

Preparation of Boc-Protected Cinnamyl-Type Alcohols: A Comparison of the Suzuki-Miyaura Coupling, Cross-Metathesis, and Horner-Wadsworth-Emmons Approaches and their Merit in Parallel Synthesis

Jan Štambaský, Andrei V. Malkov* and Pavel Kočovský,*

Department of Chemistry, WestChem, University of Glasgow, Glasgow G12 8QQ, UK

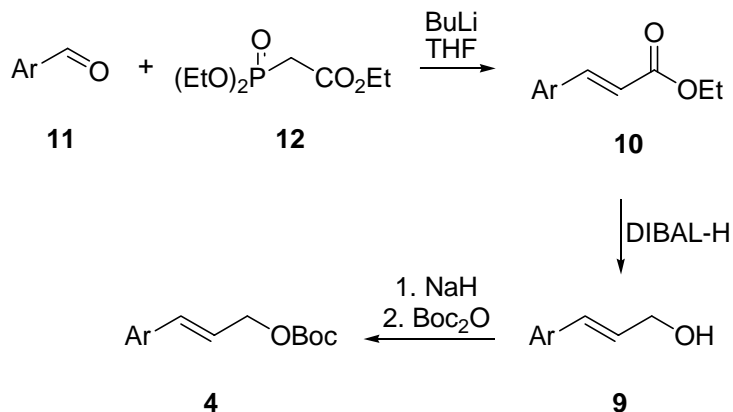
Supporting Information

Contents:

1. Horner-Wadsworth-Emmons reactions	S2
a. Scheme S1	S2
b. Spectrum S1 (Expansion E1-E3)	S3
c. Spectrum S1 (Expansion E4)	S4
d. Spectrum S2 (Expansions E1-E3)	S5
e. Spectrum S3 (Expansion E1)	S6

1. Horner-Wadsworth-Emmons reactions. The optimized reactions (Scheme S1) proved to be sufficiently selective to produce clean crude products. Sample spectra of crude reaction mixtures are provided.

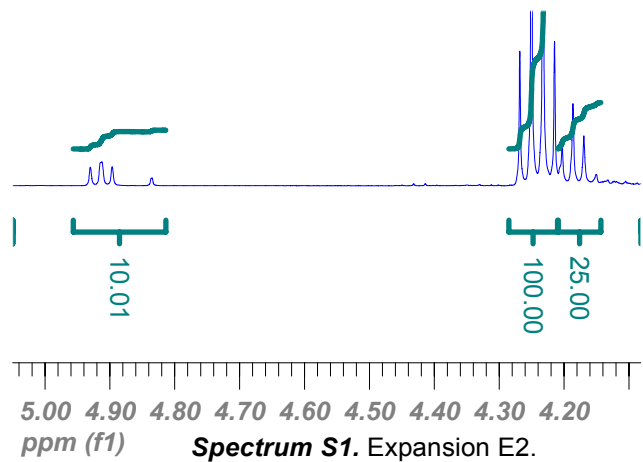
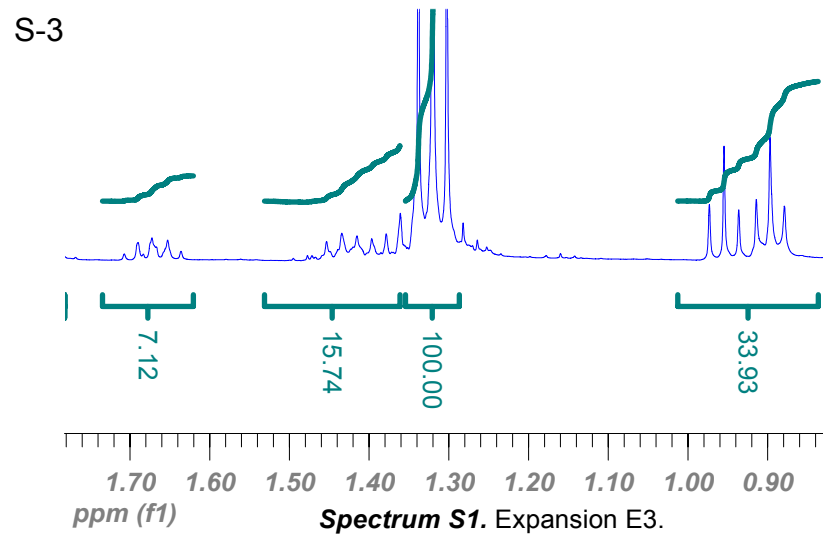
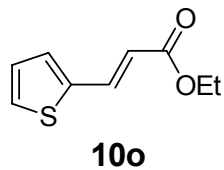
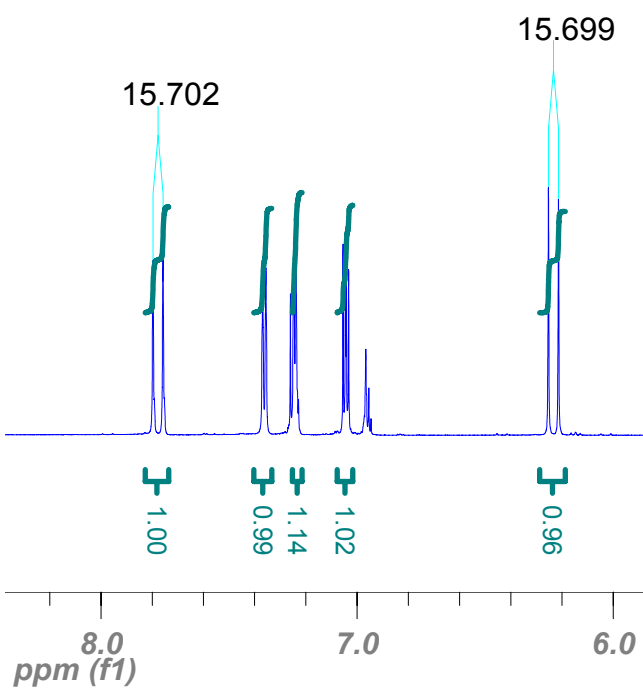
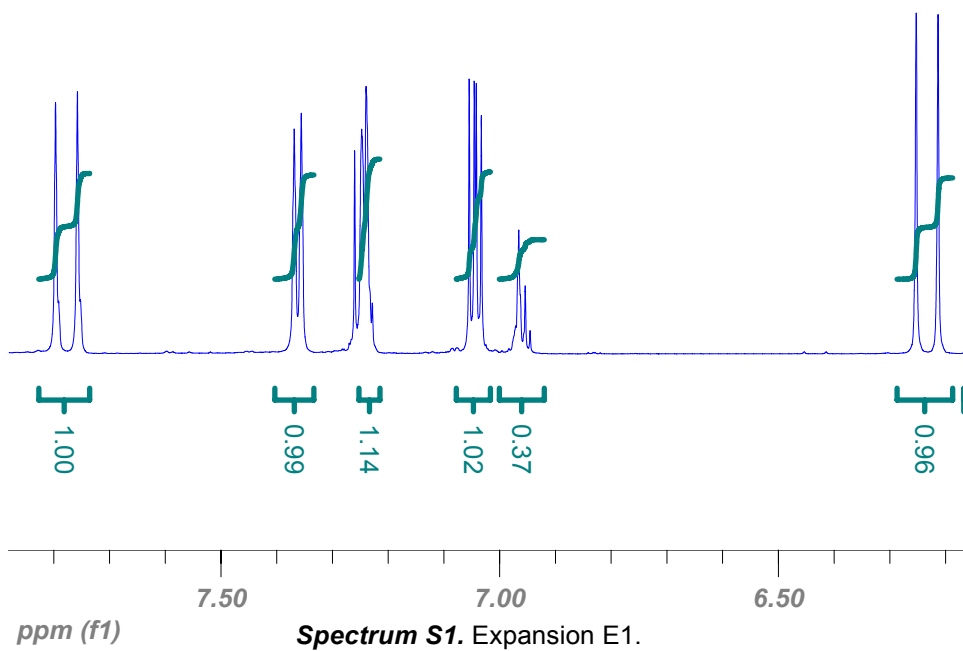
Scheme S1: Carbonates **4** via HWE approach.

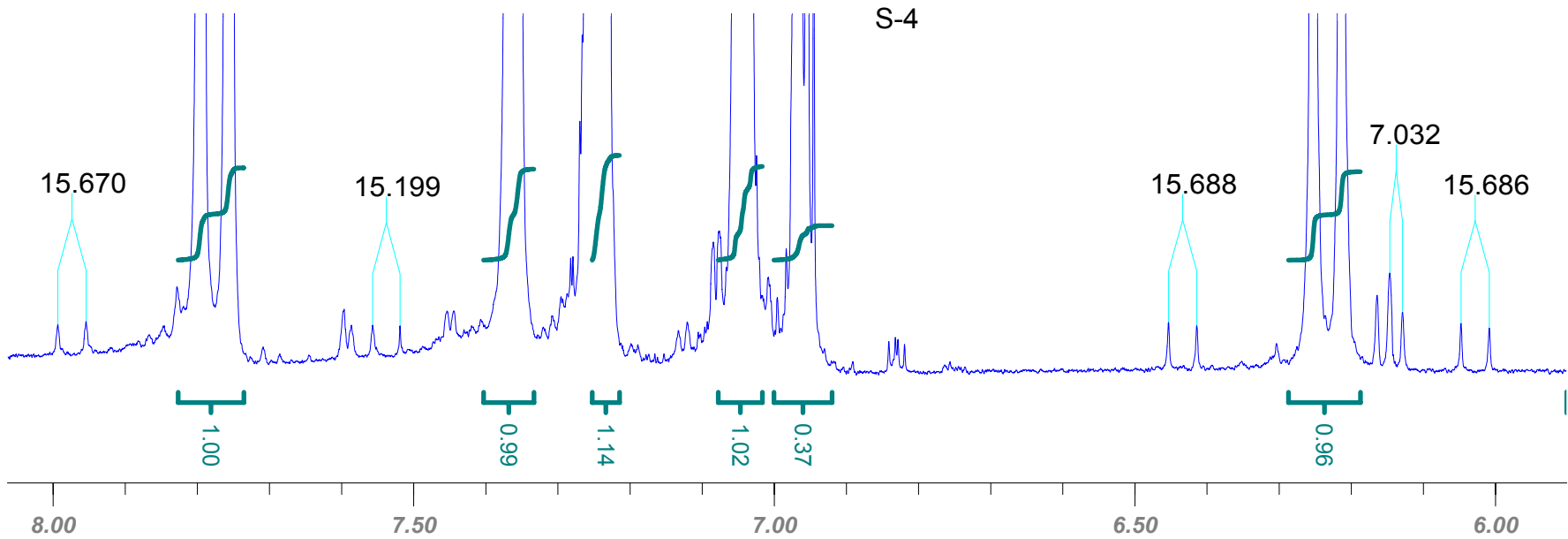


Spectrum S1 shows crude reaction mixture of ethyl acrylate **10o**. Characteristic 3J coupling constants indicate *trans*-double bond of **10o**. Expansions E1-E3 show impurities in particular regions, along with integration values relating to signals of **10o**. Expansion E4 shows 3J coupling constants of impurities, indicating that no (*Z*)-configured double bond is present.

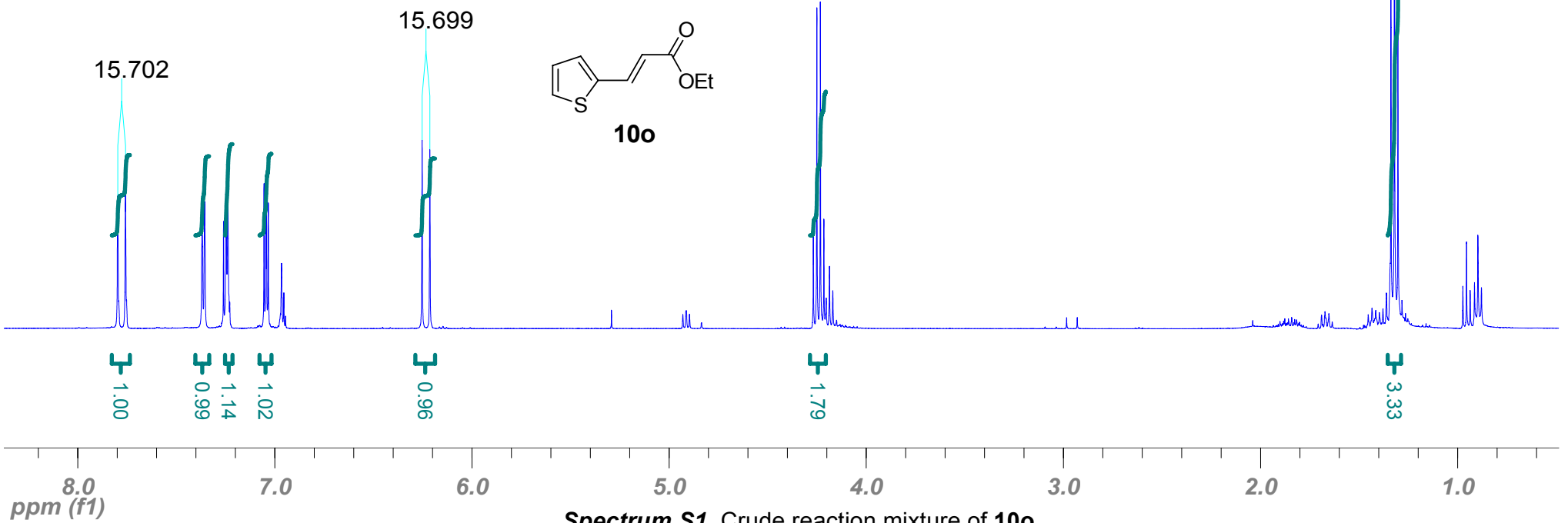
Spectrum S2 shows crude reaction mixture of ethyl acrylate **10u**. Characteristic 3J coupling constants indicate *trans*-double bond of **10u**. Expansions E1-E3 show impurities in particular regions, along with integration values relating to signals of **10u**.

Spectrum S3 shows crude reaction mixture of allyl alcohol **9u**, and along with Expansion E1 show relative purity of **9u**. This purity was sufficient for the Boc-functionalization of **9u**.



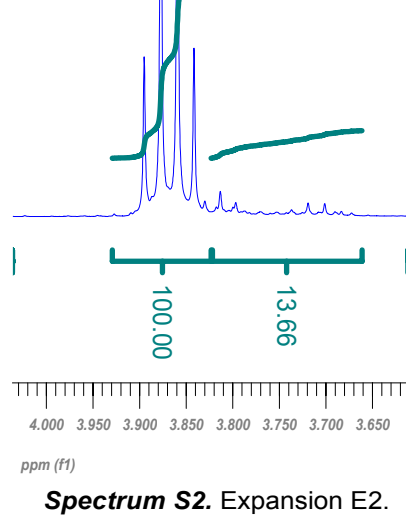
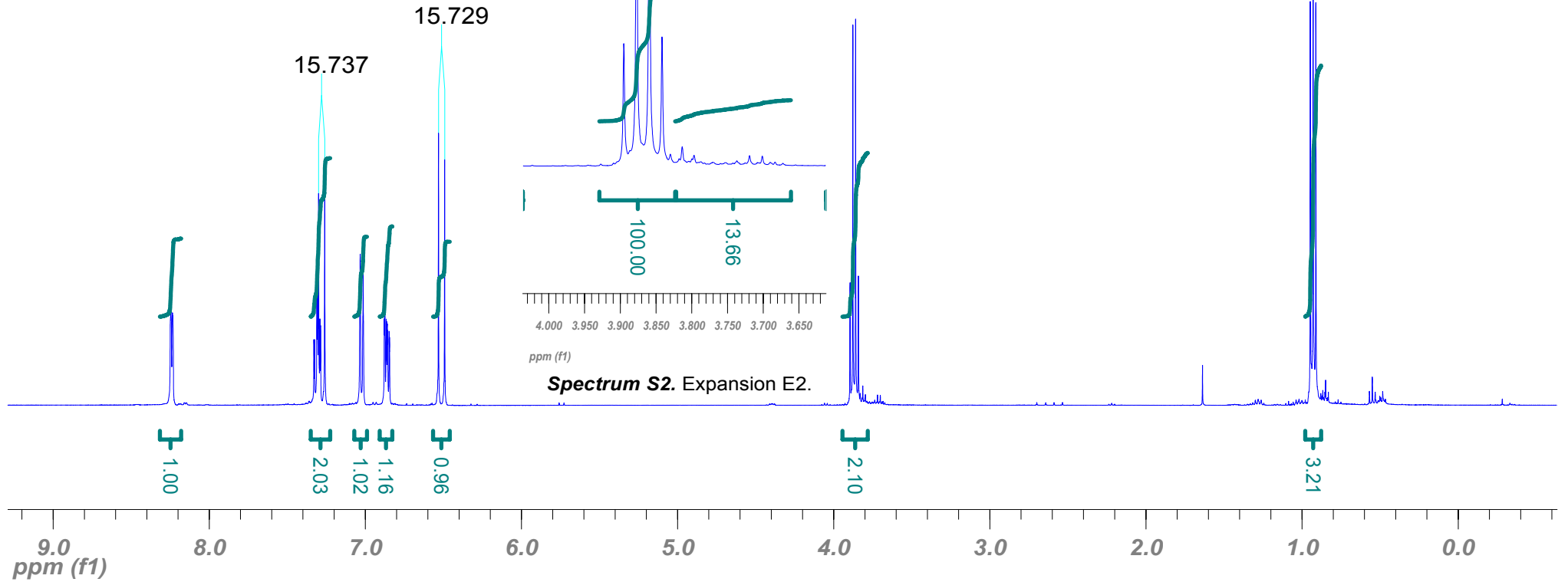
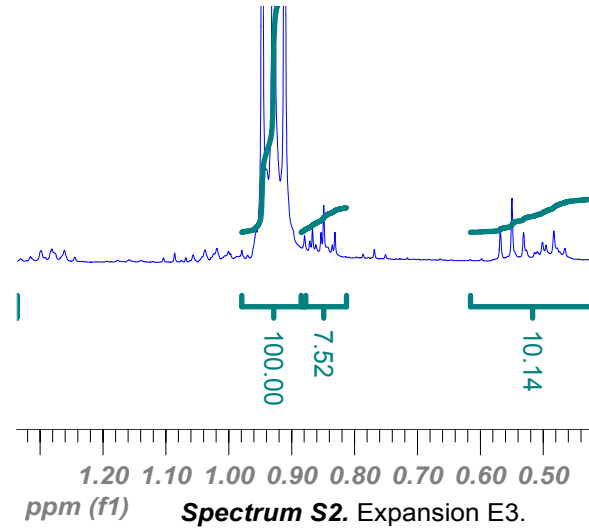
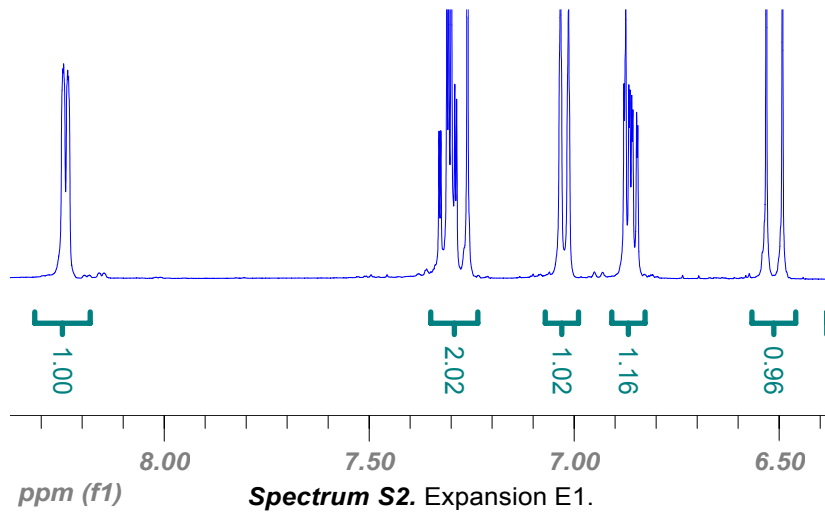
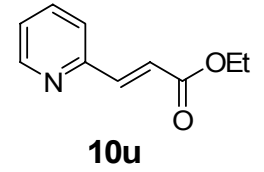


Spectrum S1. Expansion E4.

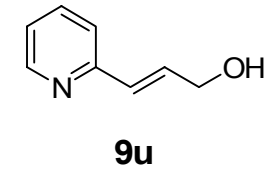
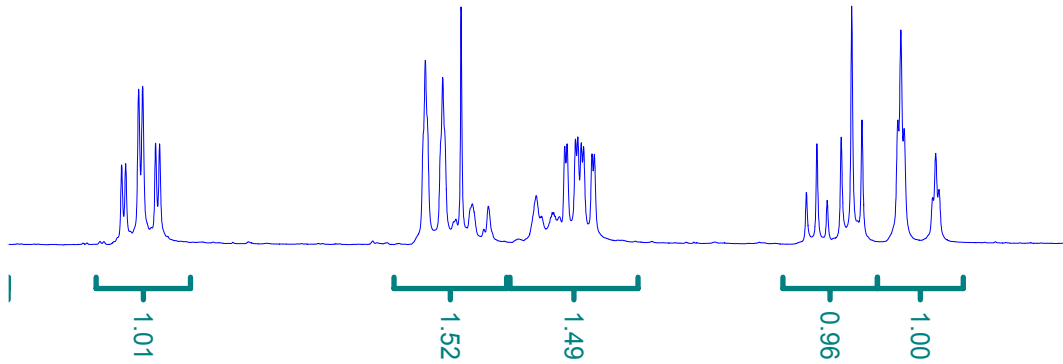


Spectrum S1. Crude reaction mixture of 10o.

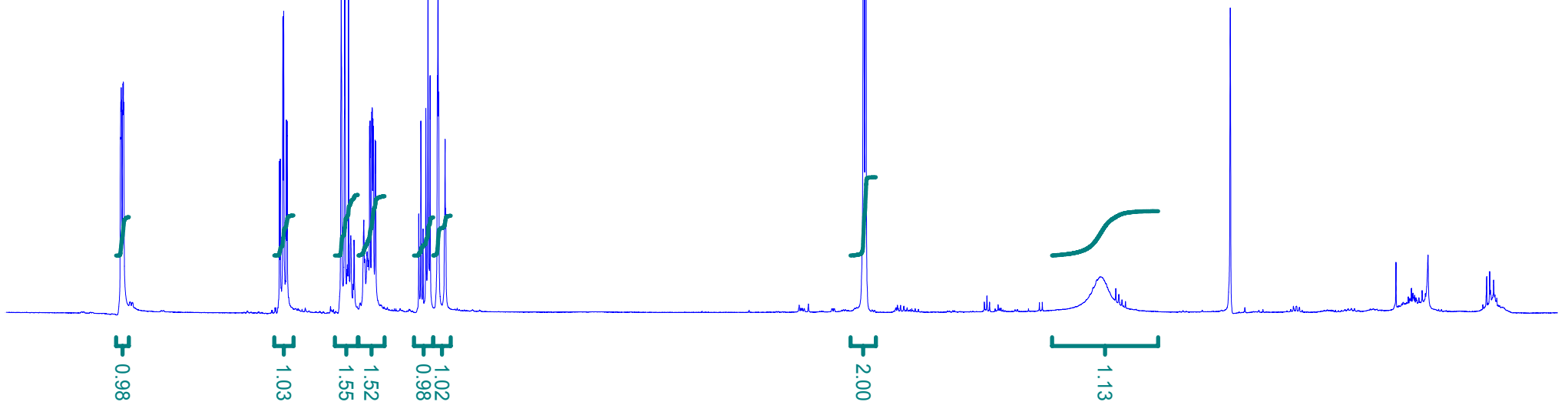
S-5



S-6



ppm (f1) 7.50 7.00 *Spectrum S3. Expansion E1.*



9.0 ppm (f1) 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 *Spectrum S3. Crude reaction mixture of 9u.*