New Journal of Chemistry

Synthesis of bio-based epoxy monomers from natural allyl- and vinyl phenols and the estimation of their affinity to the estrogen receptor α by molecular docking.

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Supporting Information

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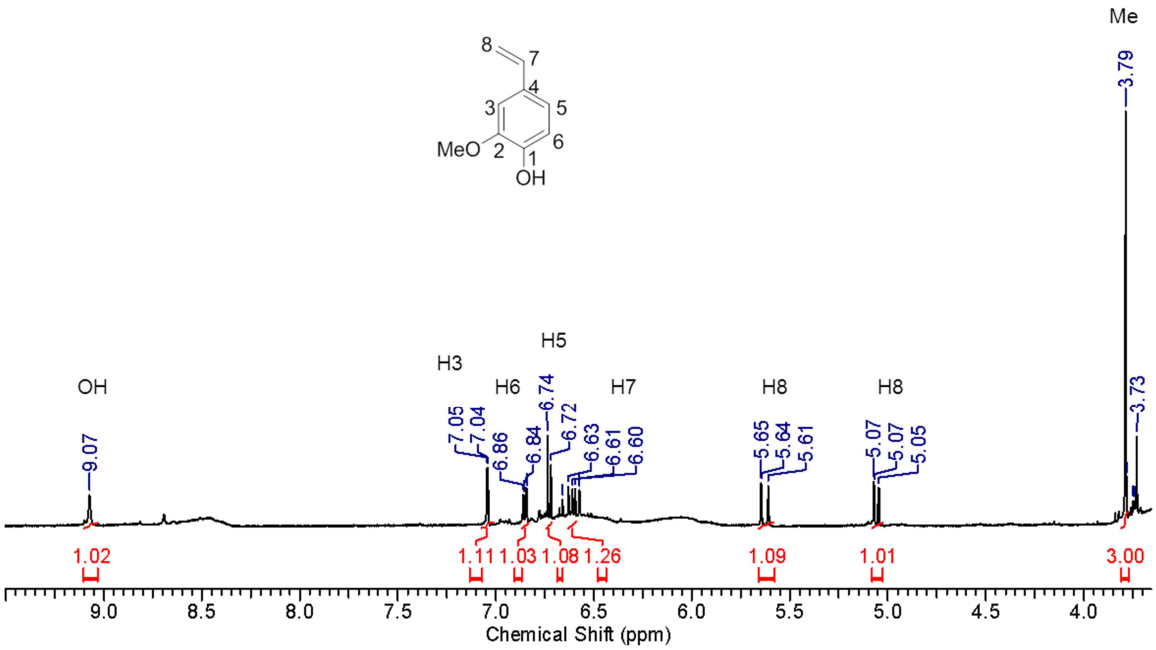
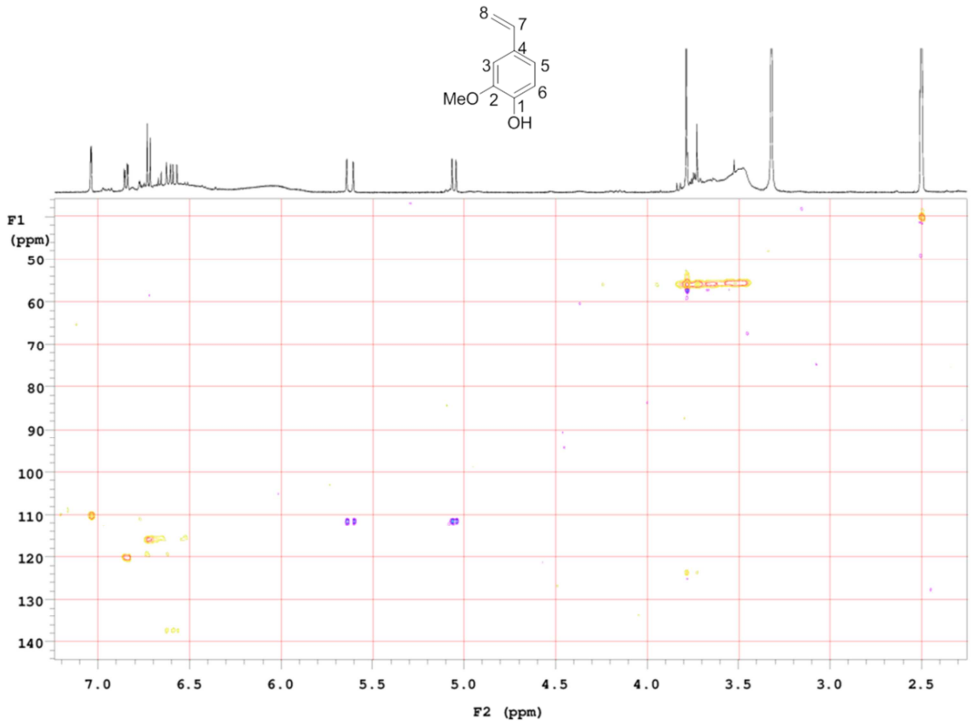
Except product **3**, all NMR spectra were acquired at 25°C in DMSO-d_6. In the edited ^{1}H-^{13}C HSQC spectra, the ^{1}JCH correlations arising from CH2 groups are phased down (in blue) and those arising from CH3 and CH groups are phased up (in red). In the ^{1}H-^{13}C HMBC spectra, some intense ^{1}JCH correlations not totally cancelled appear as undecoupled ^{1}JCH signal.

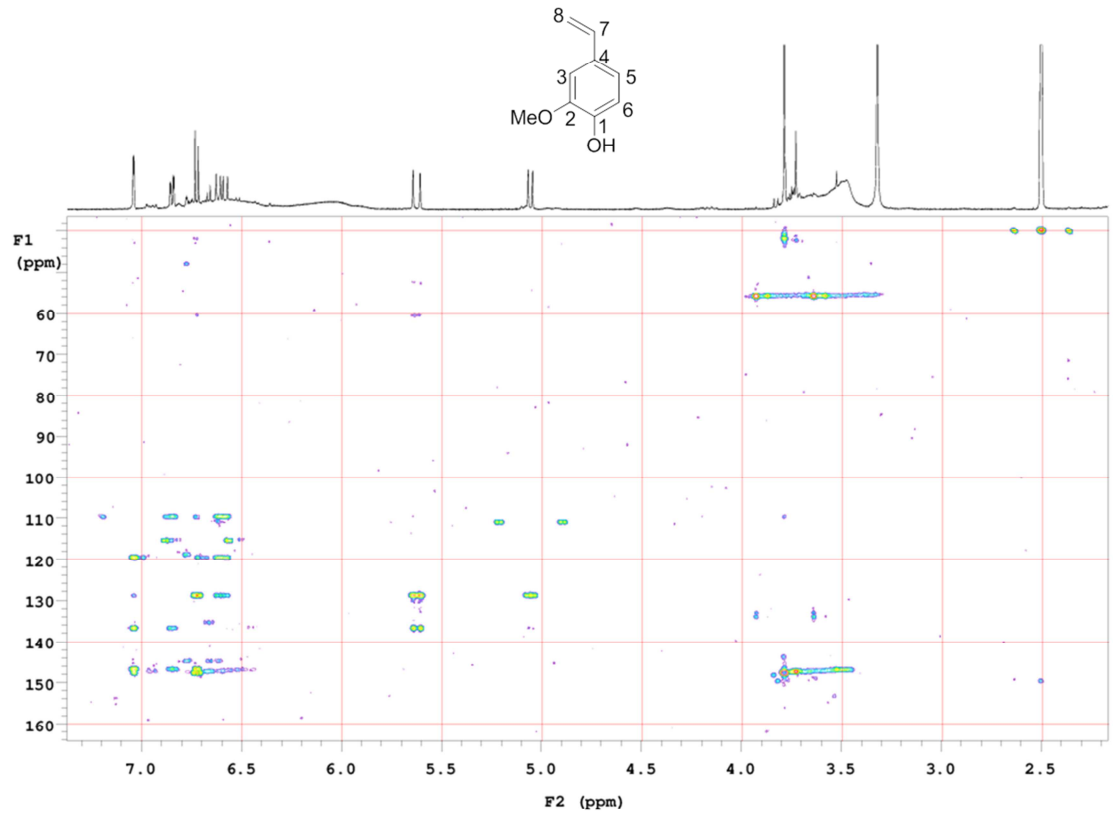
Product 2



1D ^{1}H spectrum of product **2**

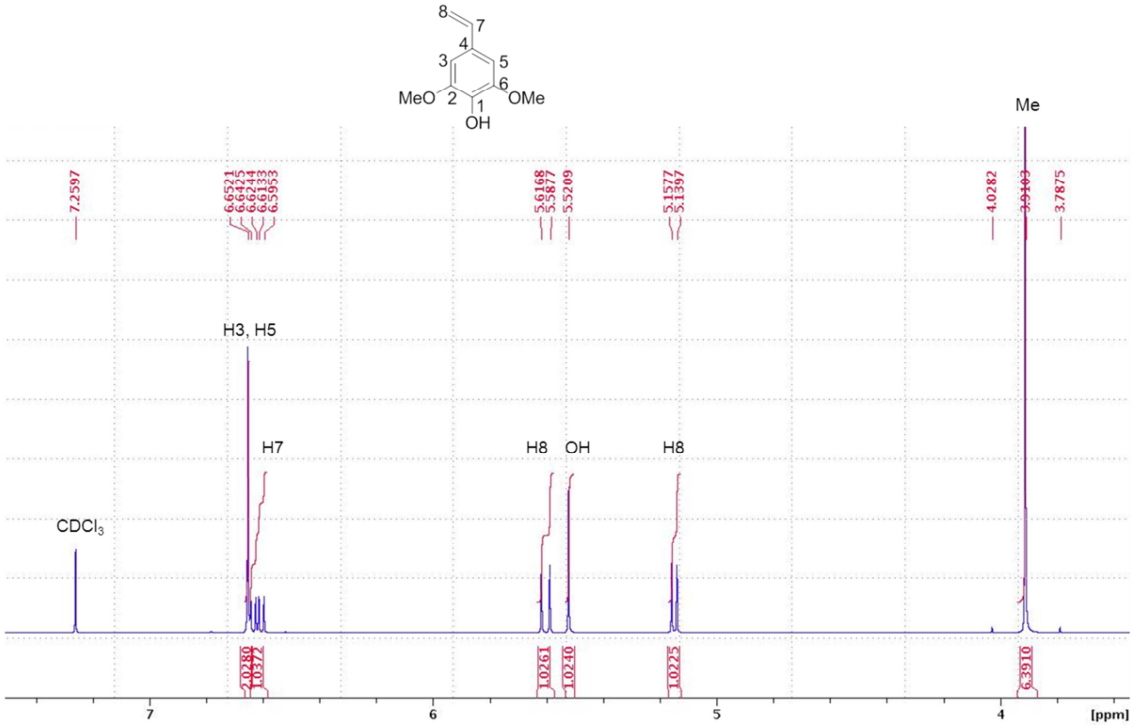


HSQC spectrum of product **2**

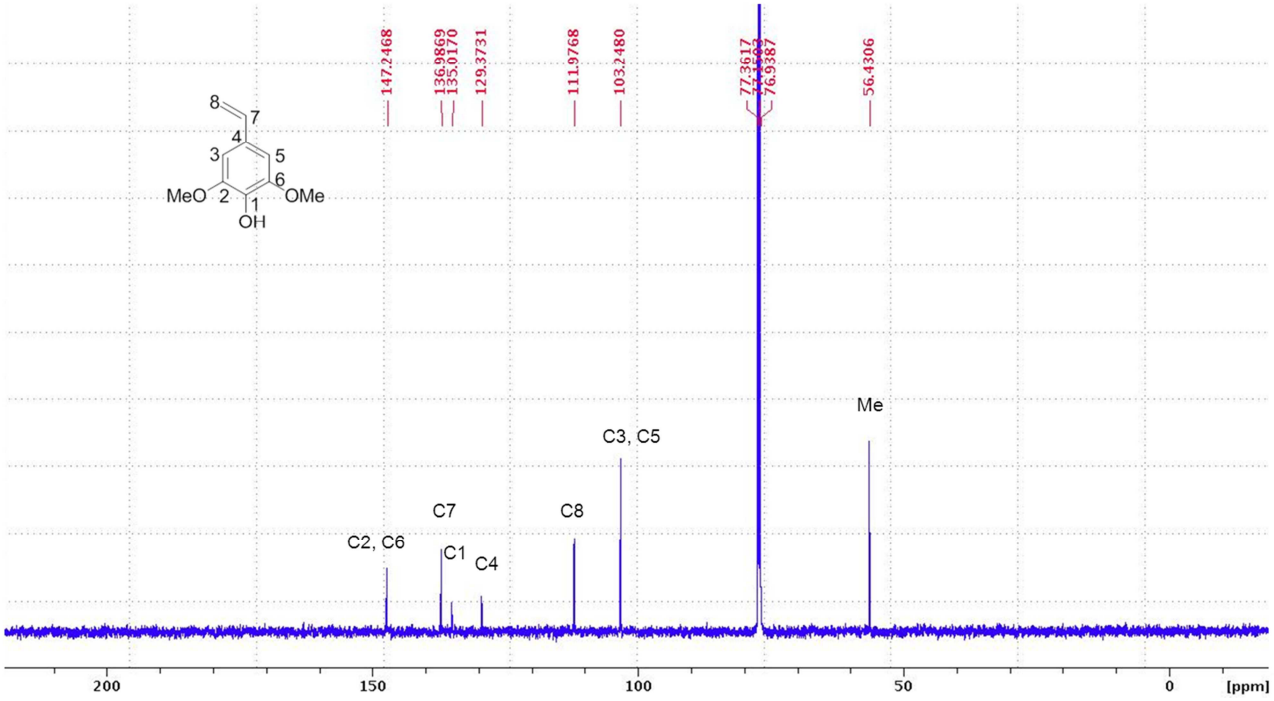


HMBC spectrum of product **2**

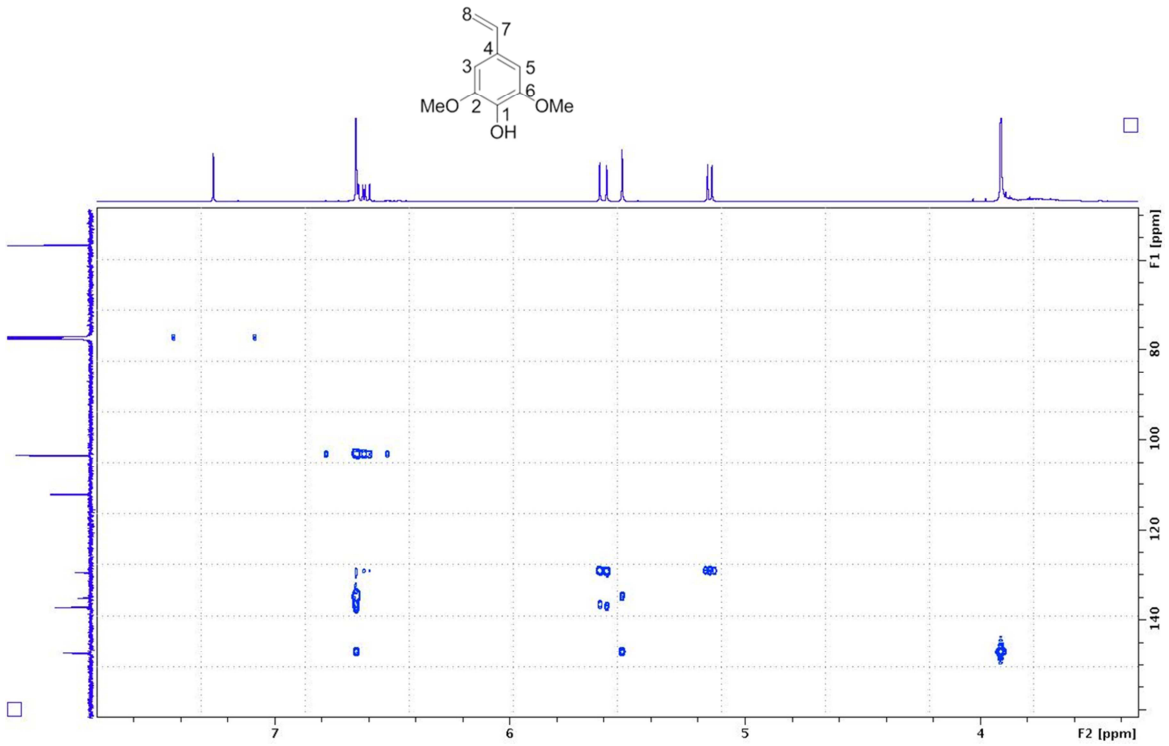
Product 3



1D ^{1}H spectrum of product **3** in $CDCl_3$

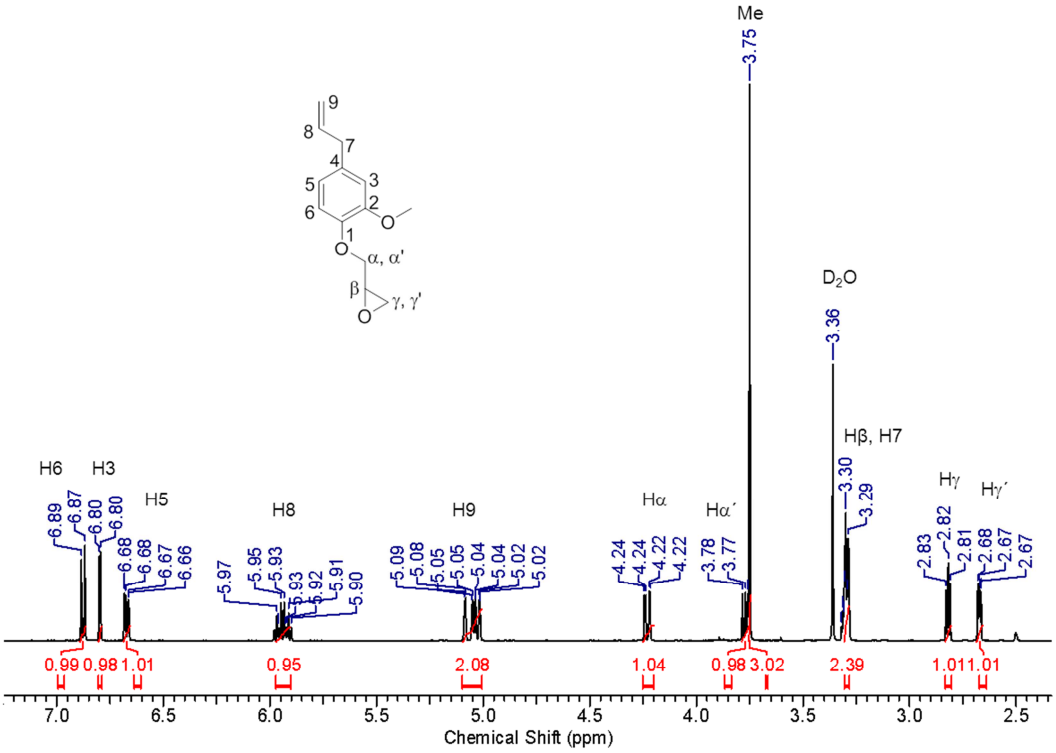


1D ^{13}C spectrum of product **3** in $CDCl_3$

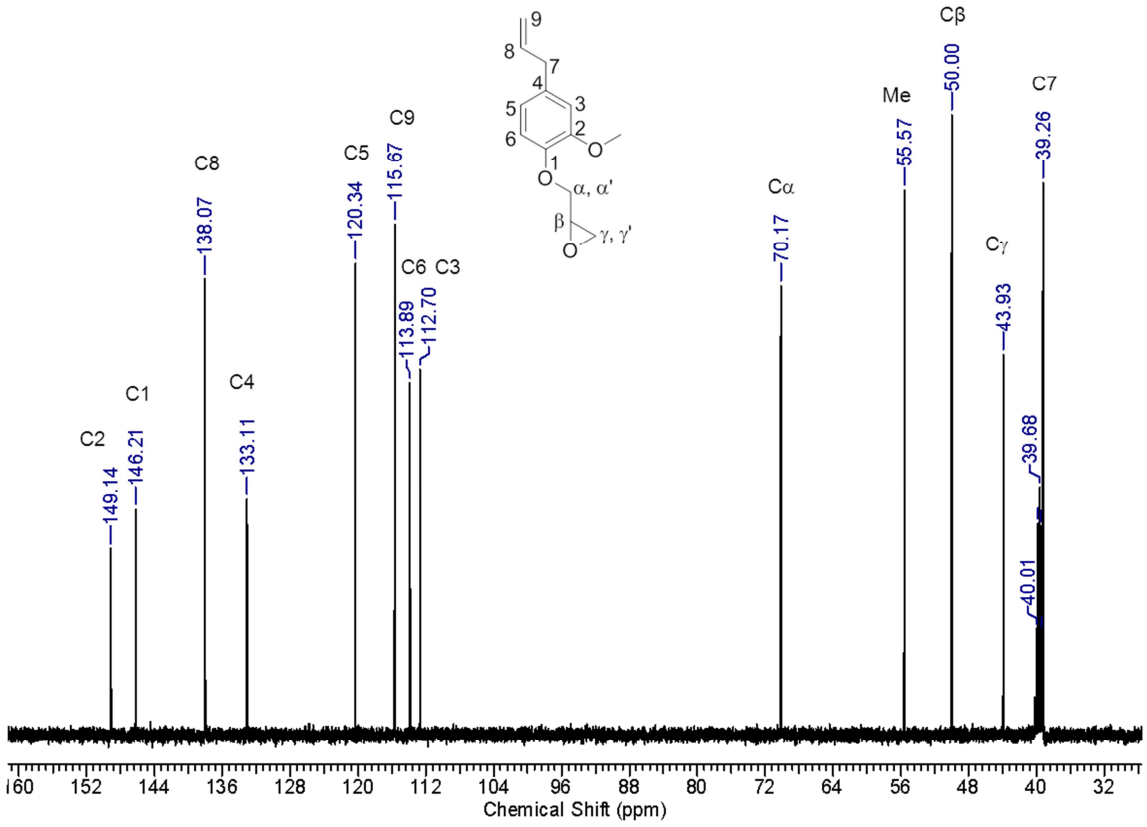


HMBC spectrum of product **3** in $CDCl_3$.

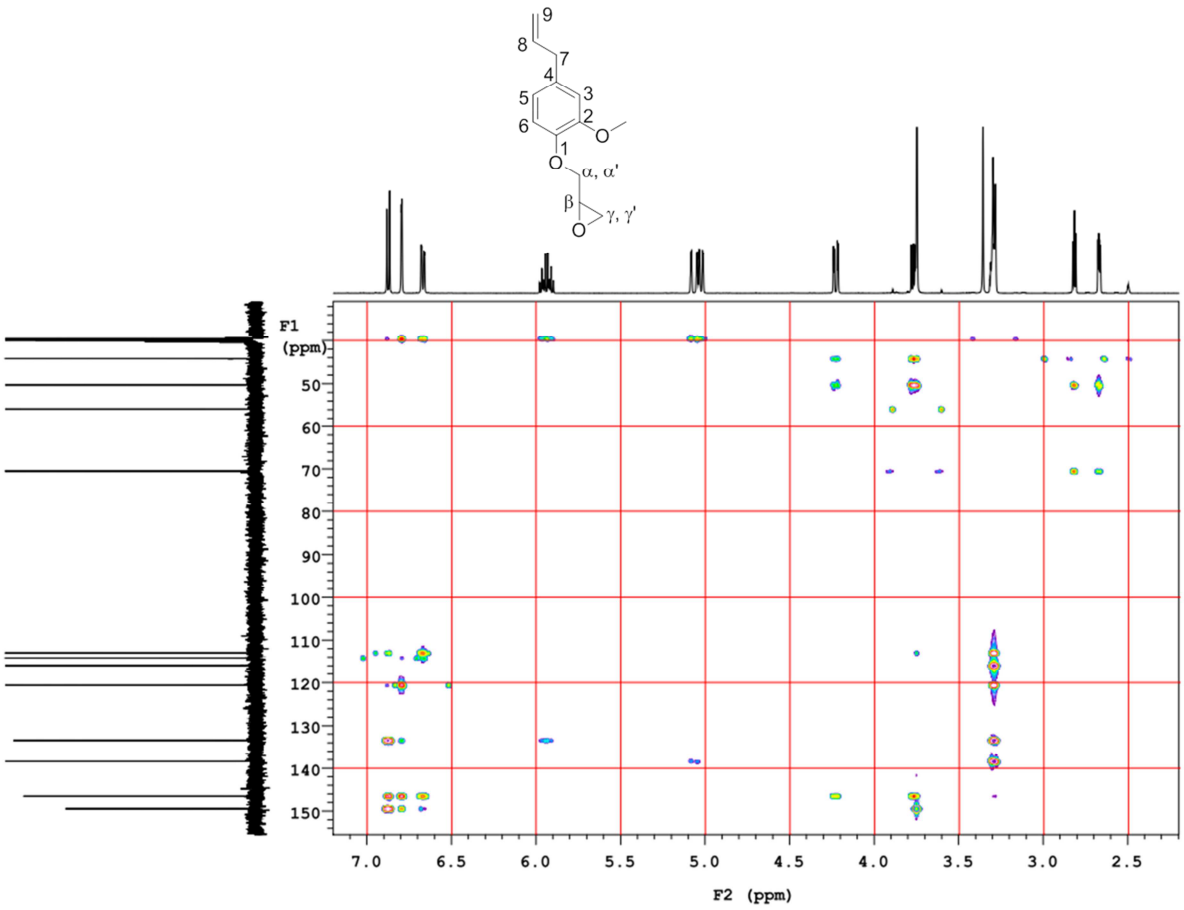
Product 4



1D ^{1}H spectrum of product **4**

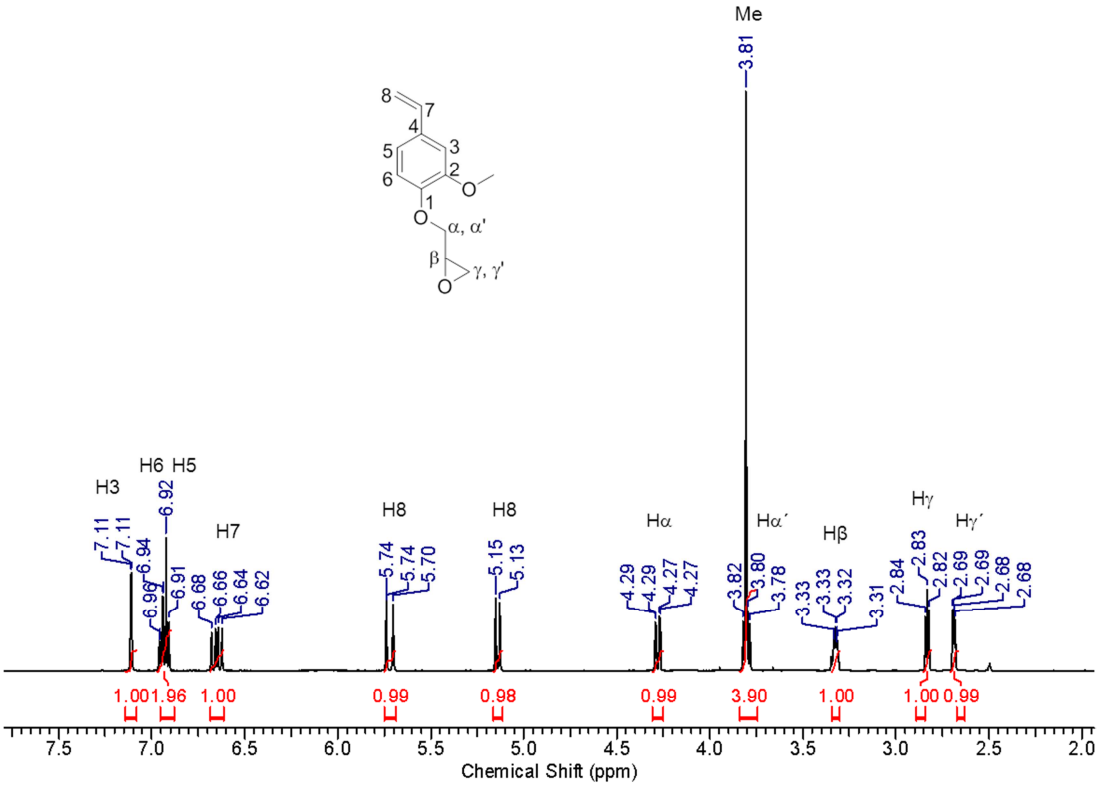


1D ^{13}C spectrum of product **4**

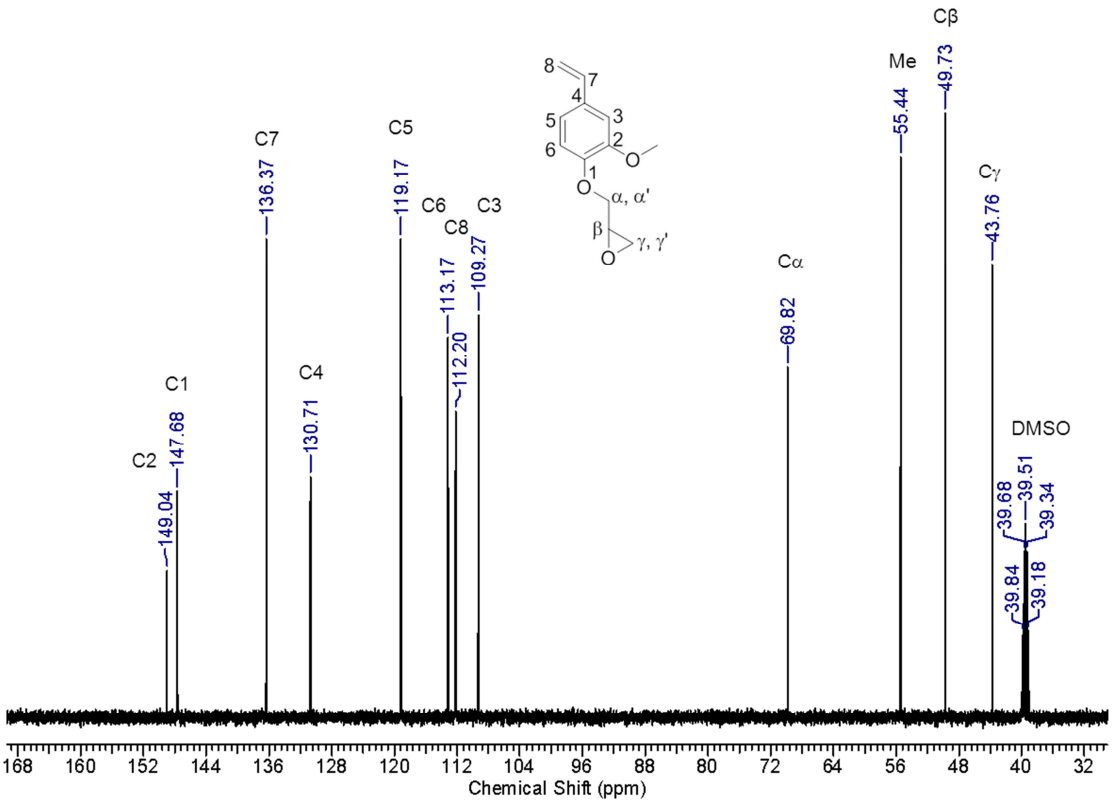


HMBC spectrum of product **4**

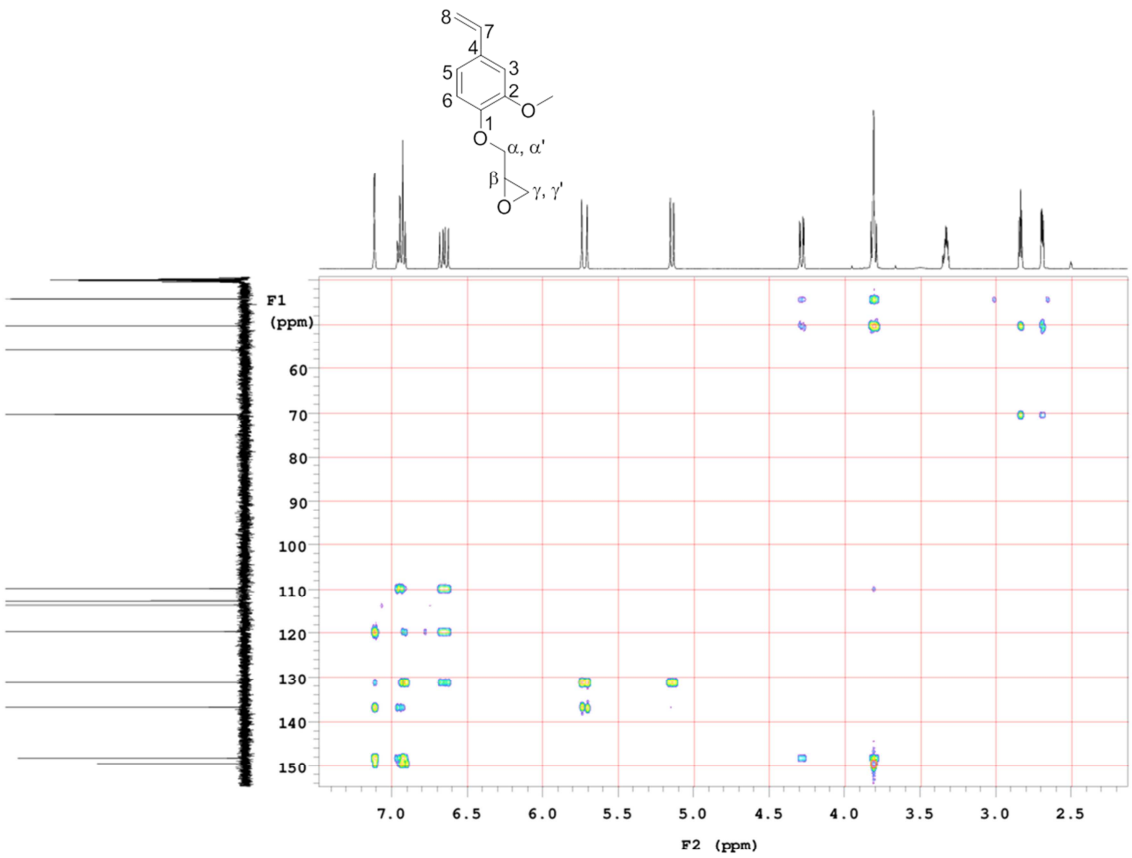
Product 5



1D ^{1}H spectrum of product **5**

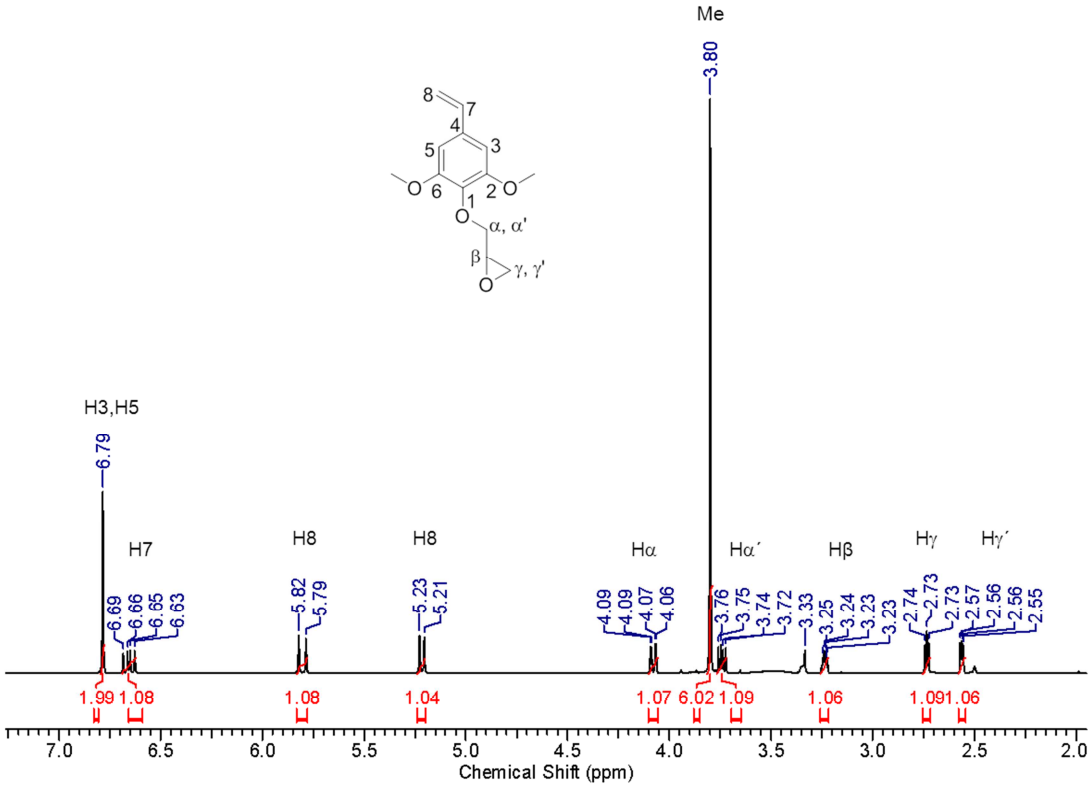


1D ^{13}C spectrum of product **8**

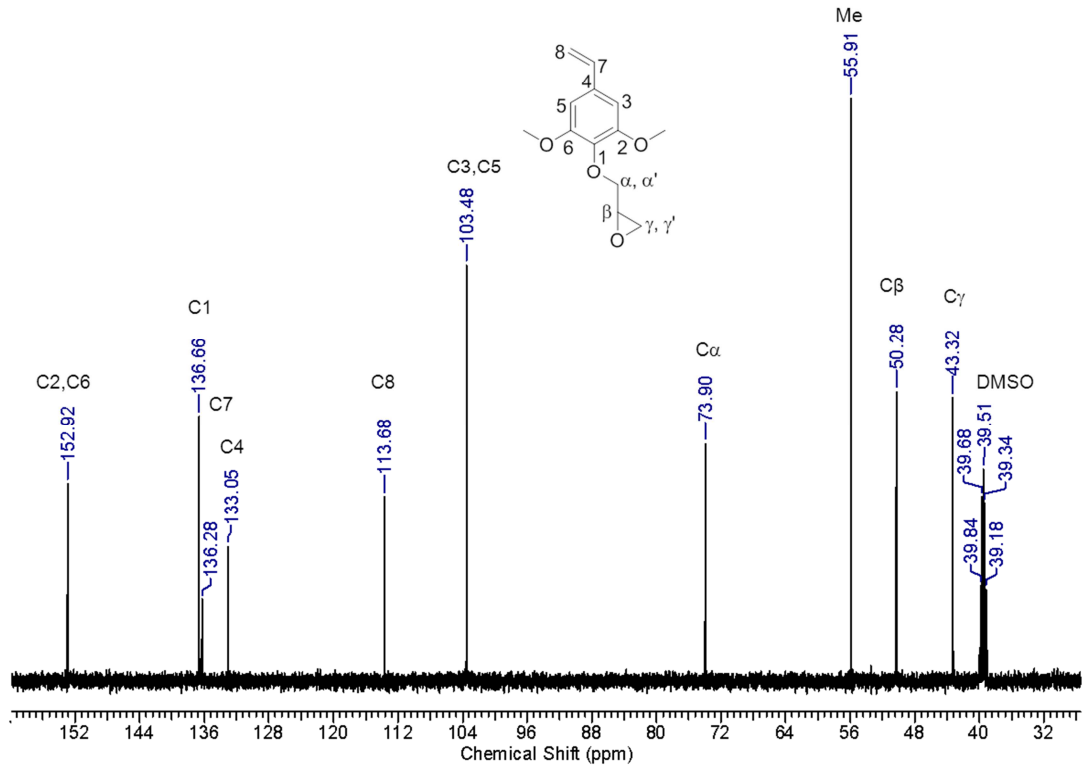


HMBC spectrum of product **5**

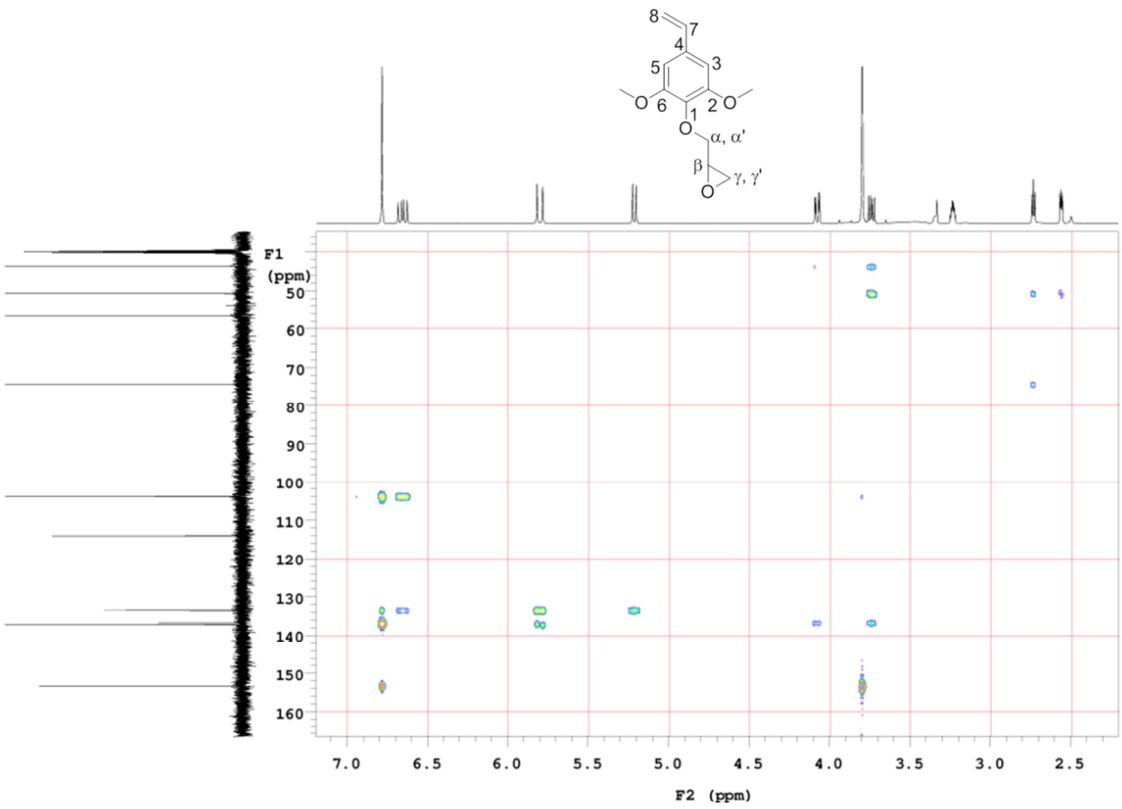
Product 6



1D ^{1}H spectrum of product **6**

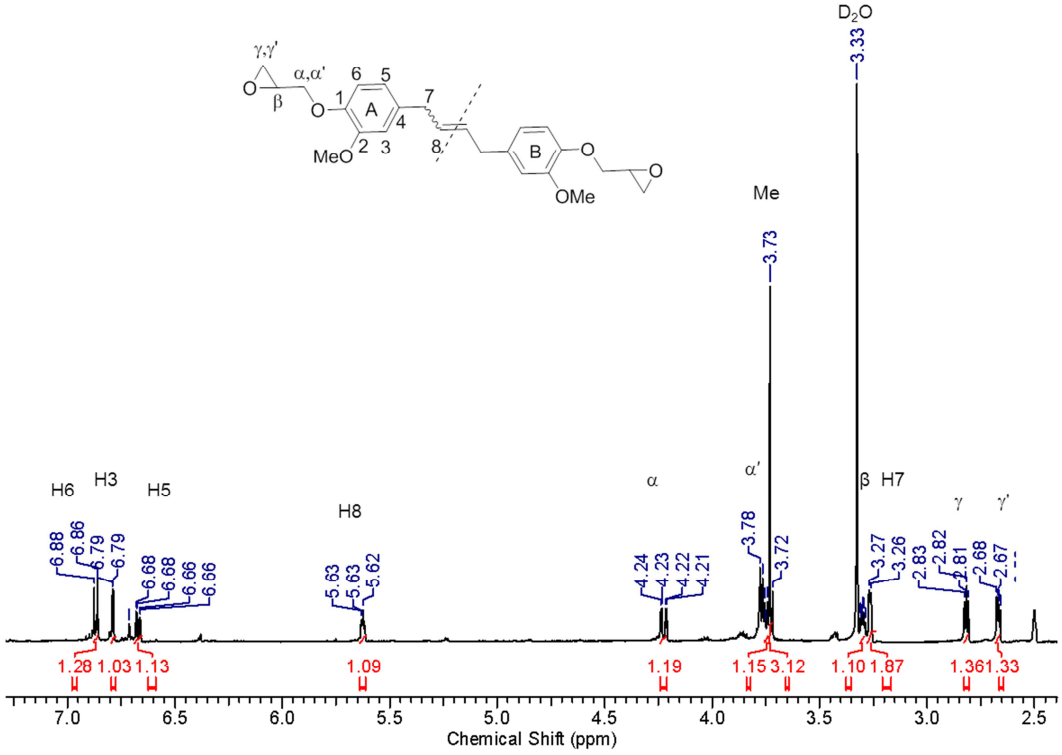


1D ^{13}C spectrum of product **6**

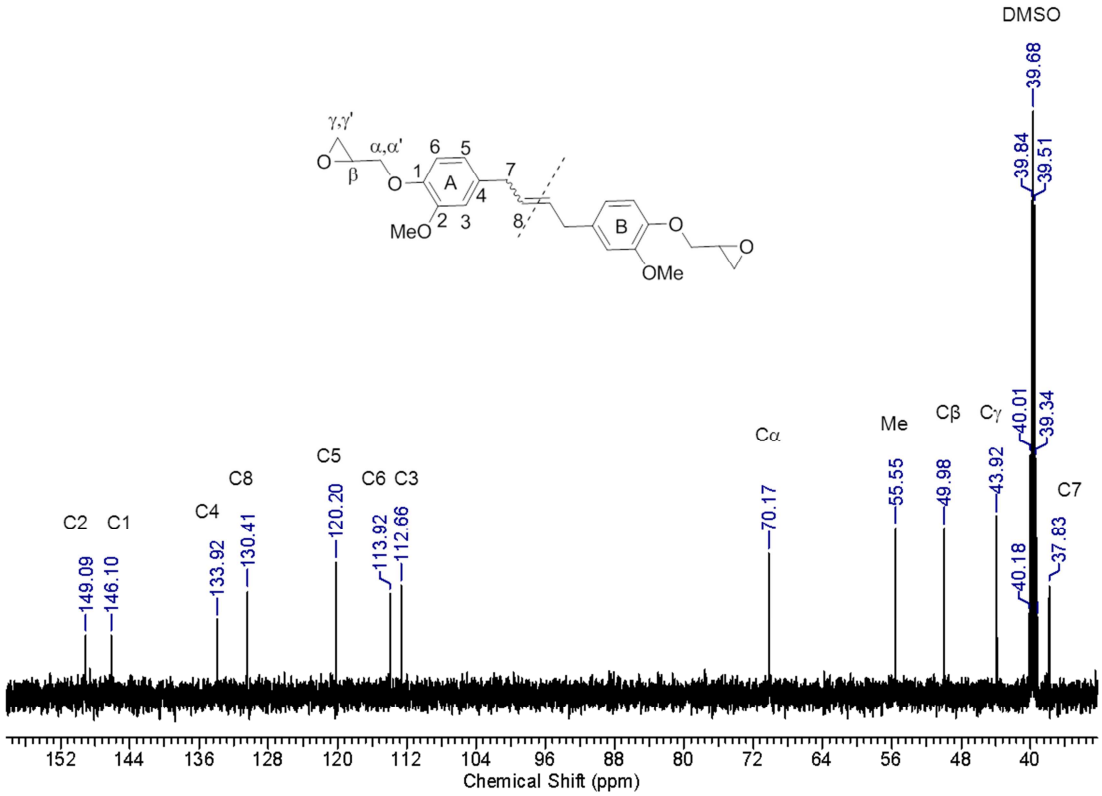


HMBC spectrum of product **6**

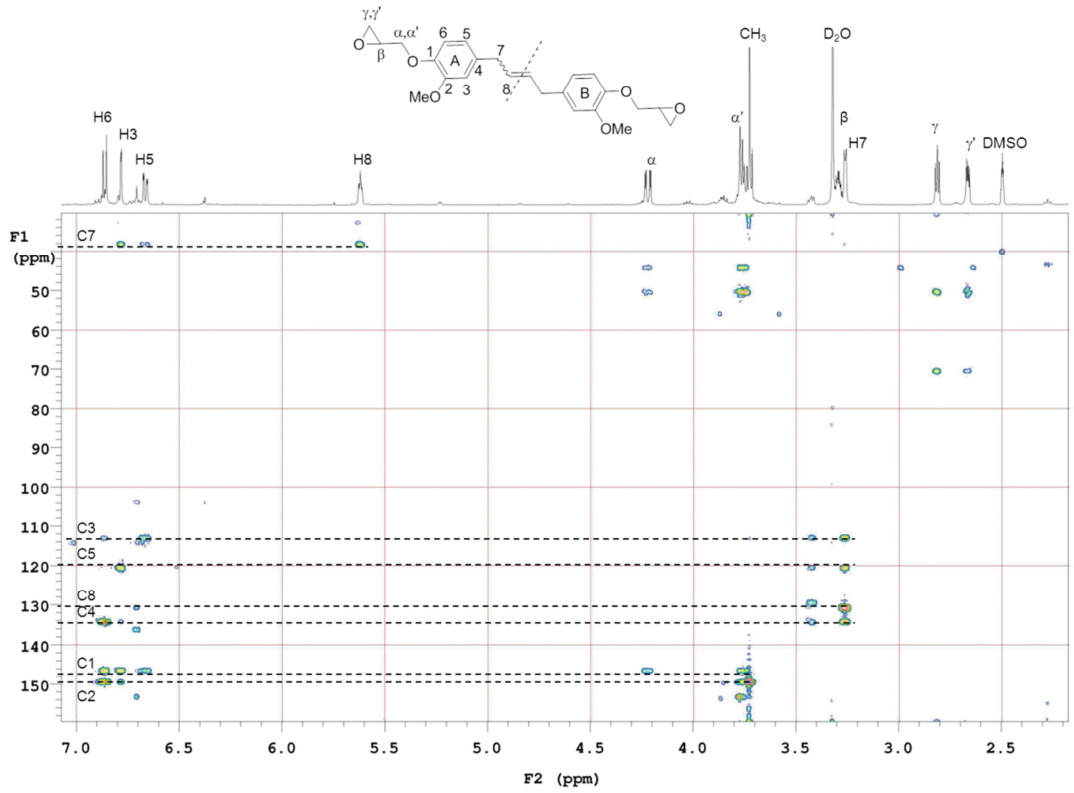
Product 7



1D ^{1}H spectrum of product **7**

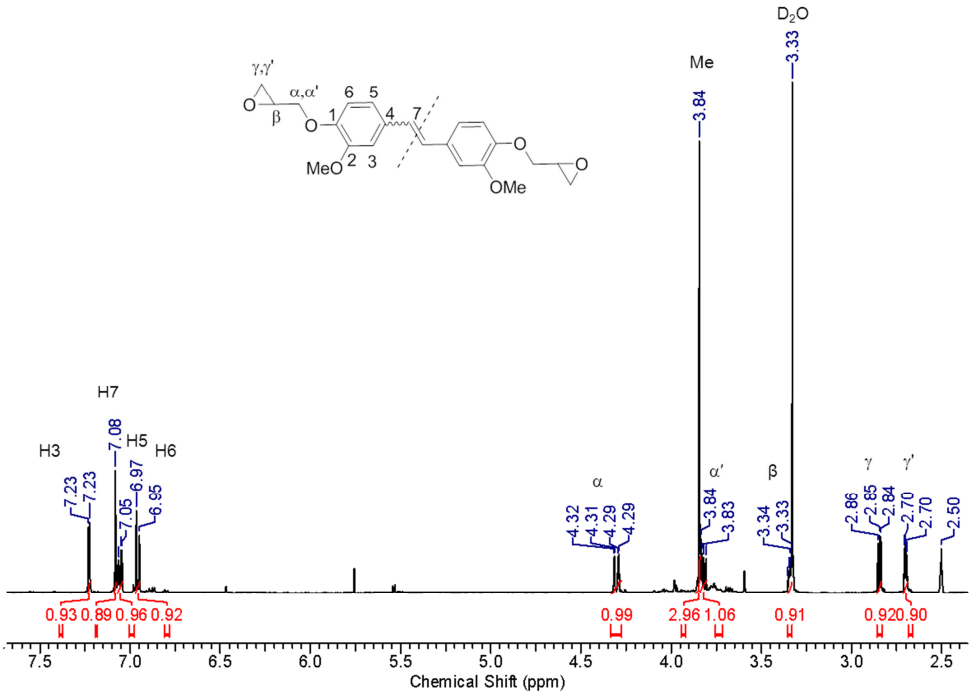


1D ^{13}C spectrum of product **7**

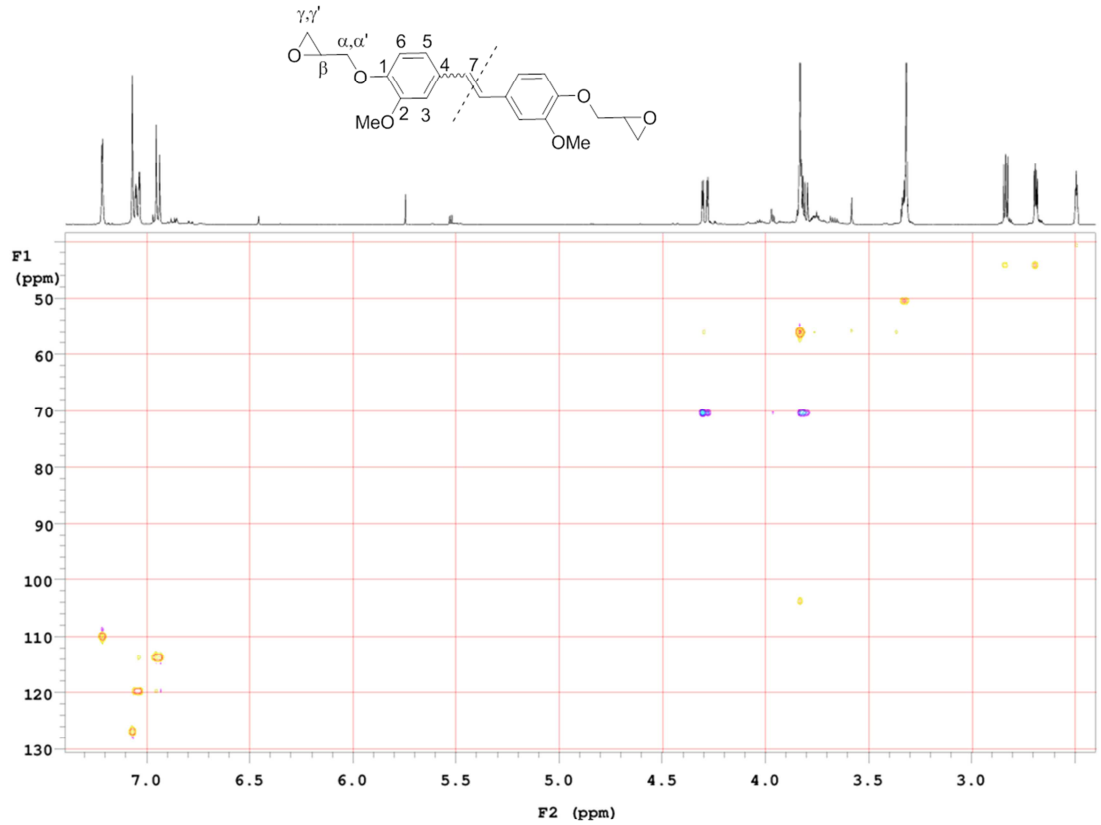


HMBC spectrum of product **7**

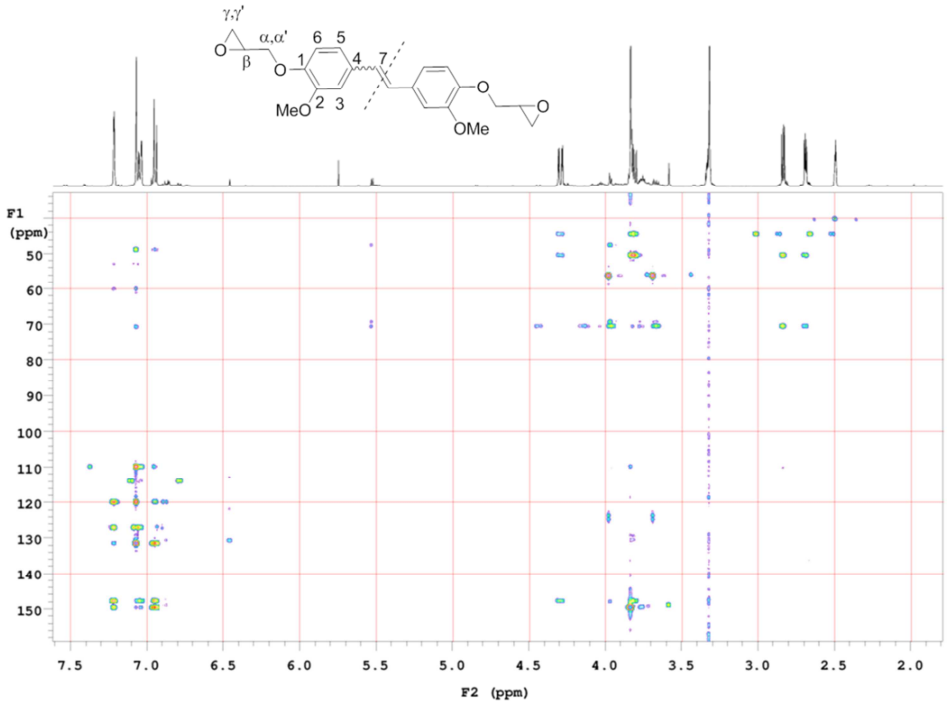
Product 8



1D ^{1}H spectrum of product **8**

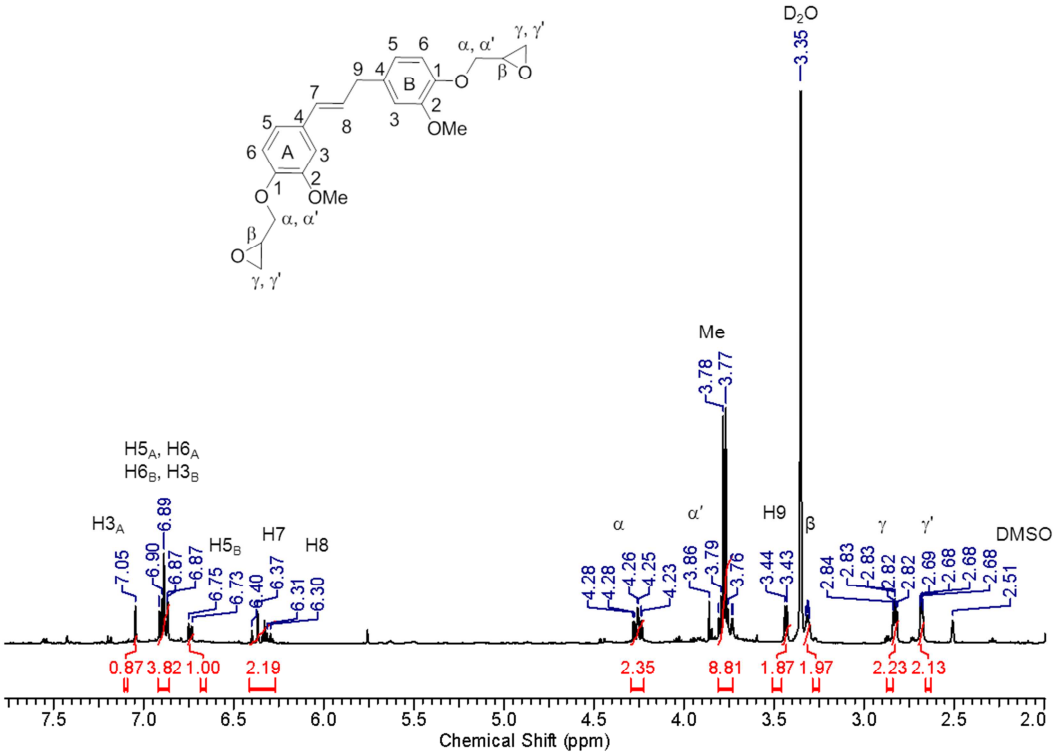


HSQC spectrum of product **8**

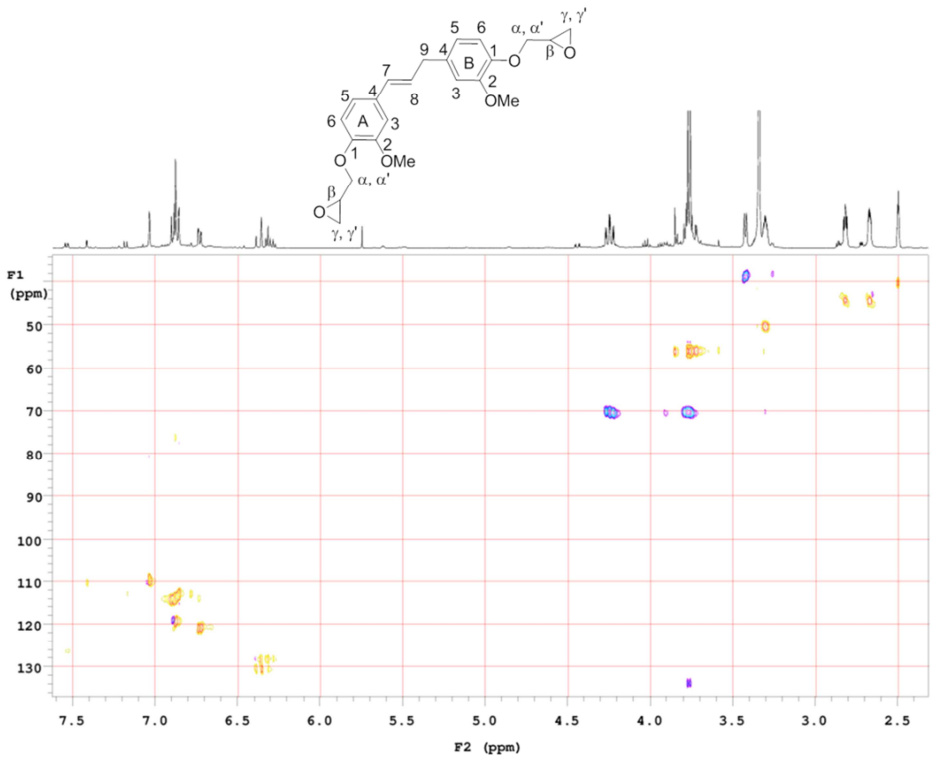


HMBC spectrum of product **8**

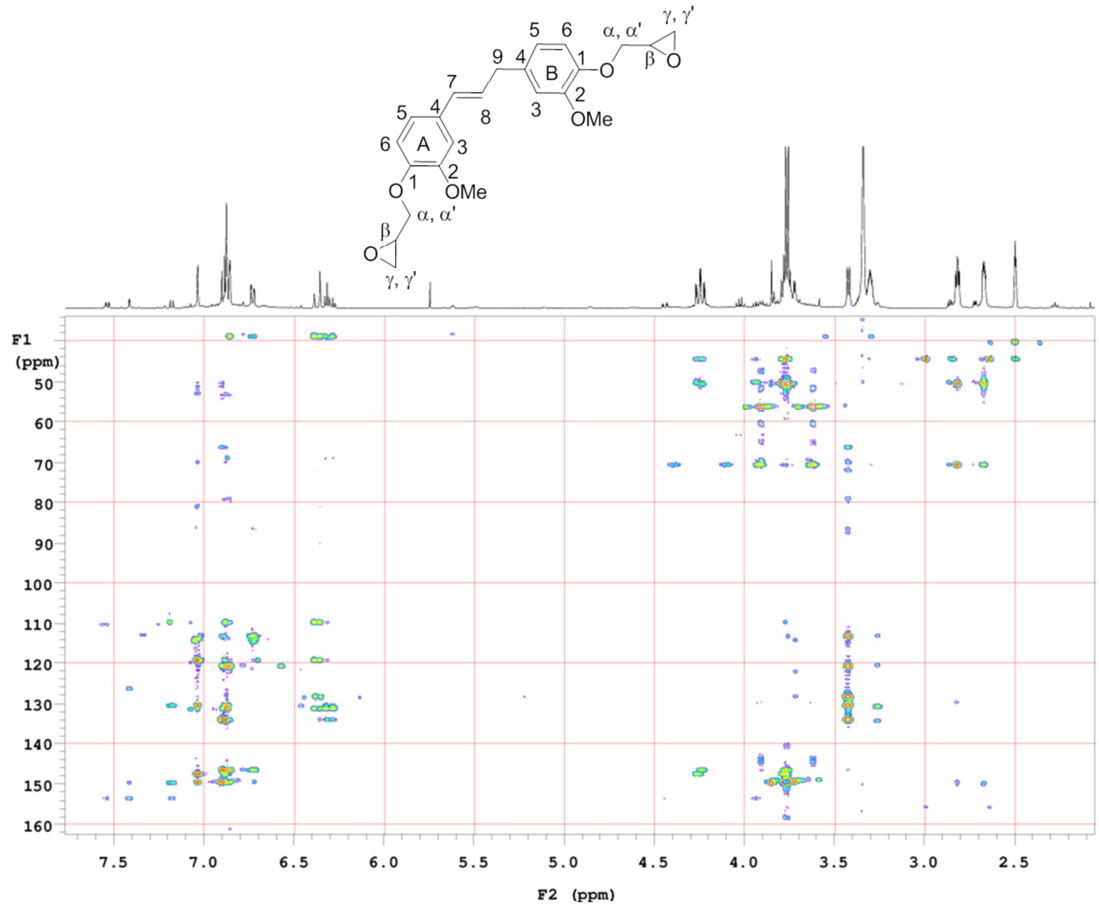
Product 9



1D ^{1}H spectrum of product **9**

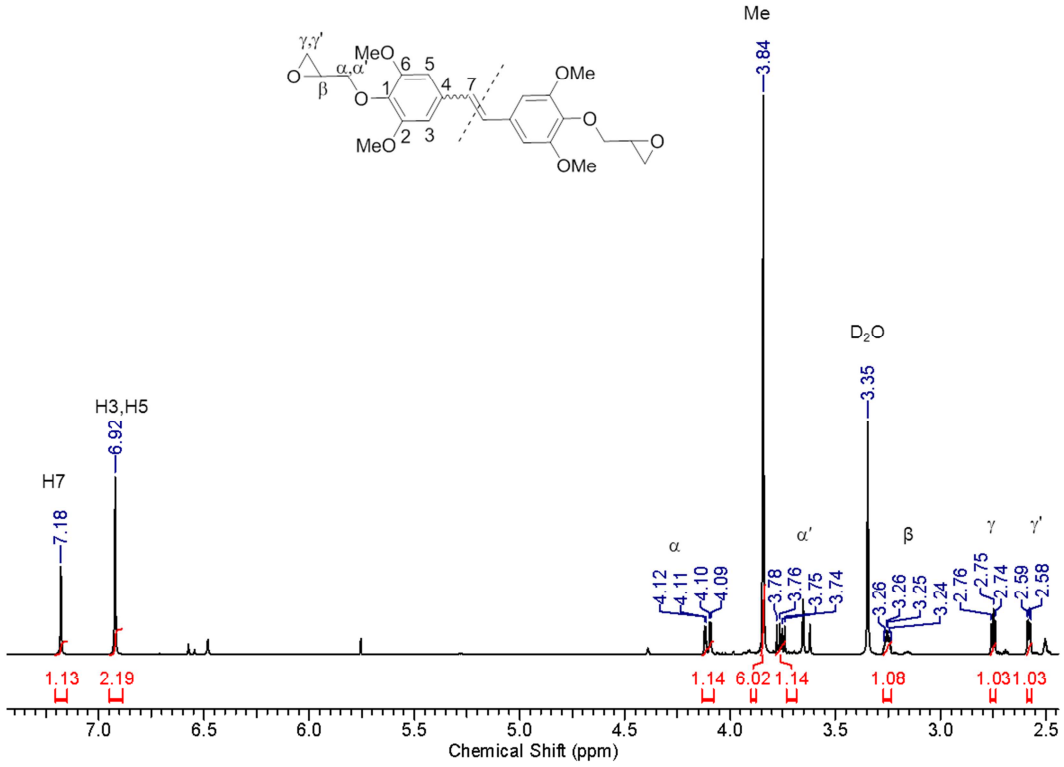


HSQC spectrum of product **9**

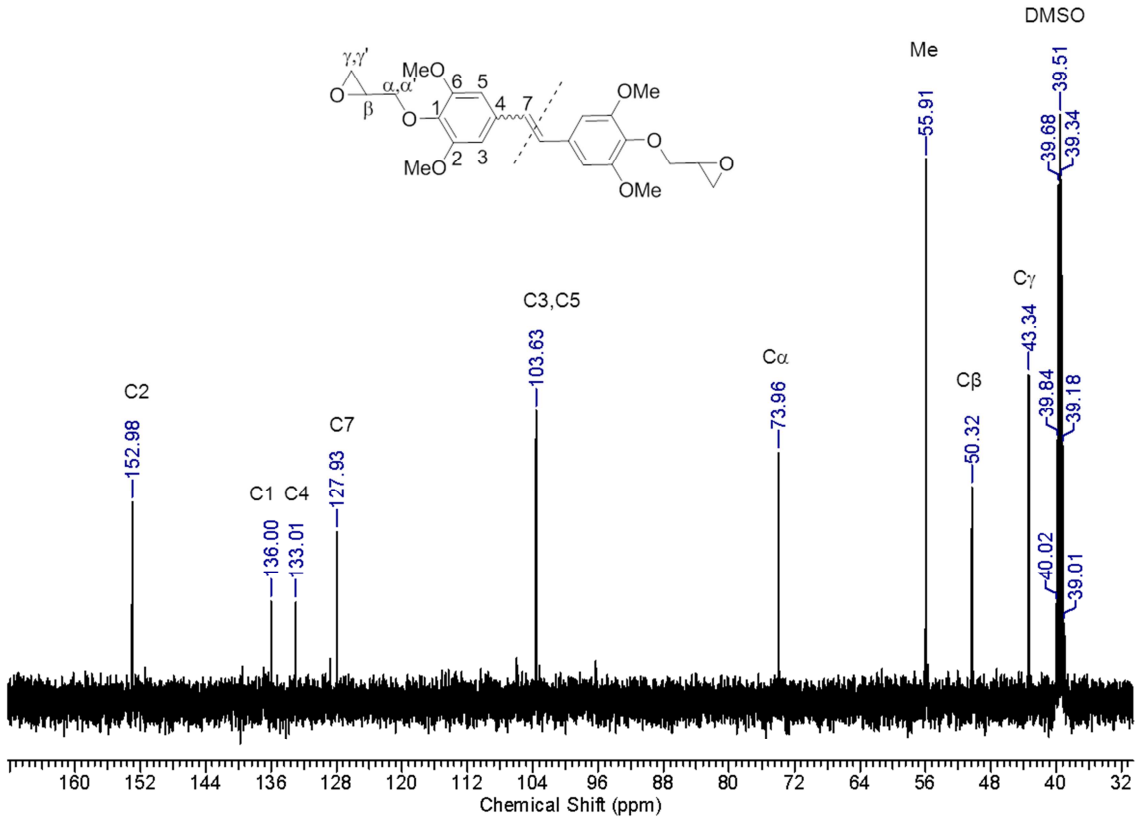


HMBC spectrum of product **9**

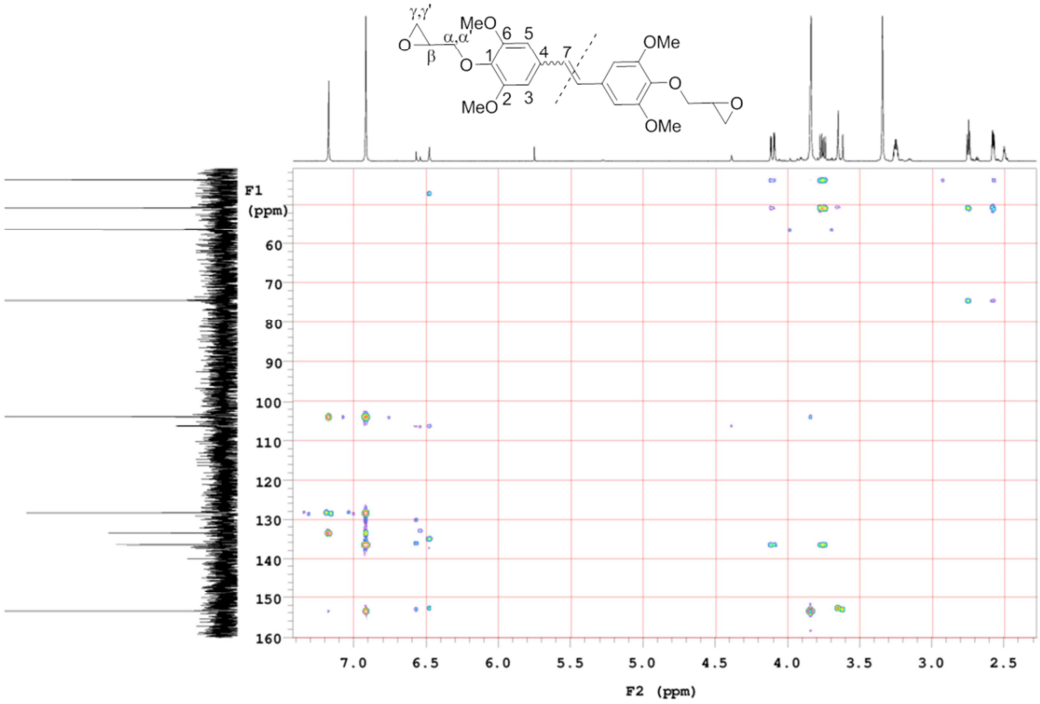
Product 10



1D ^{1}H spectrum of product **10**

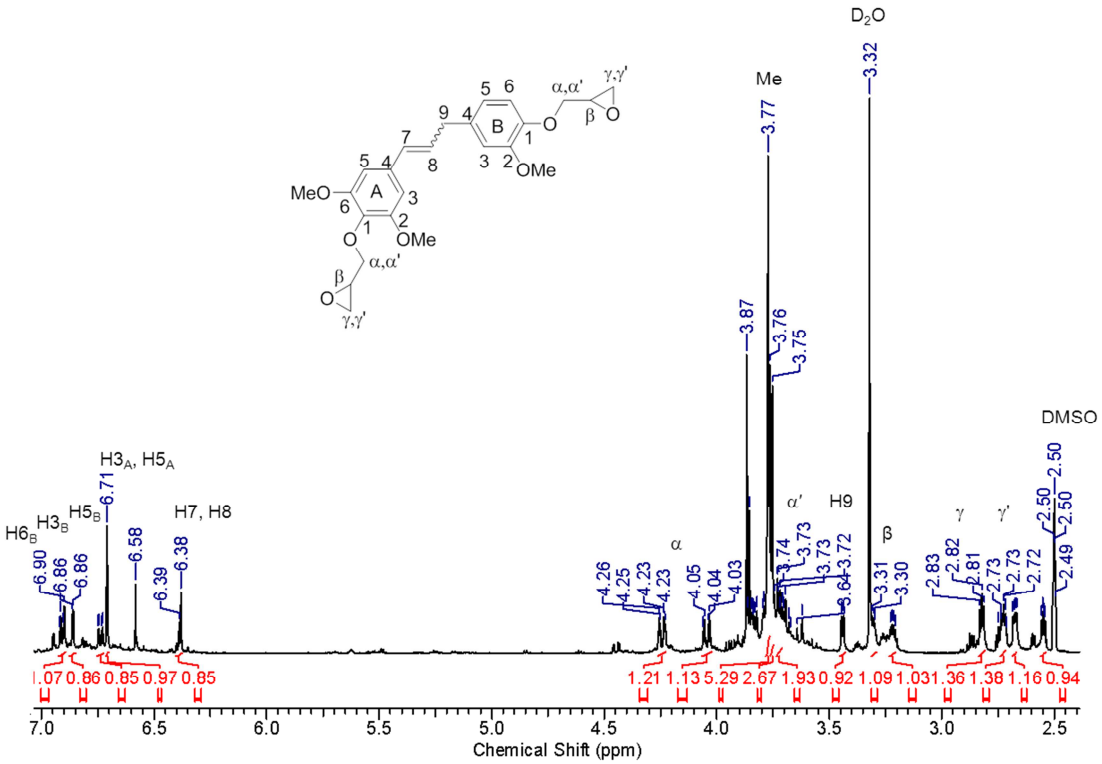


1D ^{13}C spectrum of product **10**

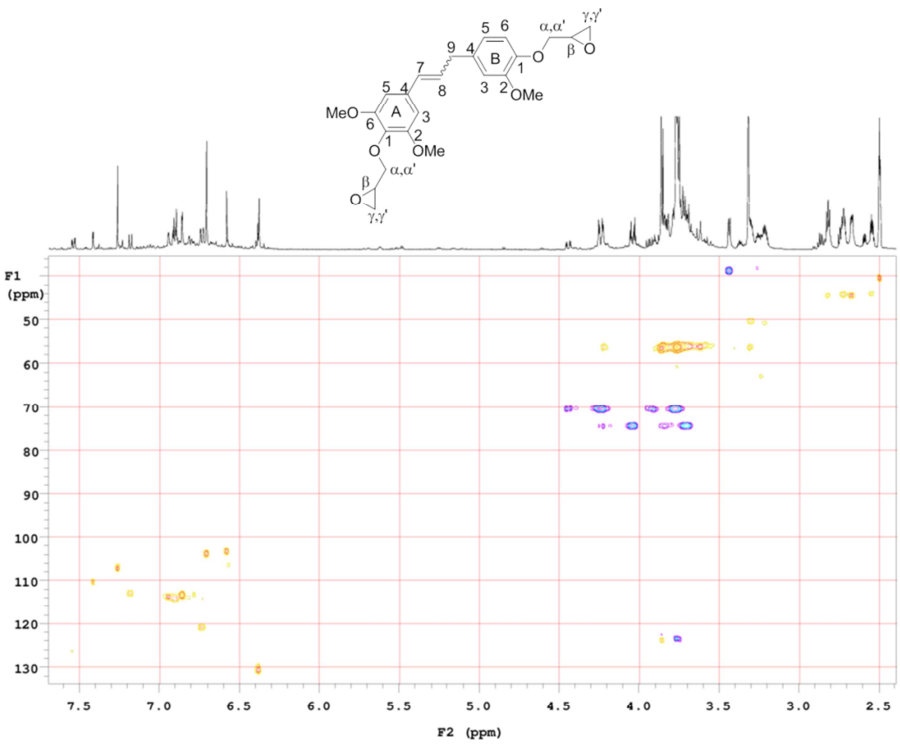


HMBC spectrum of product **10**

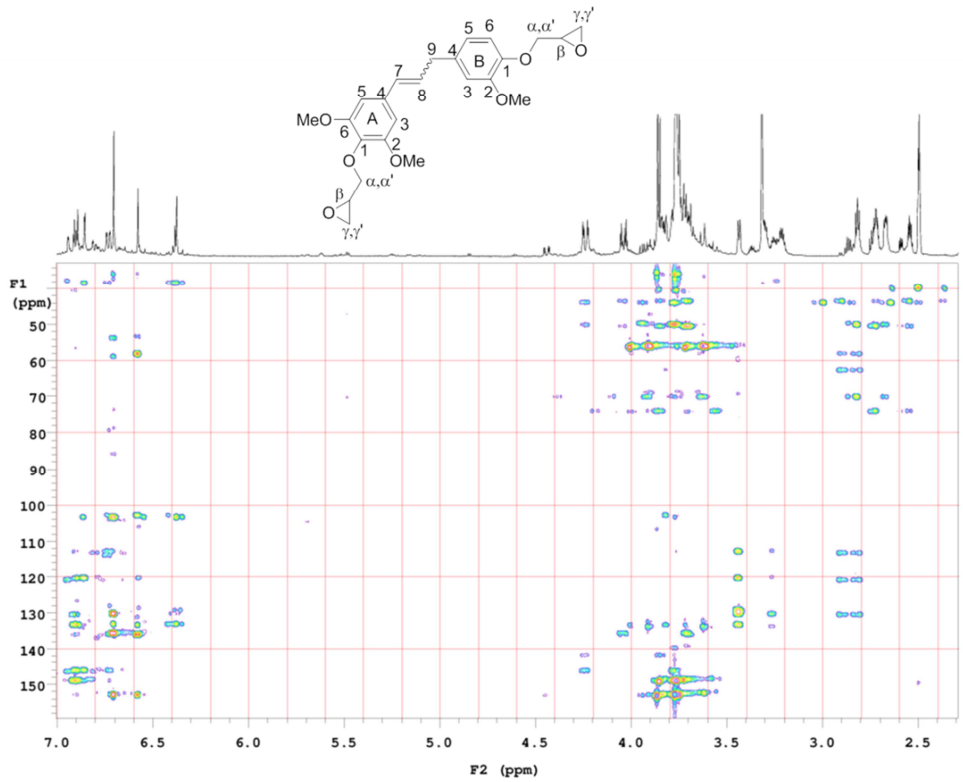
Product 11



1D ^{1}H spectrum of product **11**

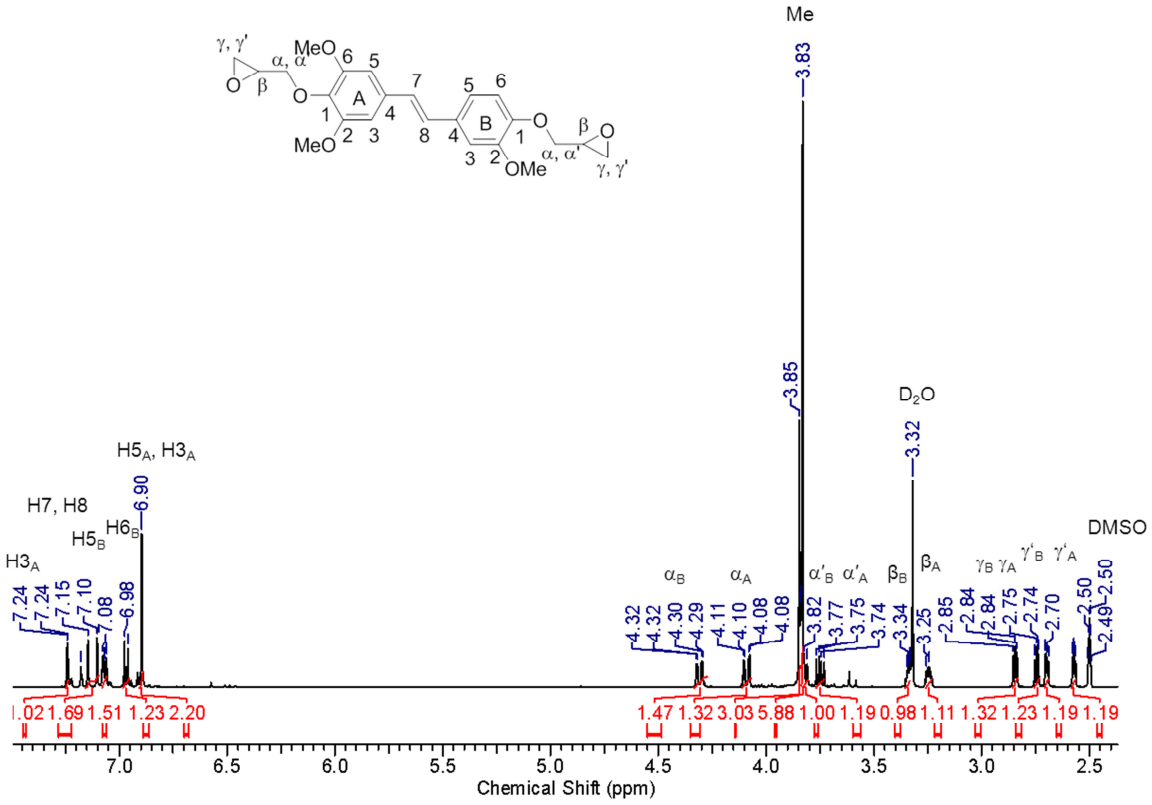


HSQC spectrum of product **11**

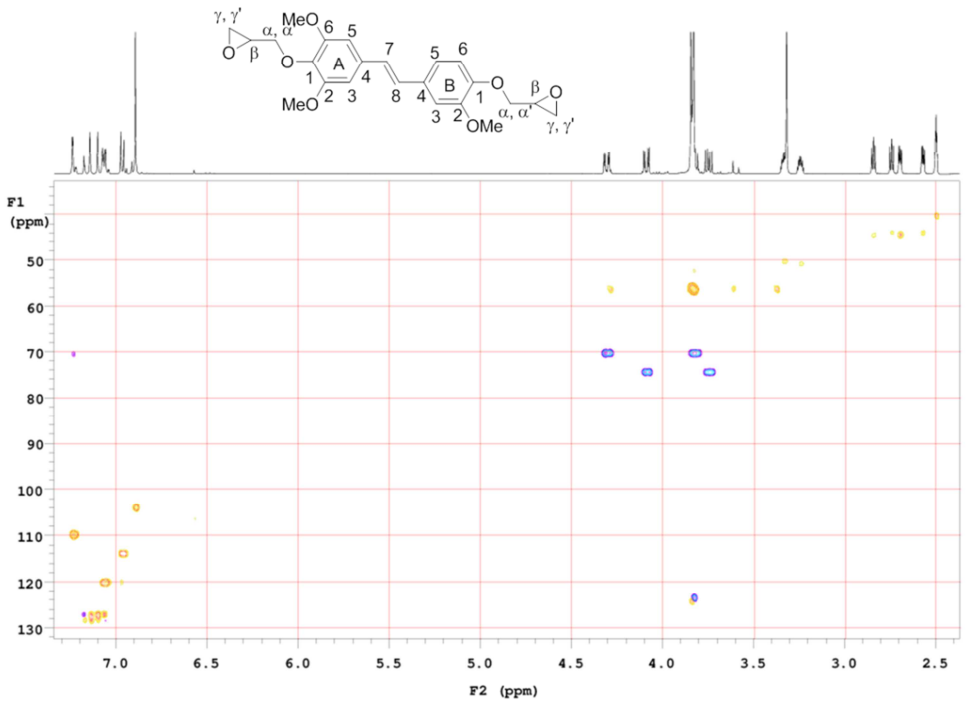


HMBC spectrum of product **11**

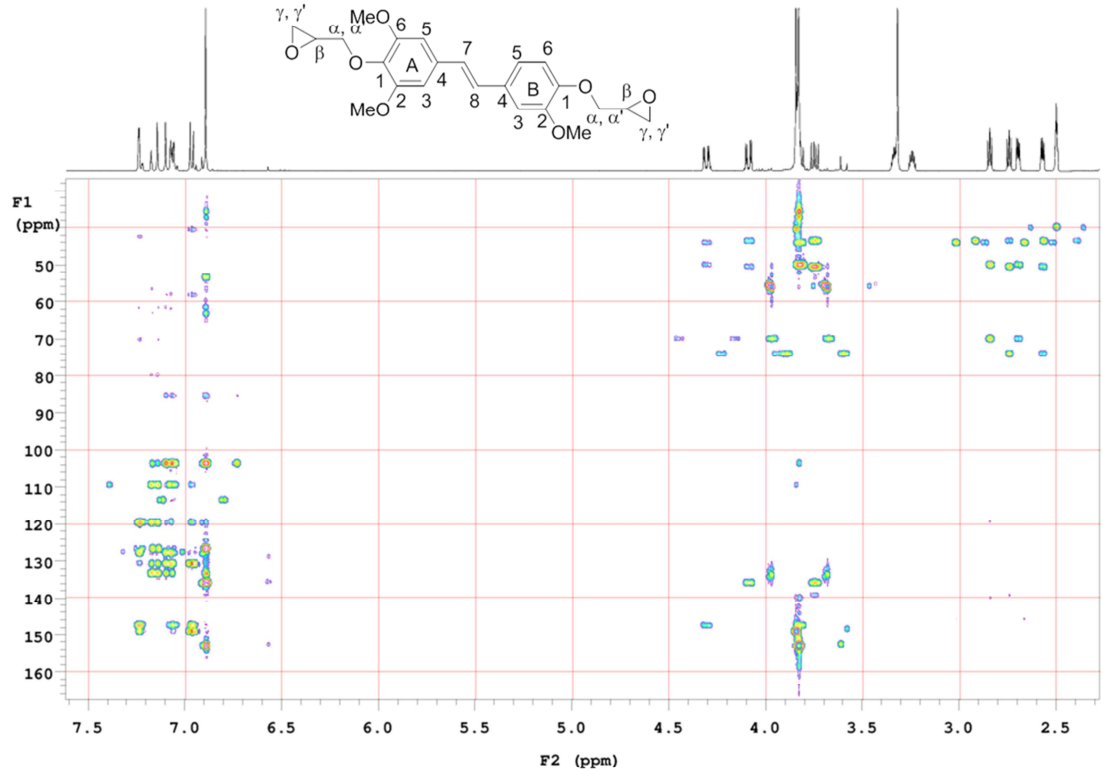
Product 12



1D ^{1}H spectrum of product **12**



HSQC spectrum of product **12**



HMBC spectrum of product **12**

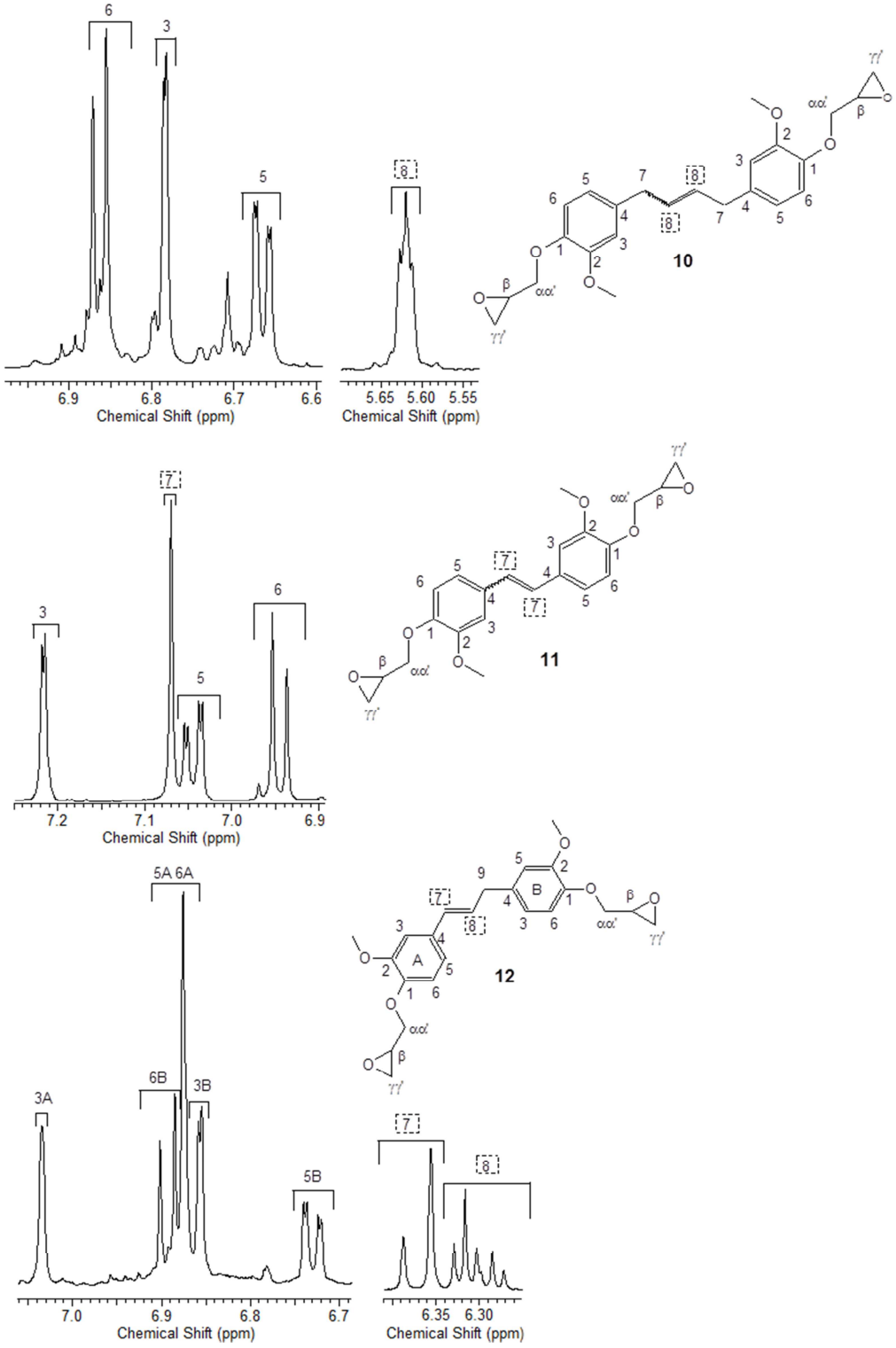


Figure 1: ^{1}H NMR spectra of compounds **7**, **8** and **9** showing the olefinic bonds signals.