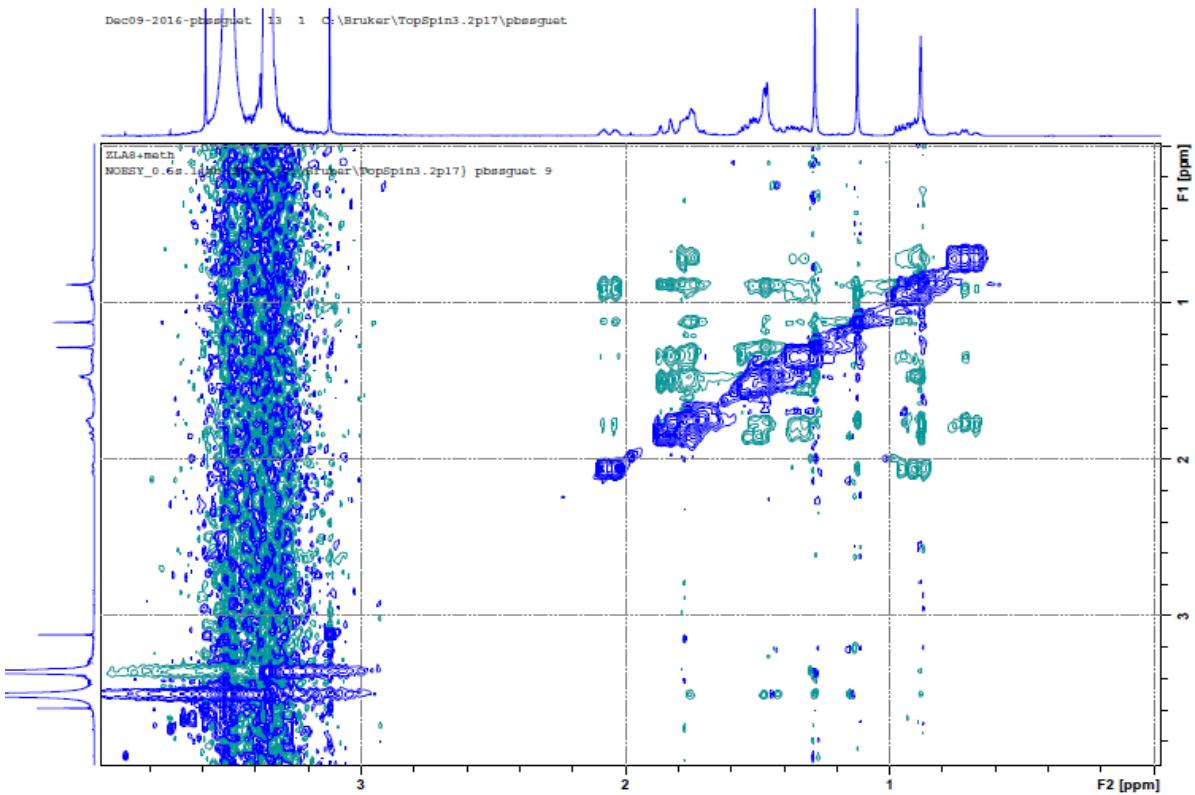
S41: HSQC (300 MHz, CDCl₃+ drops of MeOH) Spectrum of Compound **5** (*ent*-kauran-16 β -ol-19oic acid)



S42: HMBC (300 MHz, CDCl₃+ drops of MeOH) Spectrum of Compound **5** (*ent*-kauran-16 β -ol-19oic acid)



S43: NOESY (300 MHz, CDCl_3 + drops of MeOH) Spectrum of Compound **5** (*ent*-kauran-16 β -ol-19oic acid)



S44: Expansion of the NOESY Spectrum of Compound **5** (*ent*-kauran-16 β -ol-19oic acid)