

Supporting Information

Efficient Synthesis of the Anticancer β - Elemene and Other Bioactive Elemanes from Sustainable Germacrone

Alejandro F. Barrero, M. Mar Herrador,* José F. Quílez del Moral, Pilar Arteaga,
Niklas Meine, M. Carmen Pérez-Morales and Julieta V. Catalán.*

Department of Organic Chemistry, Institute of Biotechnology, Facultad de Ciencias,
University of Granada, Campus de Fuente Nueva, s/n, 18071 Granada, Spain,

afbarre@ugr.es; mmar@ugr.es.

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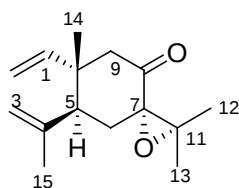
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COSY, HSQC, HMBC and NOE diff data of epoxide 13

S2

Spectra

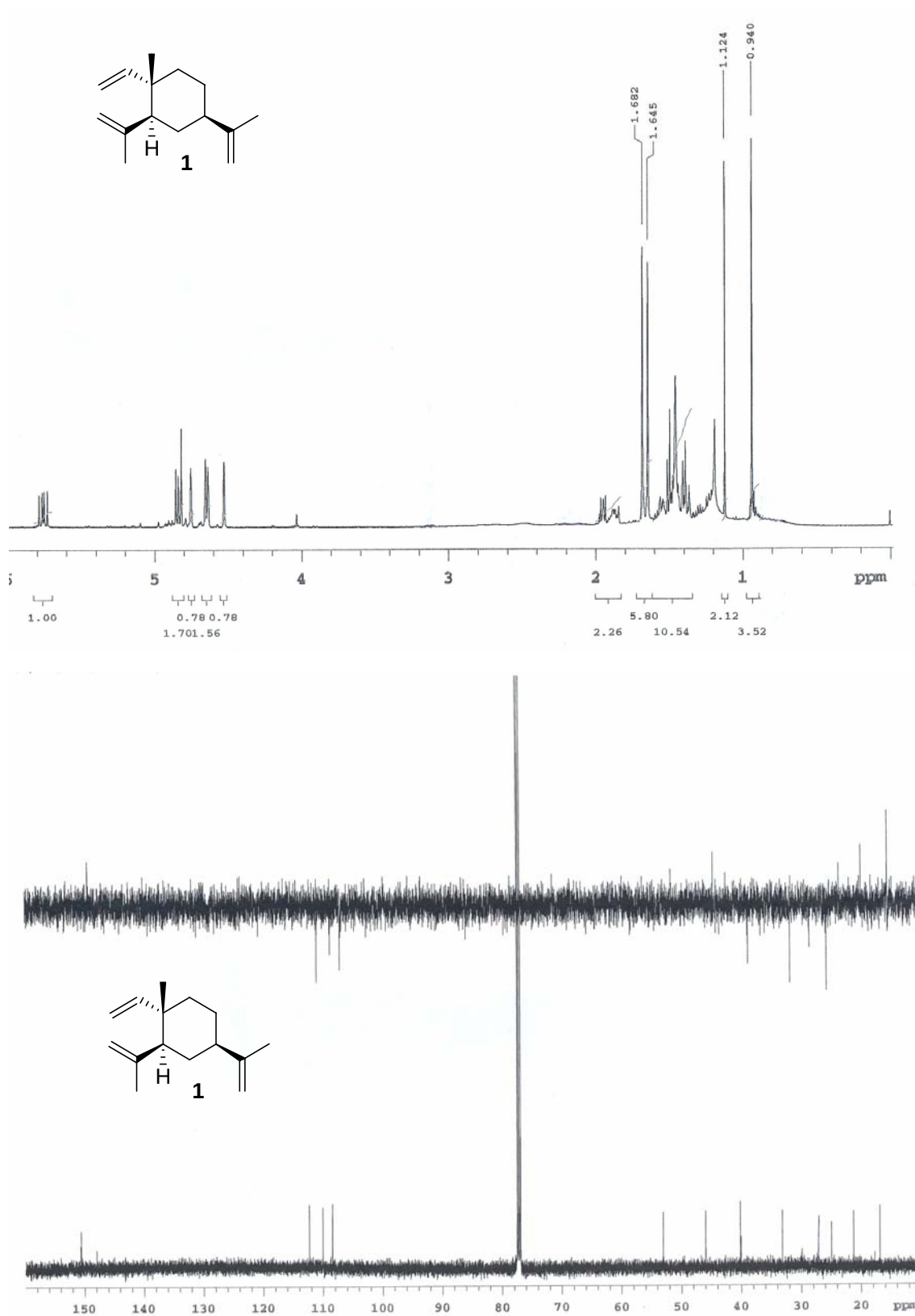
S3- S15

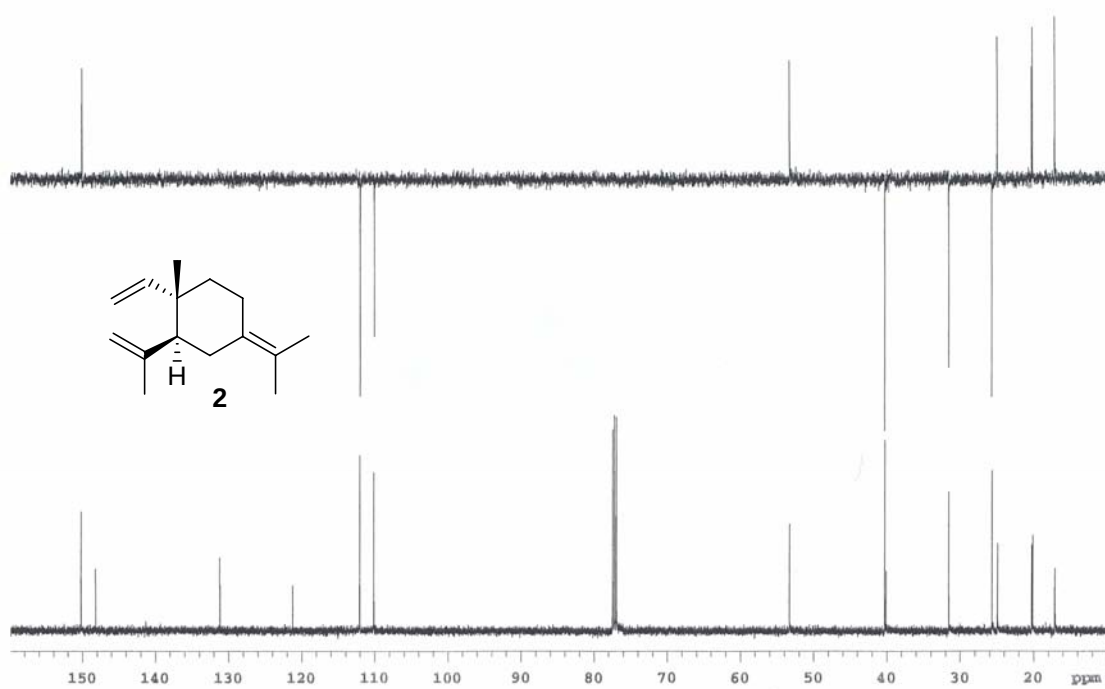
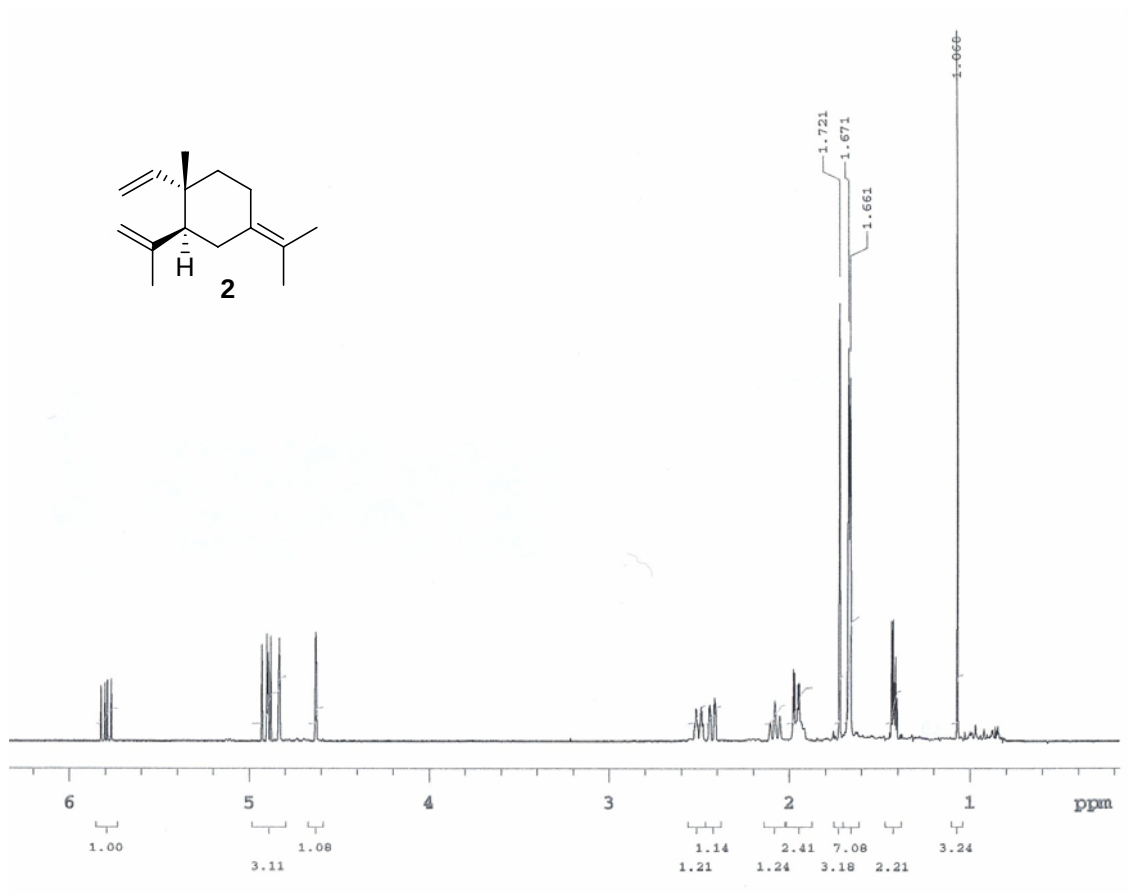


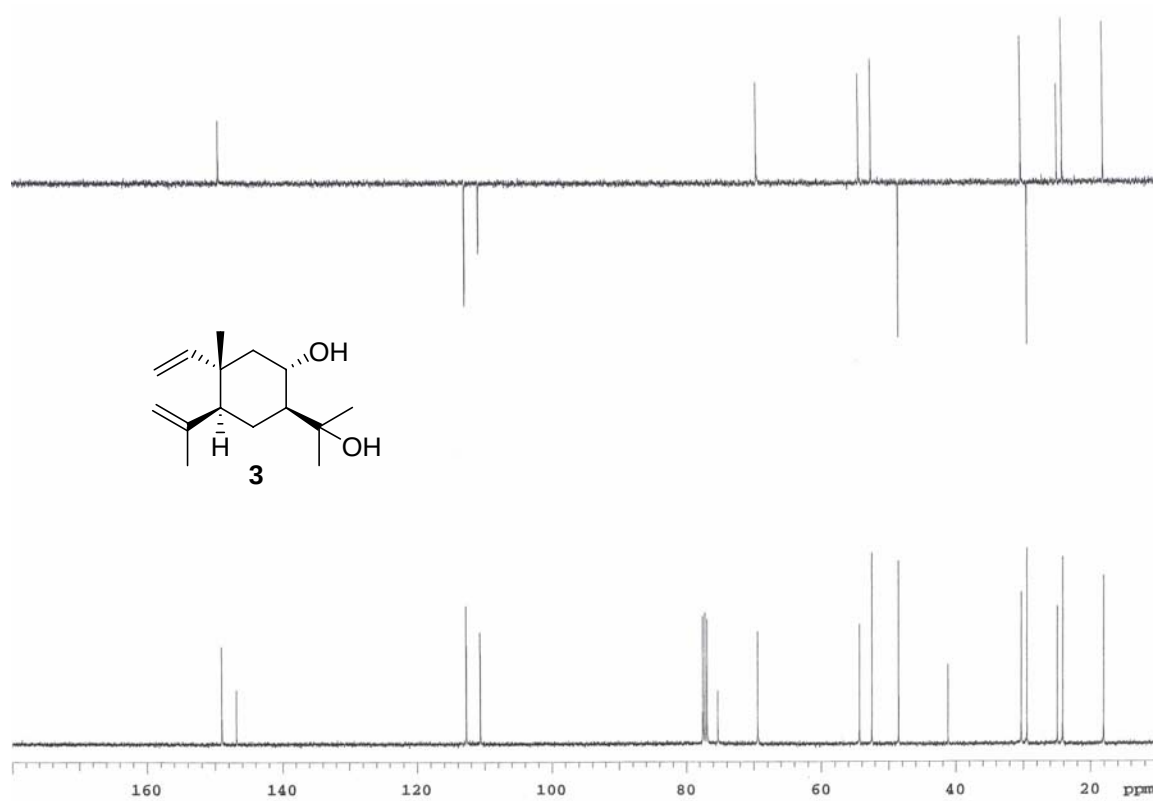
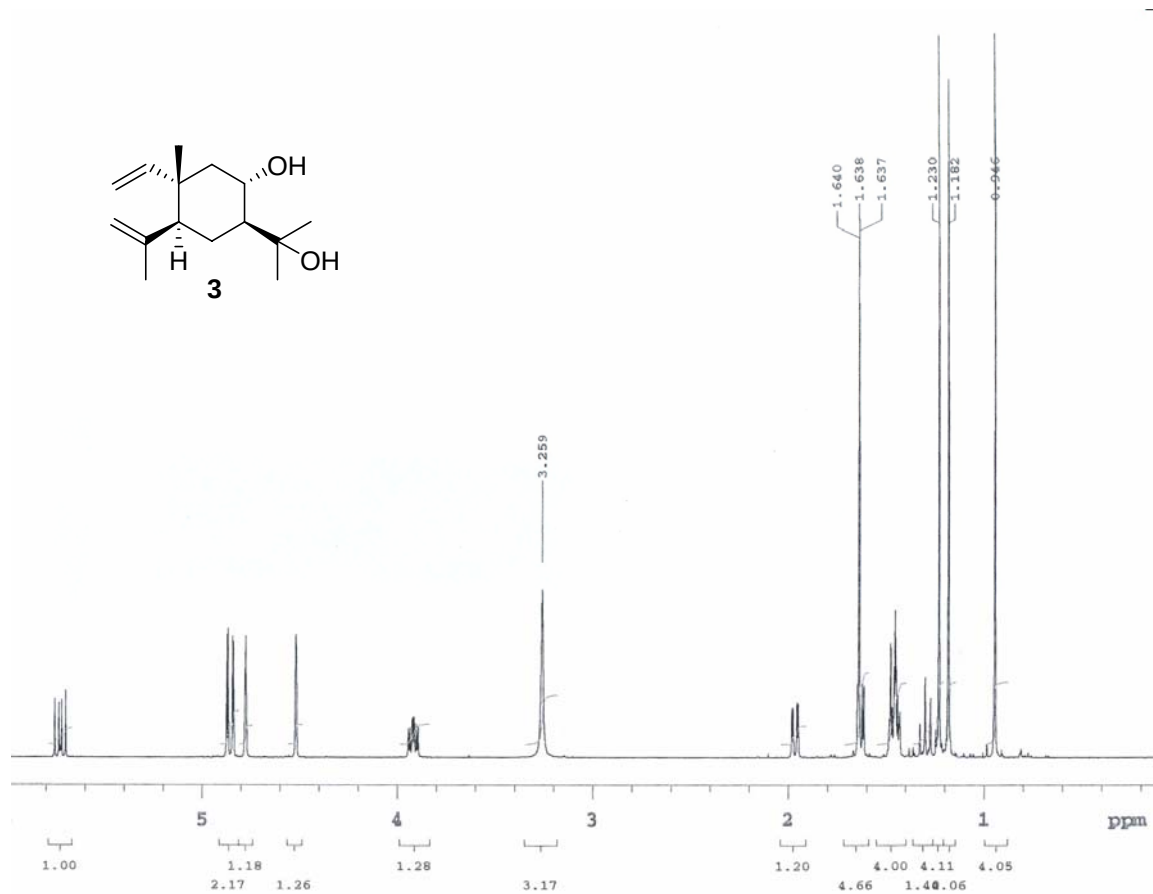
Correlation of COSY, HSQC and HMBC of (5*S*,7*R*,10*S*)-7,11-epoxyelema-1,3-dien-8-one (13)

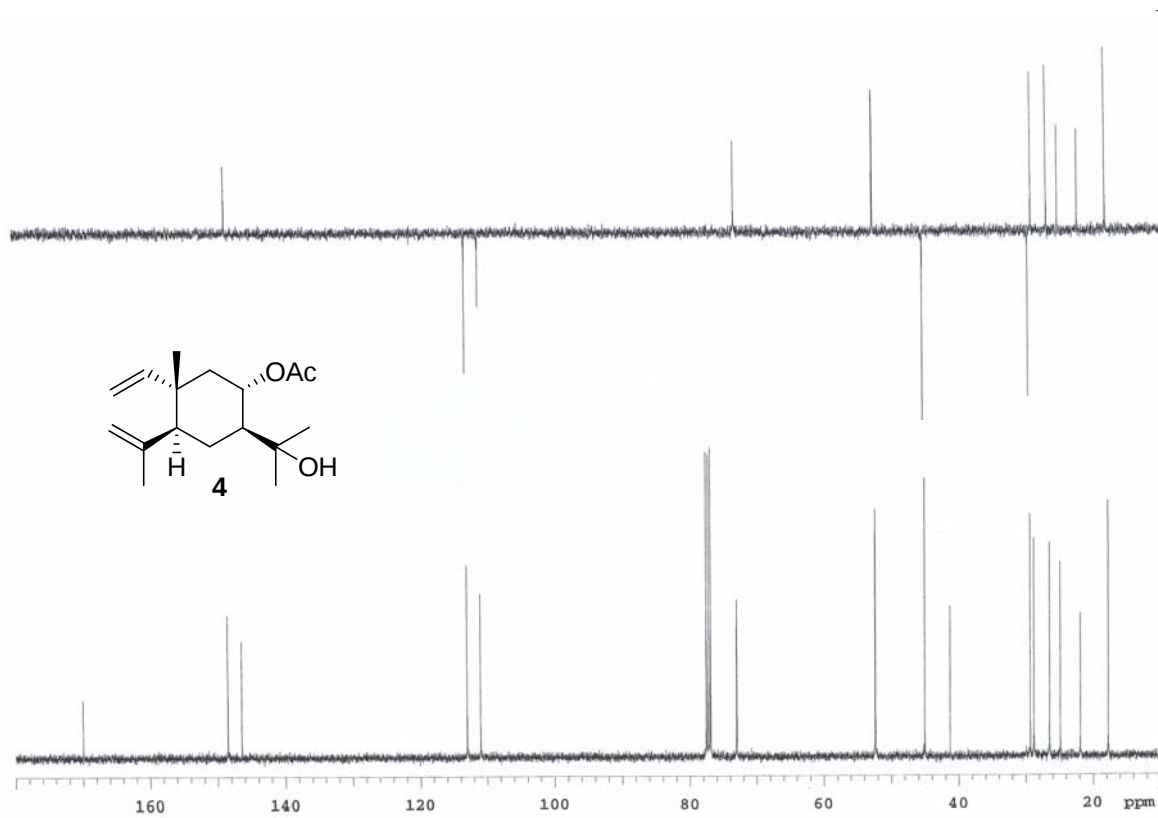
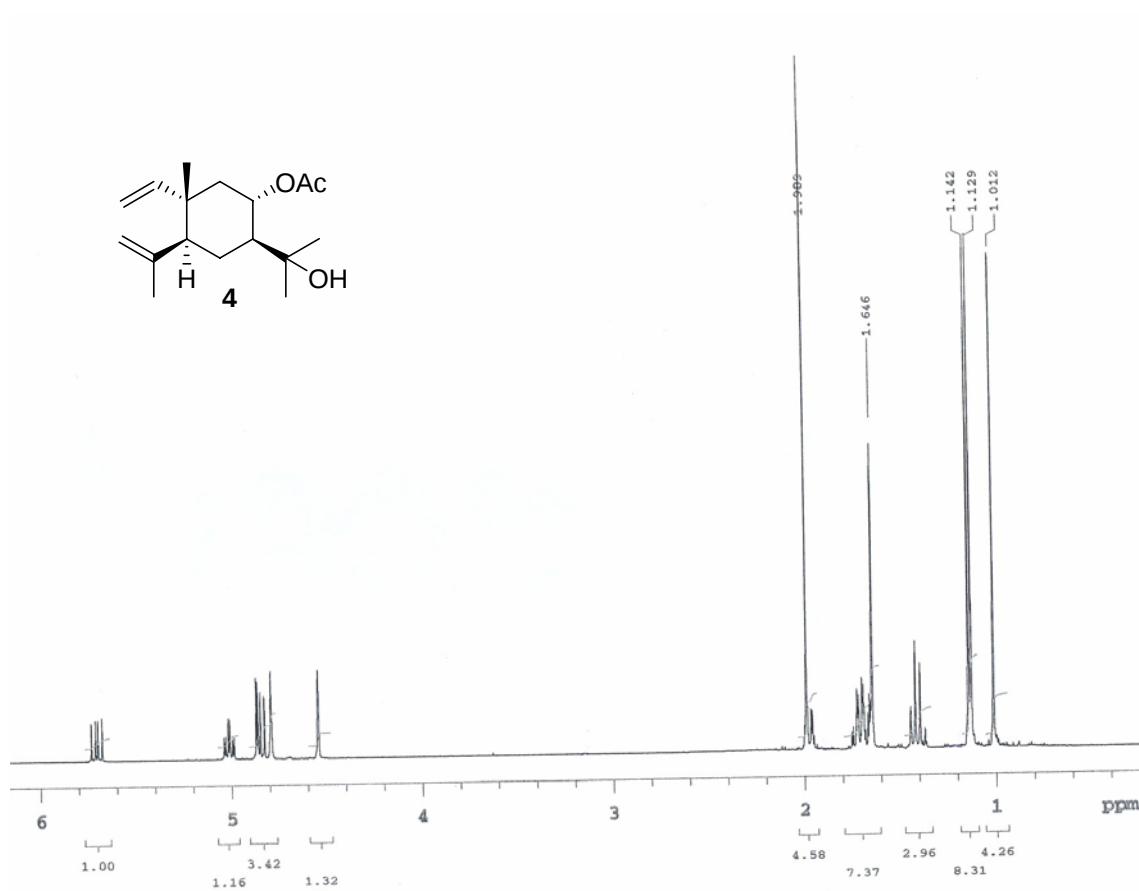
COSY	HSQC	HMBC
H-1 → H-2a, H-2b	C-1 → H-1	C-1 → H-5 α , H-9a, H-9b, H-14
H-2a → H-2b, H-1	C-2 → H-2a, H-2b	C-3 → H-5 α , H-15
H-2b → H-2a, H-1	C-3 → H-3a, H-3b	C-4 → H-3a, H-3b, H-5 α , 2 H-6, H-15
H-3a → H-3b, H-15	C-5 → H-5 α	C-5 → H-3a, H-3b, 2 H-6, H-9a, H-9b, H-14, H-15
H-3b → H-3a, H-15	C-6 → H-6a, H-6b	C-6 → H-5 α
H-5 α → 2 H-6	C-9 → H-9a, H-9b	C-7 → 2 H-6, H-9a, H-9b, H-12, H-13
2 H-6 → H-5 α , H-12	C-12 → H-12	C-8 → 2 H-6, H-9a, H-9b
H-9a → H-9b	C-13 → H-13	C-9 → H-1, H-14
H-9b → H-9a	C-14 → H-14	C-10 → H-1, H-2a, H-2b, H-5 α , 2 H-6, H-9a, H-9b, H-14
H-12 → 2 H-6	C-15 → H-15	C-11 → 2 H-6, H-12, H-13
H-15 → H-3a, H-3b		C-12 → H-13
		C-13 → H-12
		C-14 → H-1, H-9a, H-9b
		C-15 → H-3a, H-3b, H-5 α

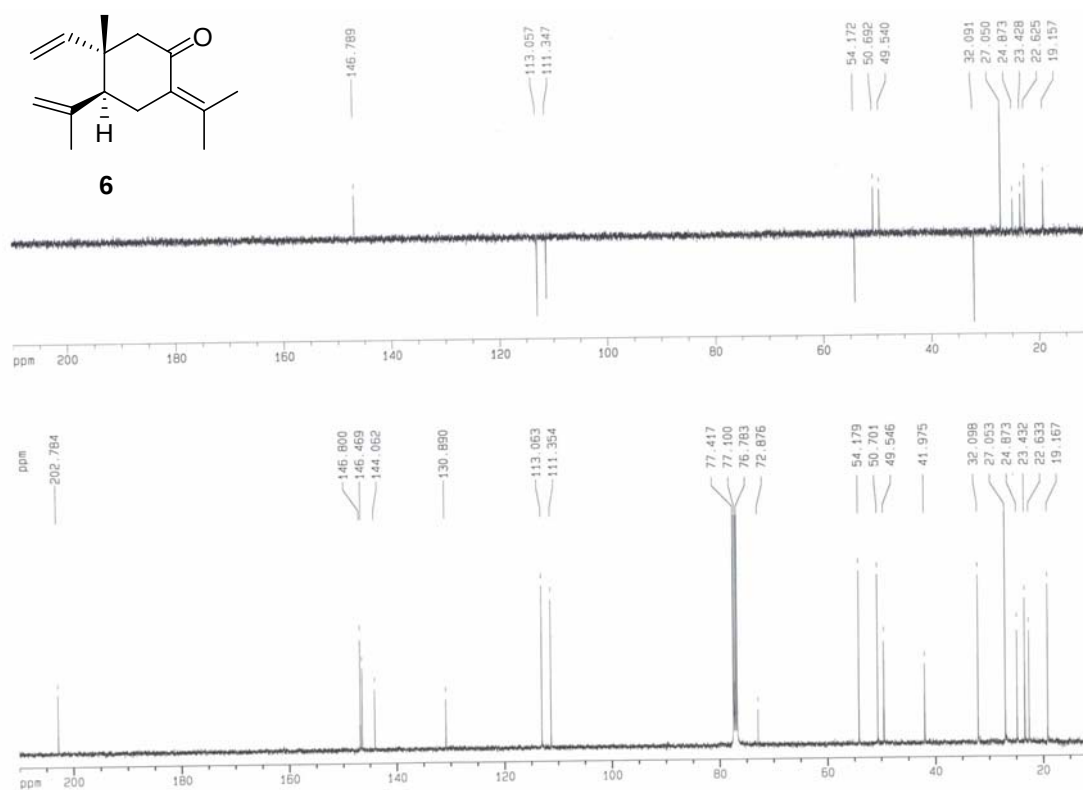
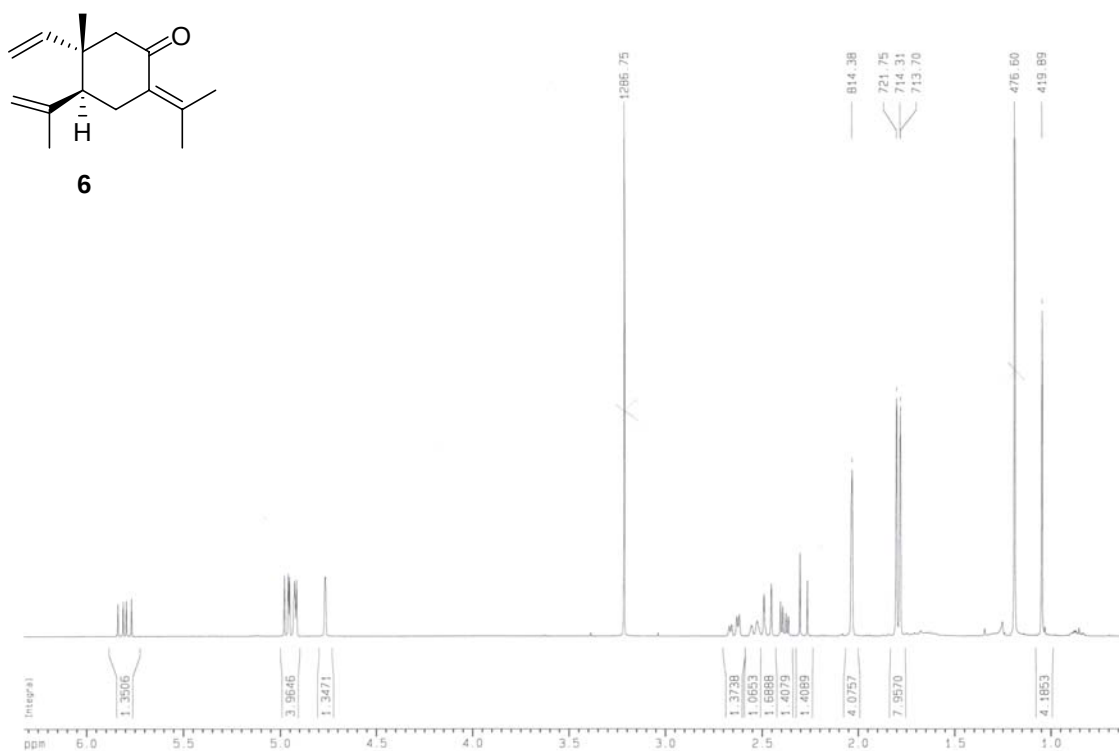
NOE diff.: H-13 with H-12 and H-6; H-12 with H-13.

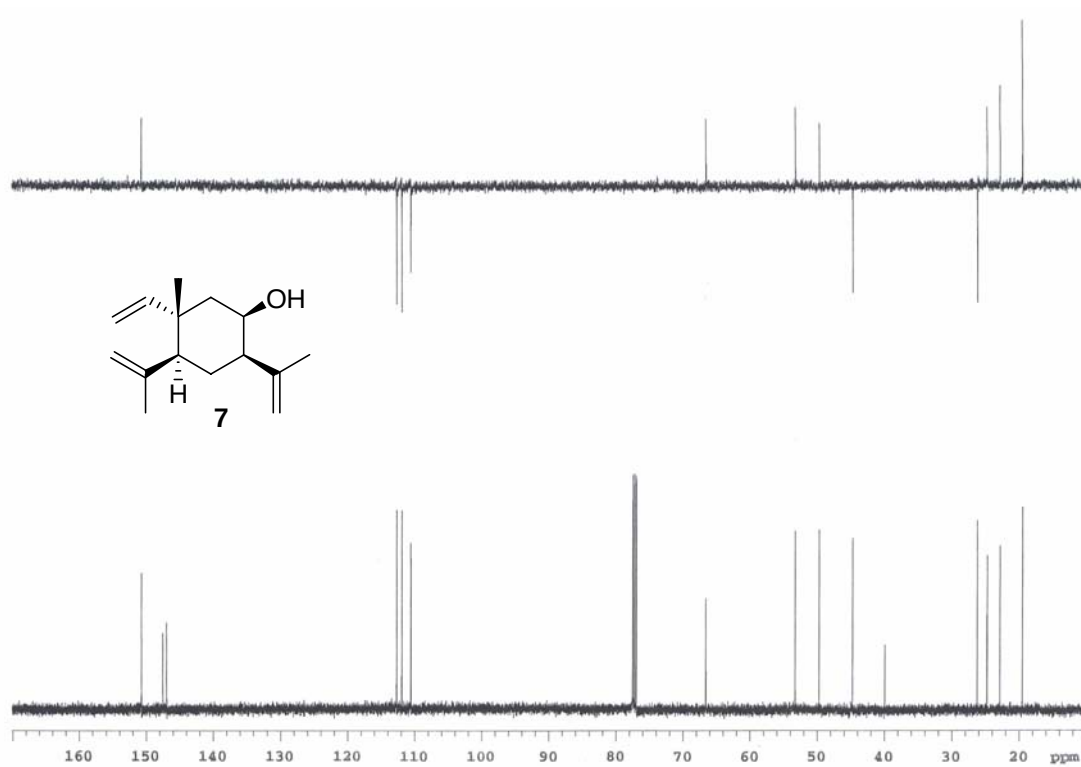
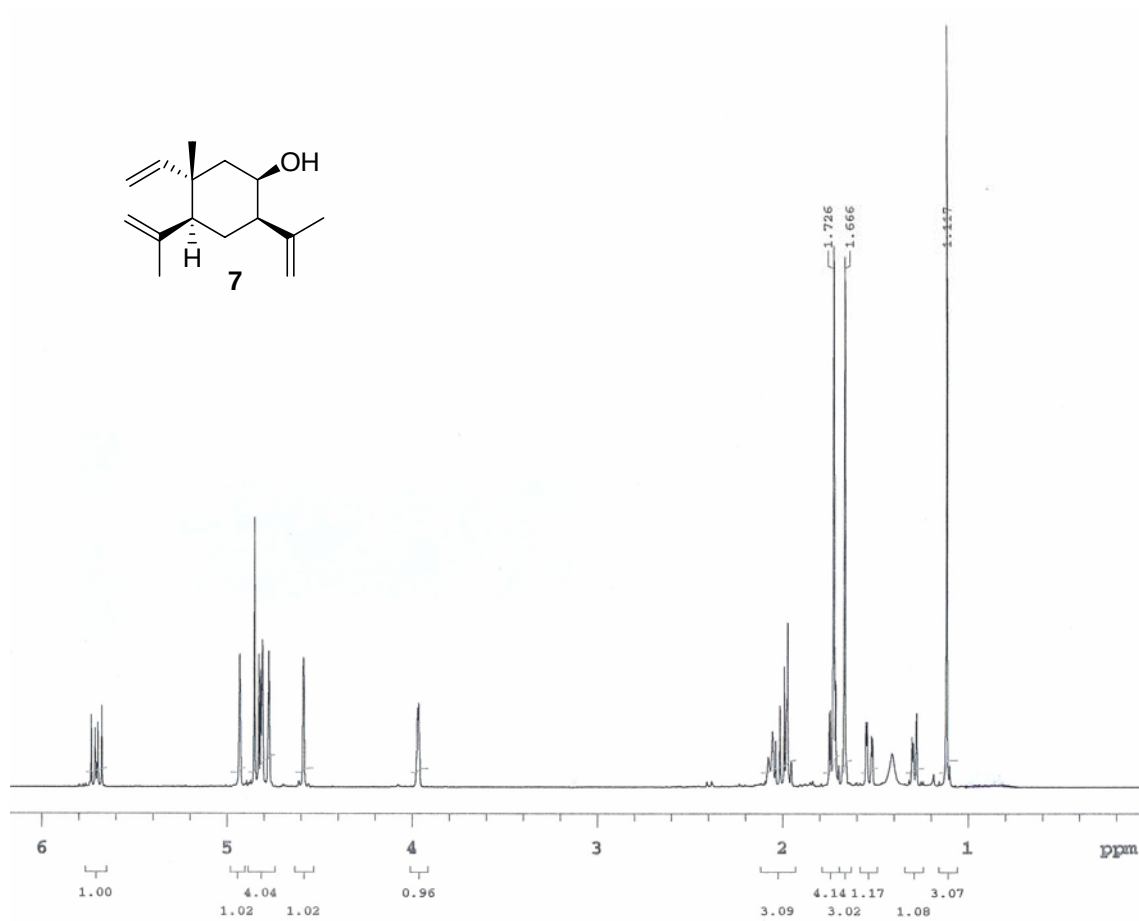


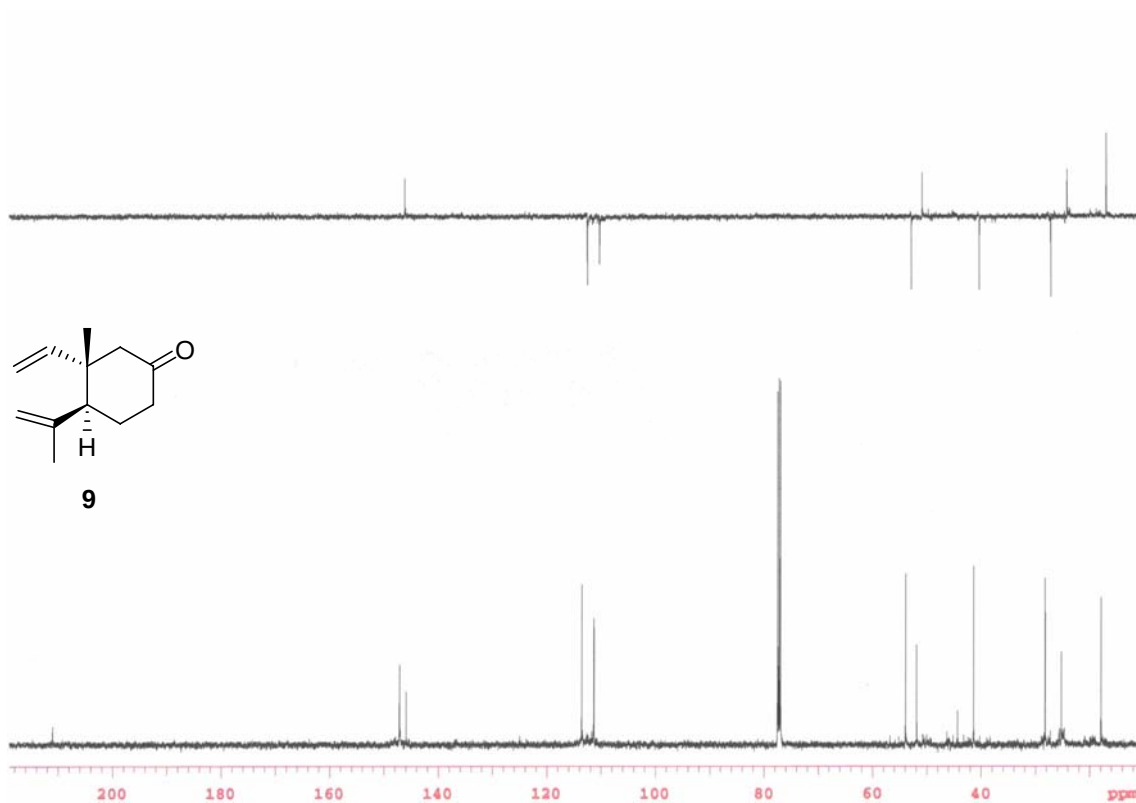
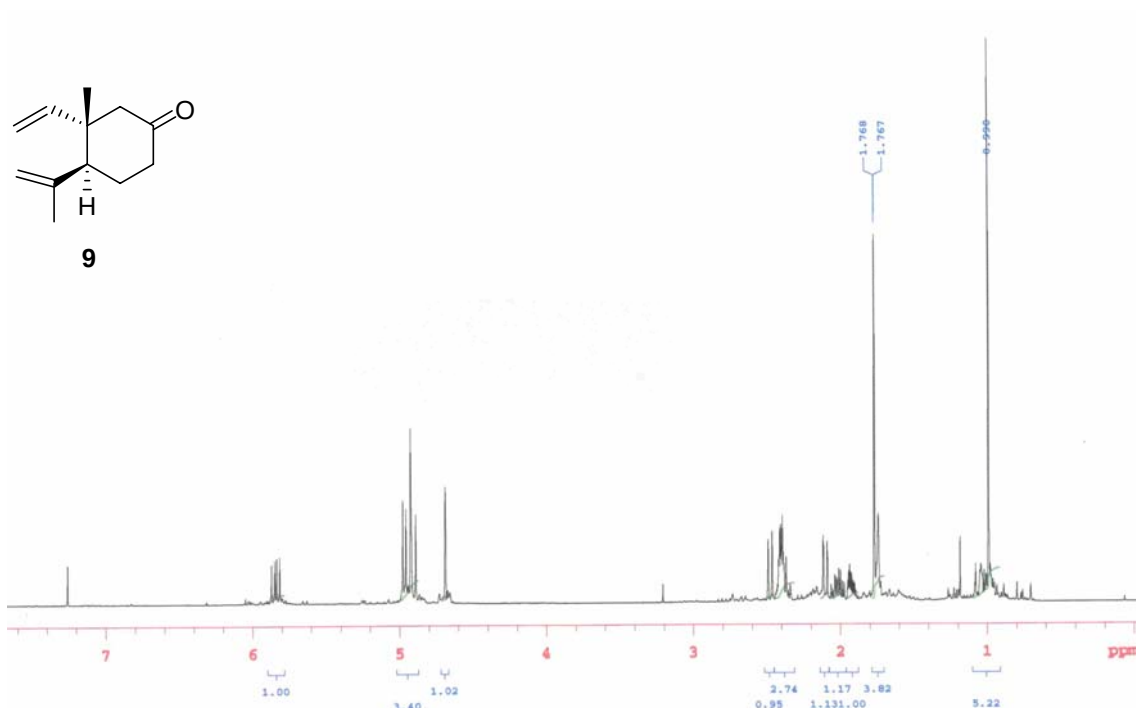


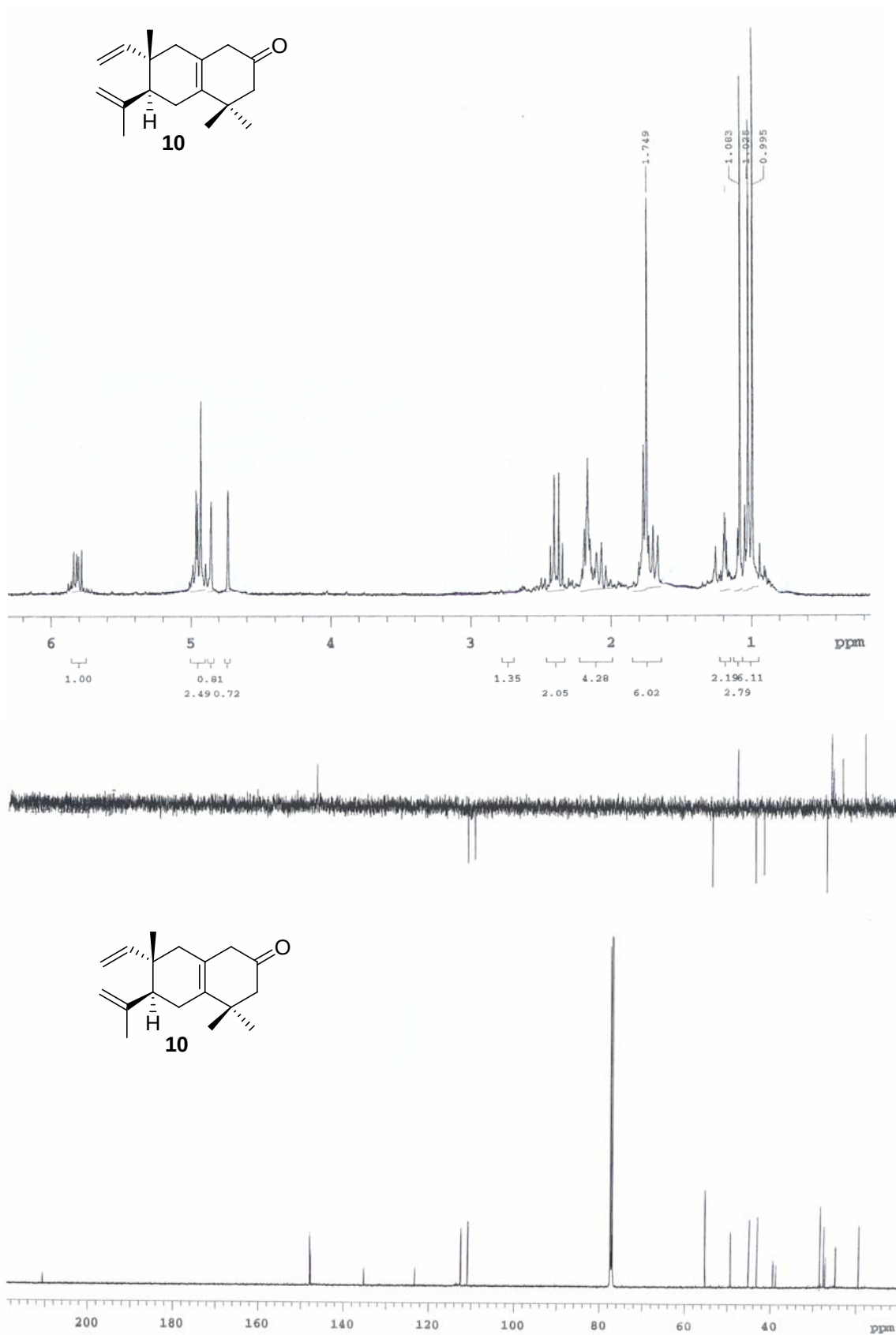


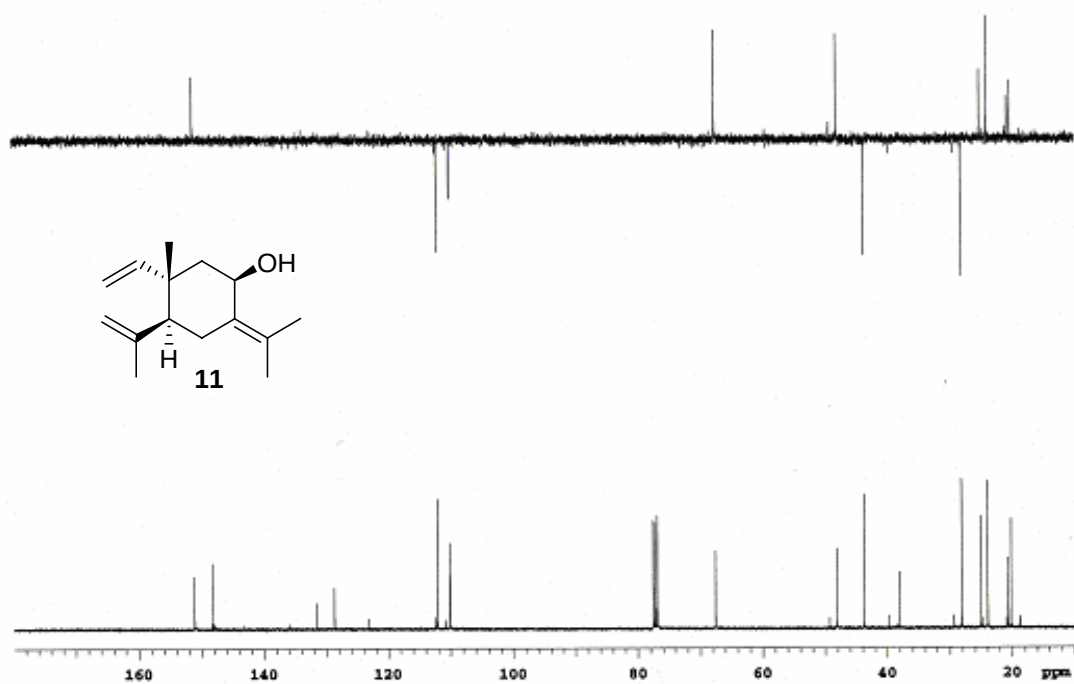
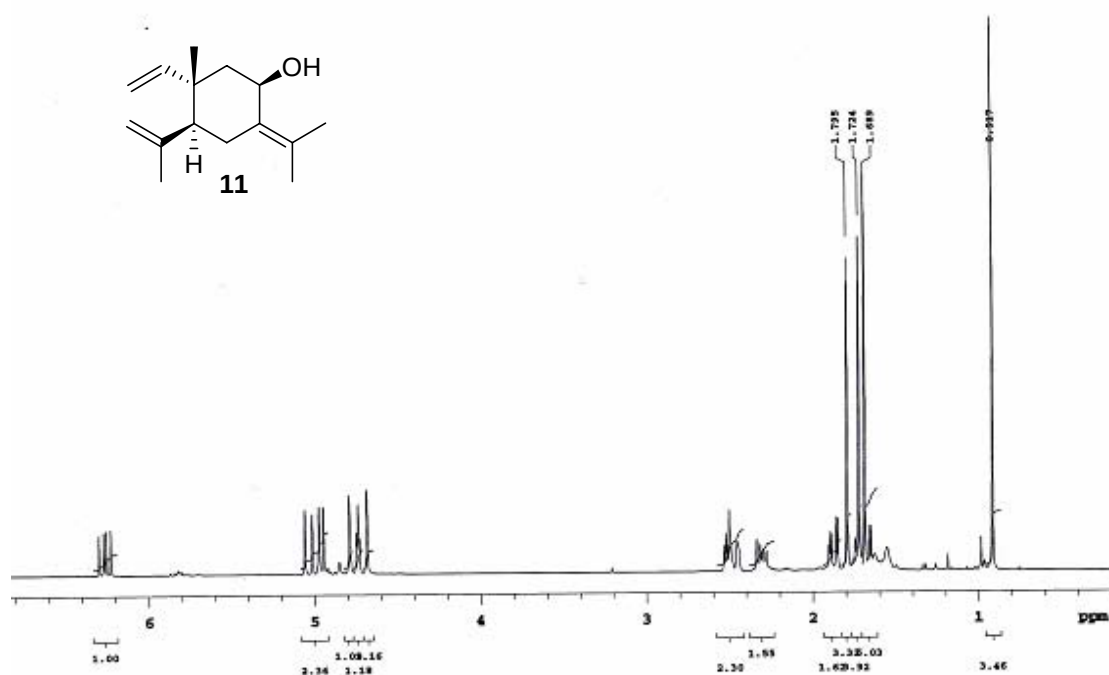


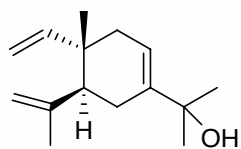




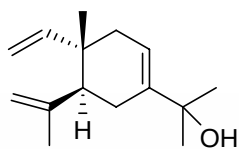
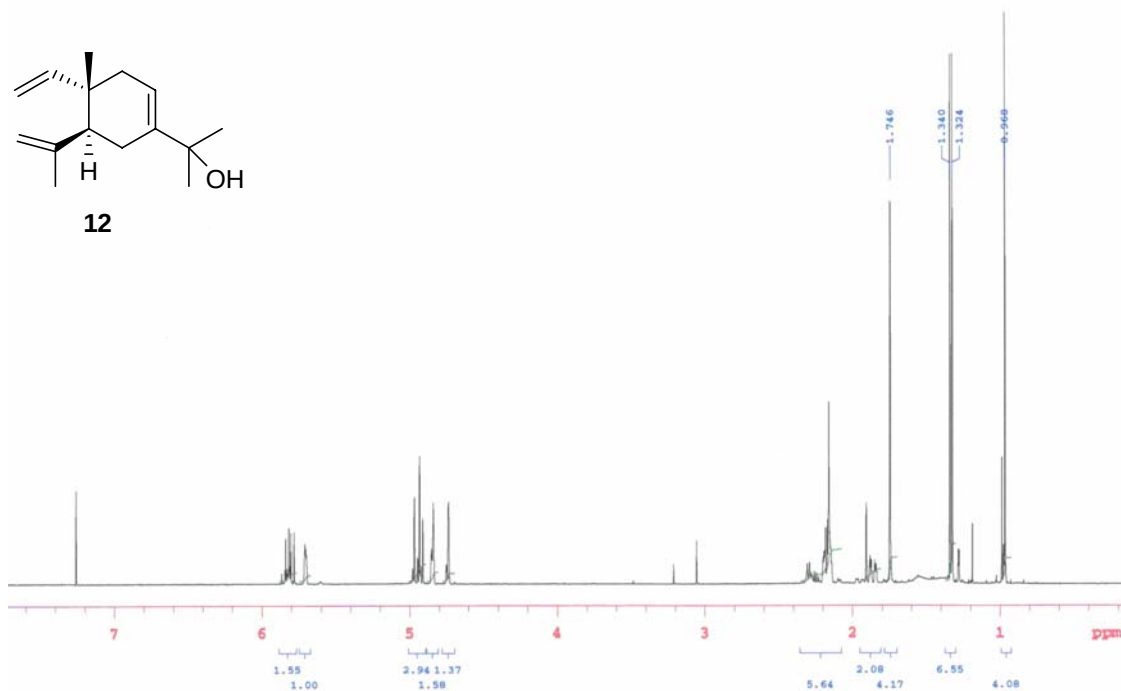




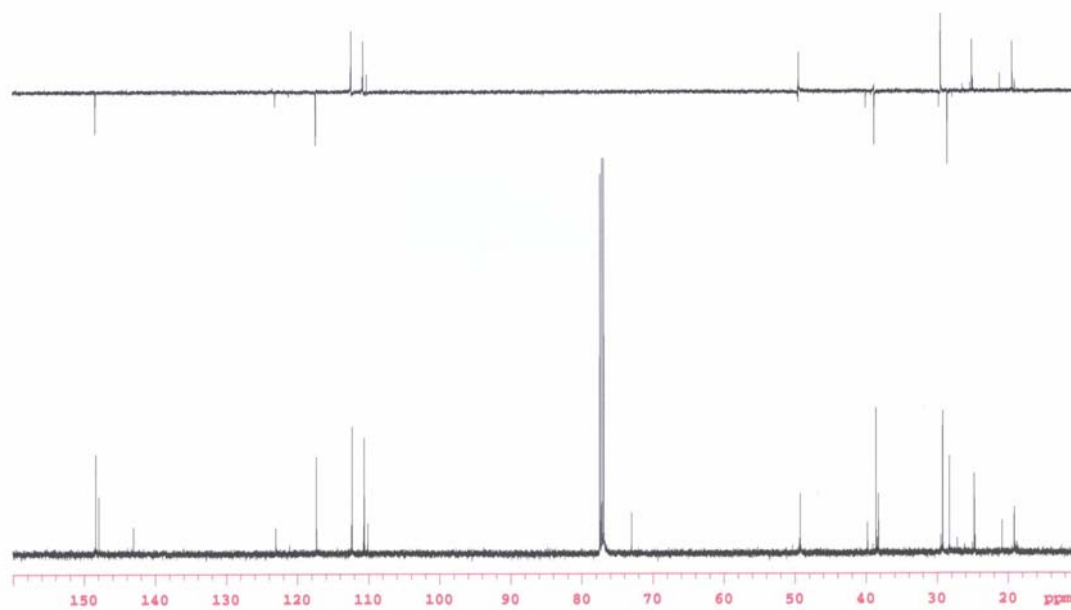


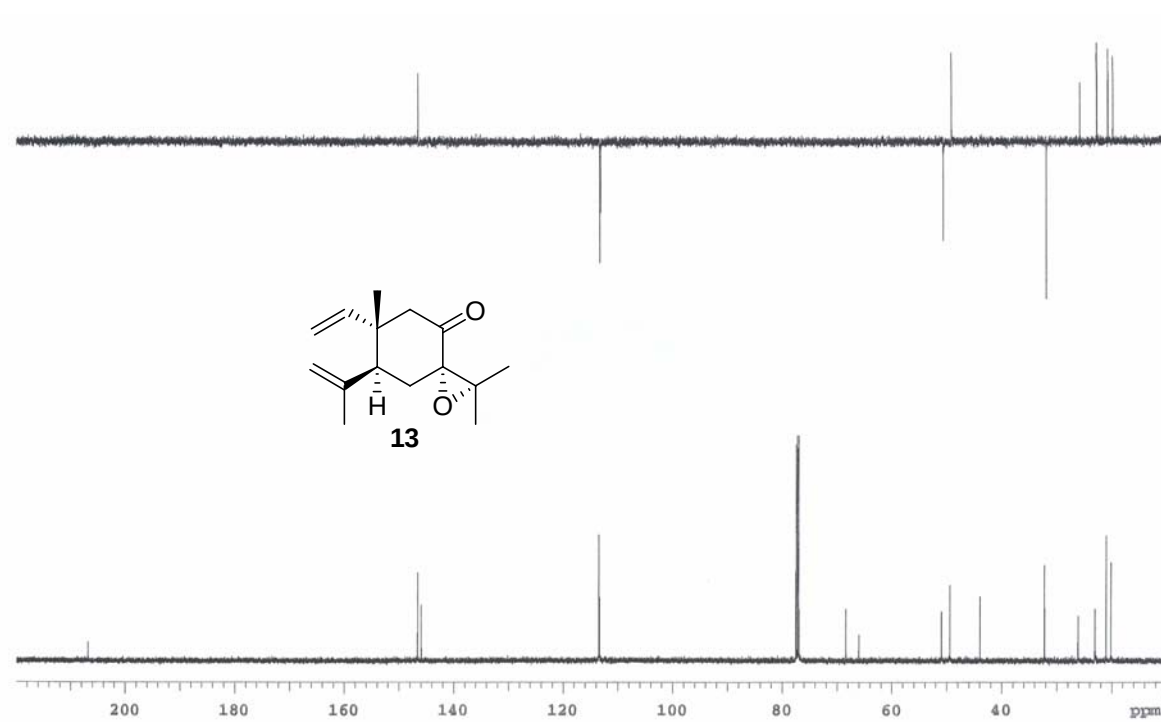
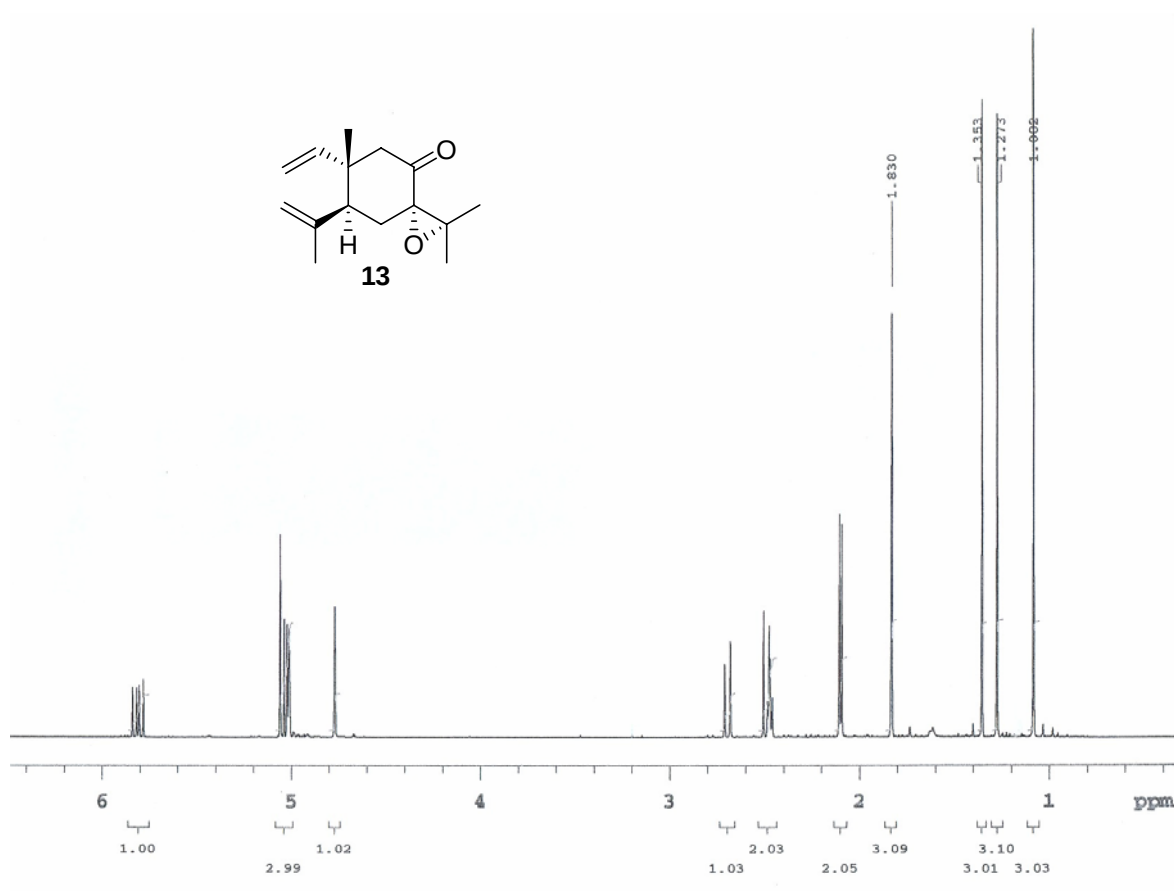


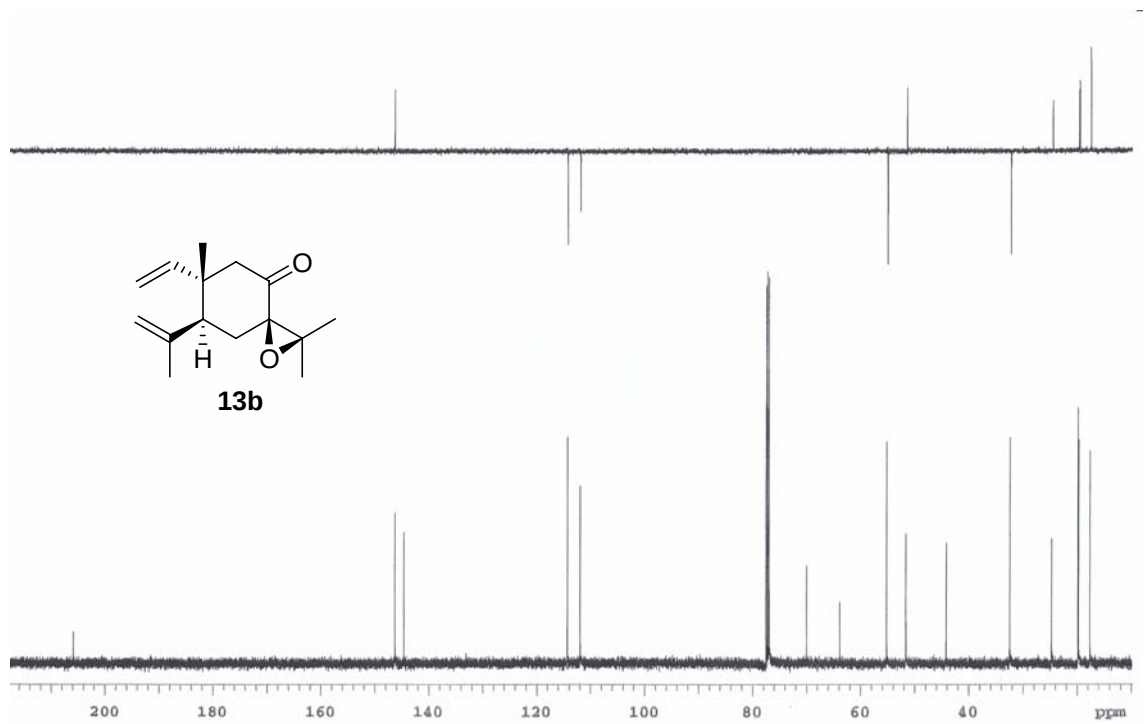
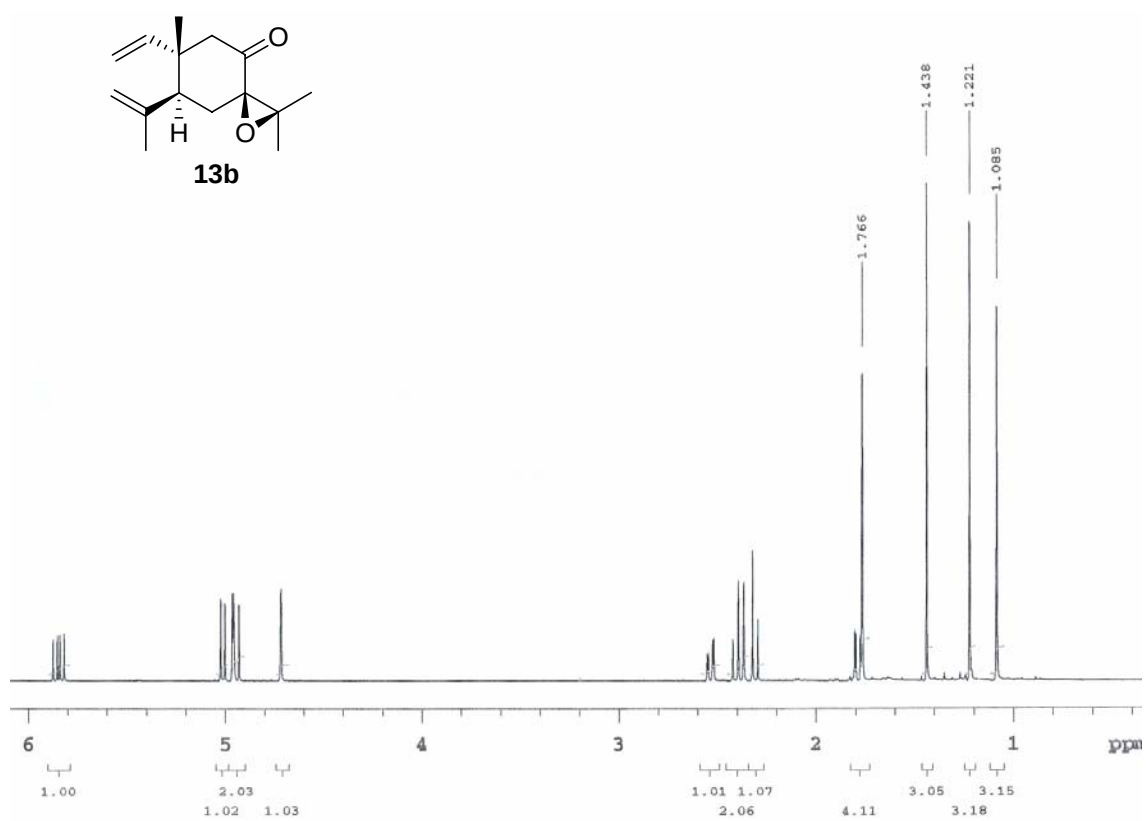
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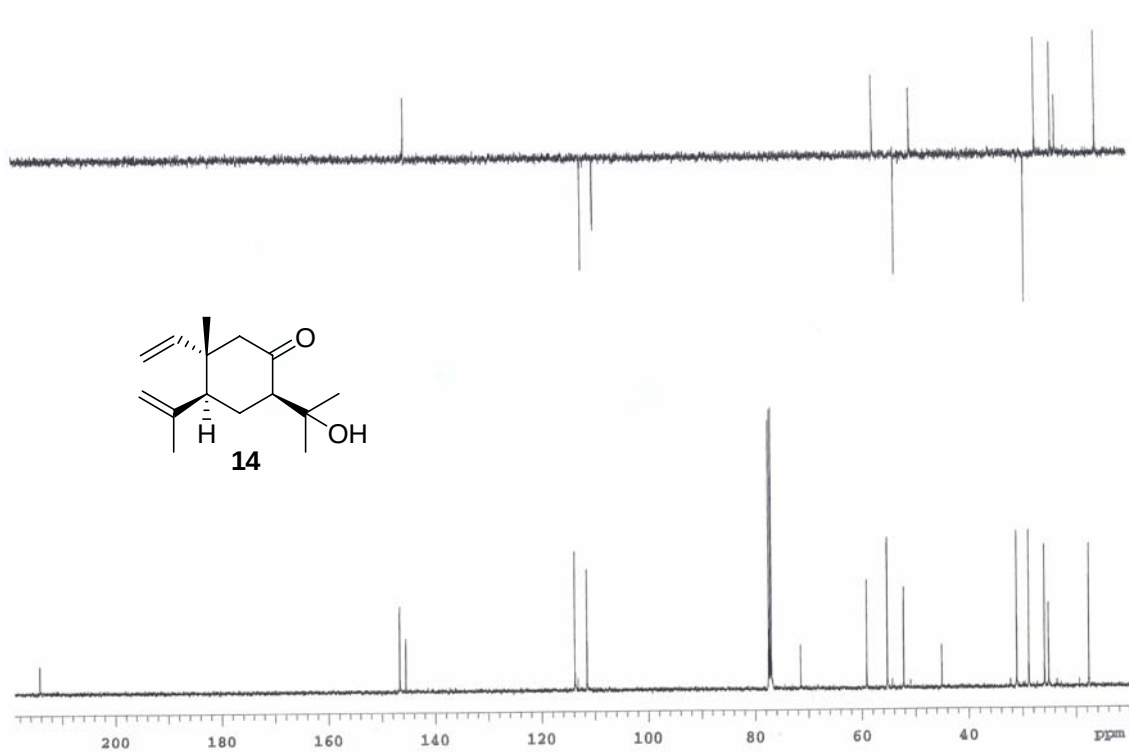
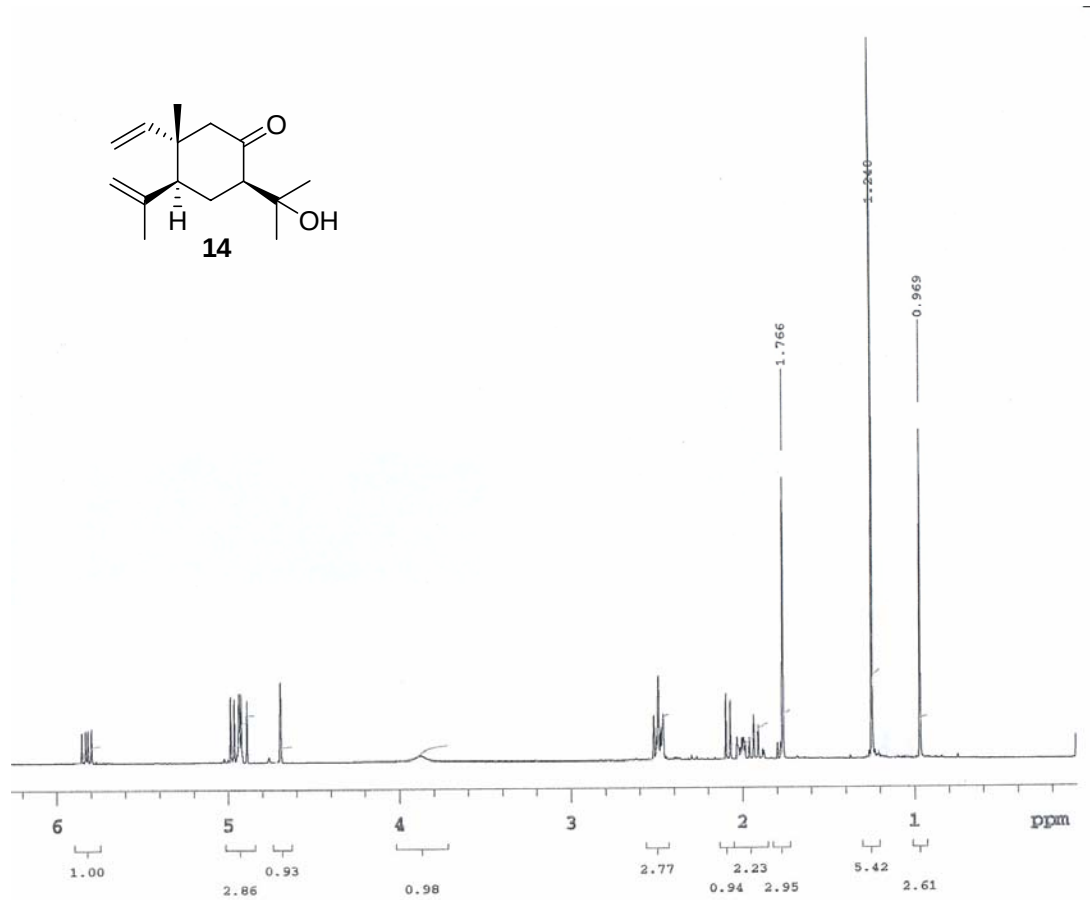


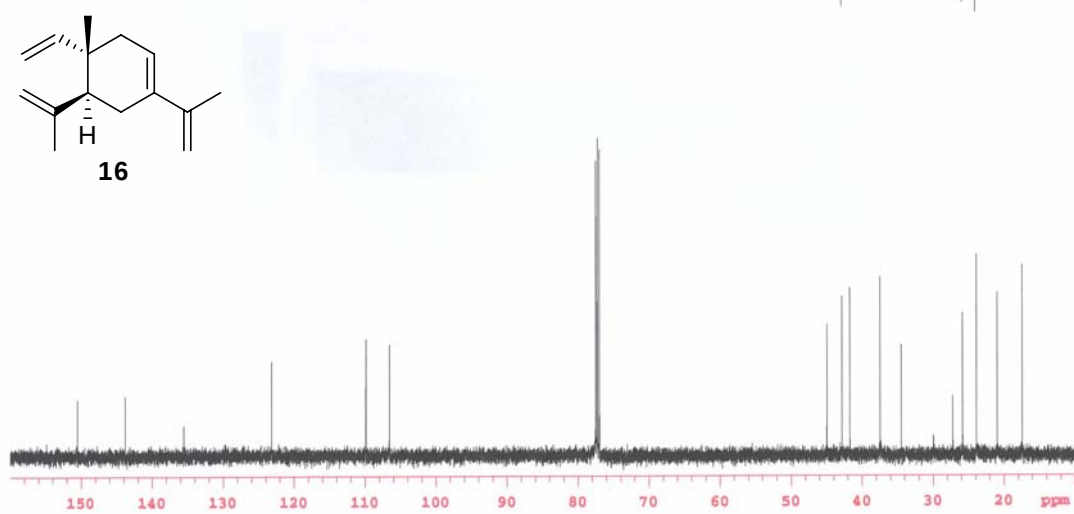
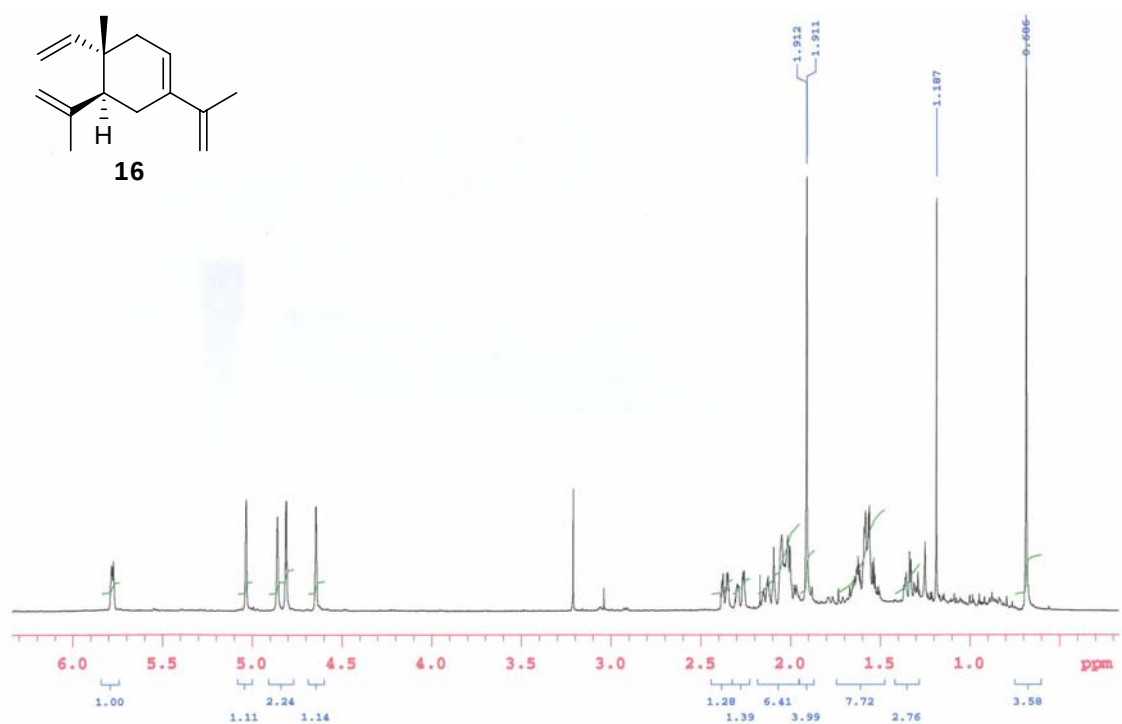
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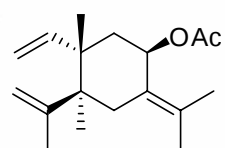












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