Supplementary Material

BF_3OEt_2 and $MeSO_3H$-Promoted reactions of phenols and ethyl phenylpropiolate as a synthetic routes to neoflavones and a potential route to flavones

Nayang Kgakatsi, Runner R. T. Majinda, and Ishmael B. Masesane

Department of Chemistry, University of Botswana, Private Bag 00704, Gaborone, Botswana
Email: masesane@ub.ac.bw

Table of Contents

Typical Procedure for $BF_3.OEt_2$-promoted reaction of phenols and ethyl phenylpropiolate

A mixture of phenol **1** (0.50 g, 5.3 mmol) with ethyl phenylpropiolate **2** (0.93 g, 5.3 mmol) in the presence of excess BF_3OEt_2 (3 mL, 24.3 mmol) and DMF (1.88 mL, 24.3 mmol) was refluxed for 3 h. The reaction was quenched with water and extracted with chloroform. The extract was concentrated using rotavapor and adsorbed on silica before been subjected to column chromatography and eluted with *n*-hexane-ethyl acetate (8: 3)

Typical Procedure for $MeSO_3H$-promoted reaction of phenols and ethyl phenylpropiolate

A mixture of phenol **1** (0.5 g, 5.3 mmol) and ethyl phenylpropiolate **2** (0.93 g, 5.3 mmol) in the presence of excess methanesulfonic acid (3 mL, 46.2 mmol) was stirred at room temperature for 2 h. The reaction was quenched with a saturated aqueous solution of $NaHCO_3$ and extracted with chloroform. The extract was then concentrated using rotavapor and subjected to column chromatography eluting with *n*-hexane-ethyl acetate (8:3).

^{1}H and ^{13}C SPECTRA OF THE PREPARED COMPOUNDS

Figure 1. ^{1}H NMR (500 MHz, chloroform-d) spectrum of neoflavone **4.**

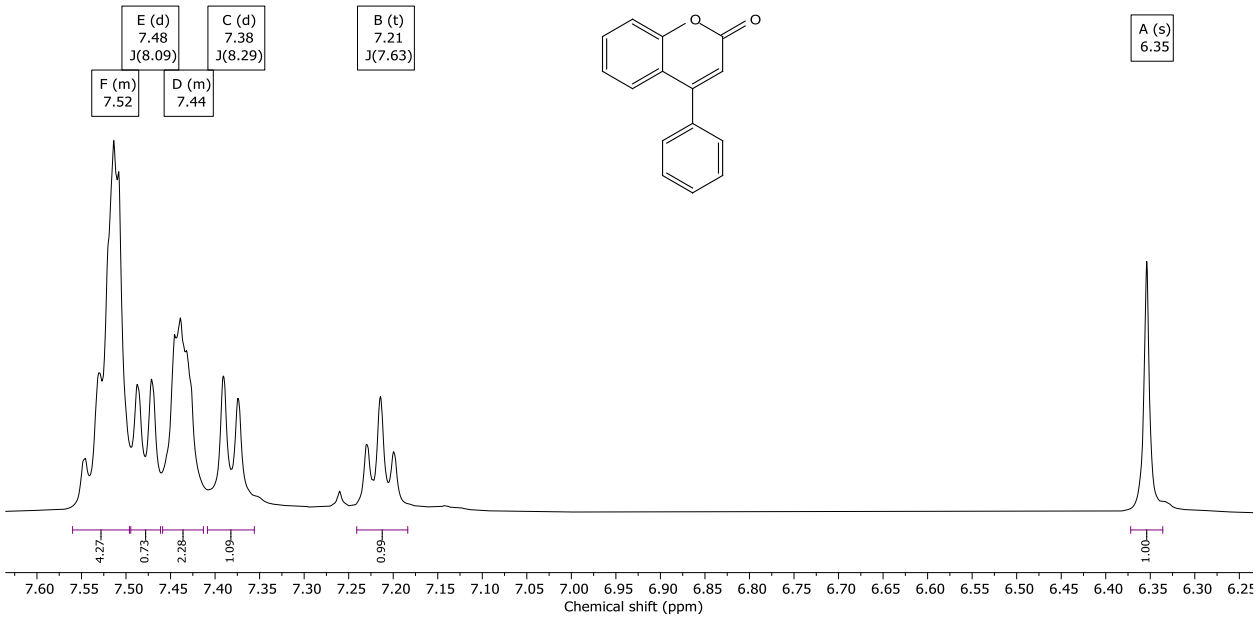

Figure 2. ^{13}C NMR (125 MHz, chloroform-d) spectrum of neoflavone **4.**

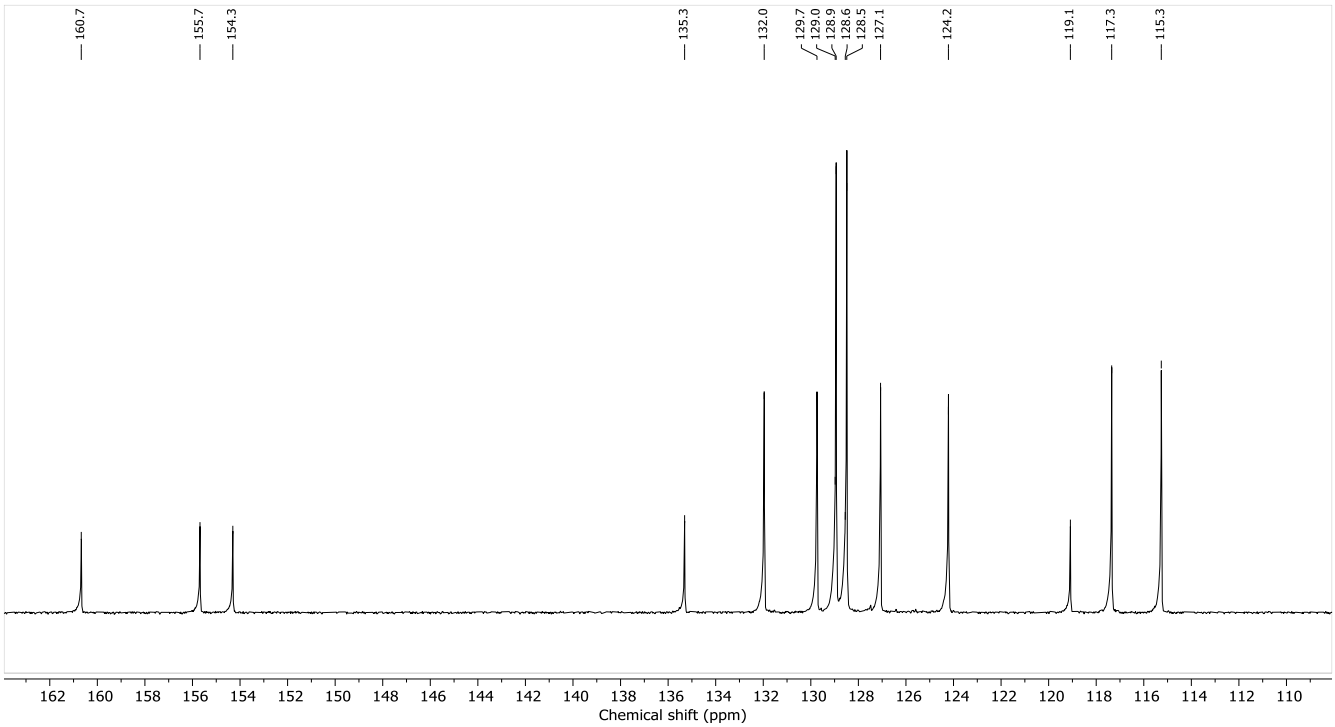

Figure 3. ^{1}H NMR (500 MHz, chloroform-d) spectrum of flavone **6.**

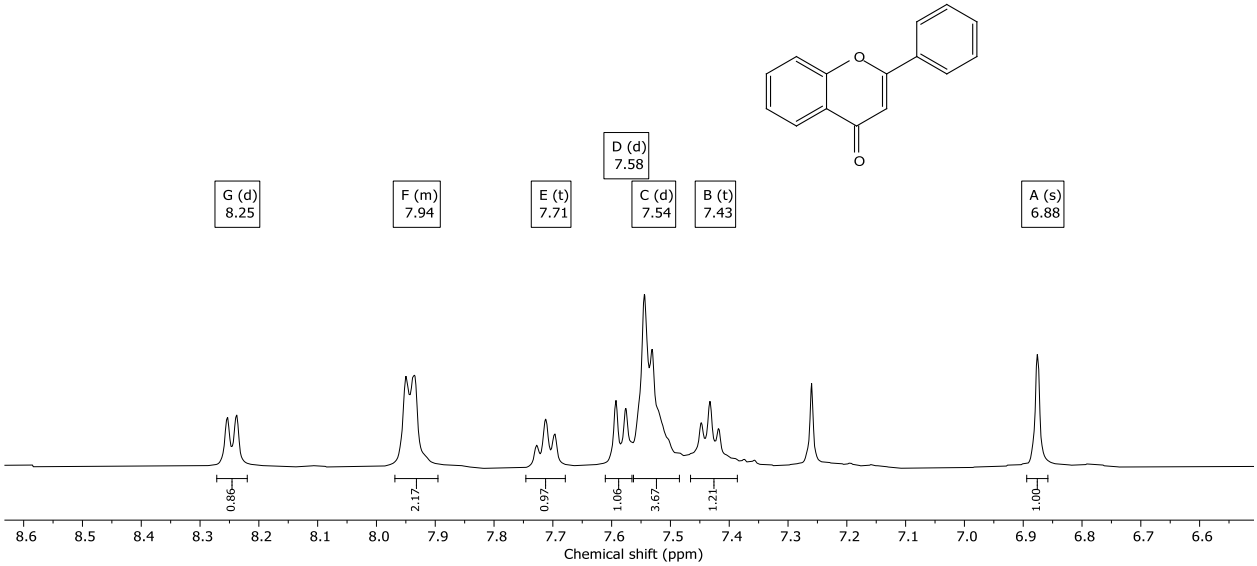

Figure 4. ^{13}C NMR (125 MHz, chloroform-d) spectrum of flavone **6.**

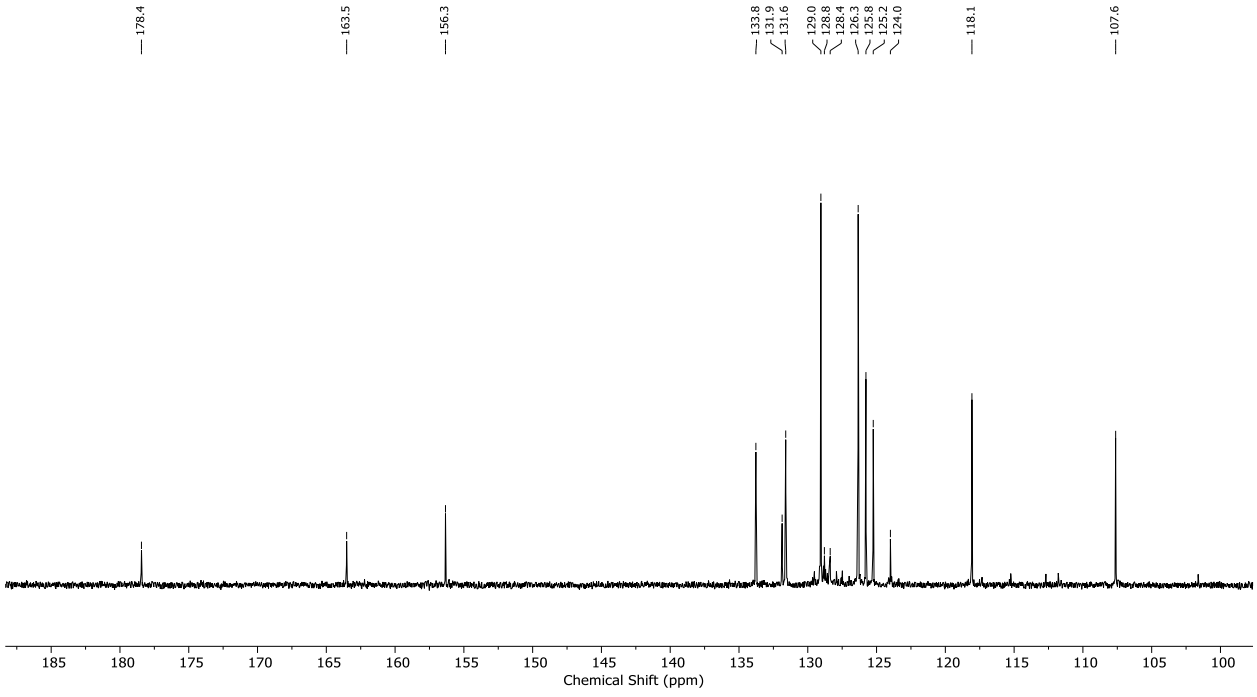

Figure 5. ^{1}H NMR (500 MHz, chloroform-d) spectrum of neoflavone **8.**

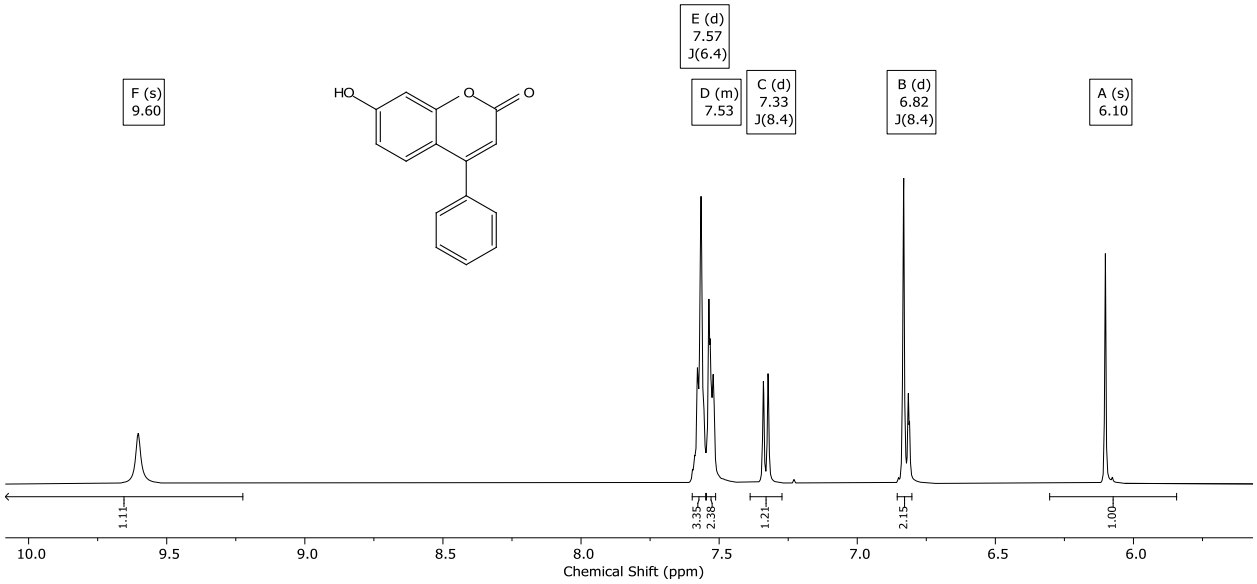

Figure 6. ^{13}C NMR (125 MHz, chloroform-d) spectrum of Neoflavone **8.**

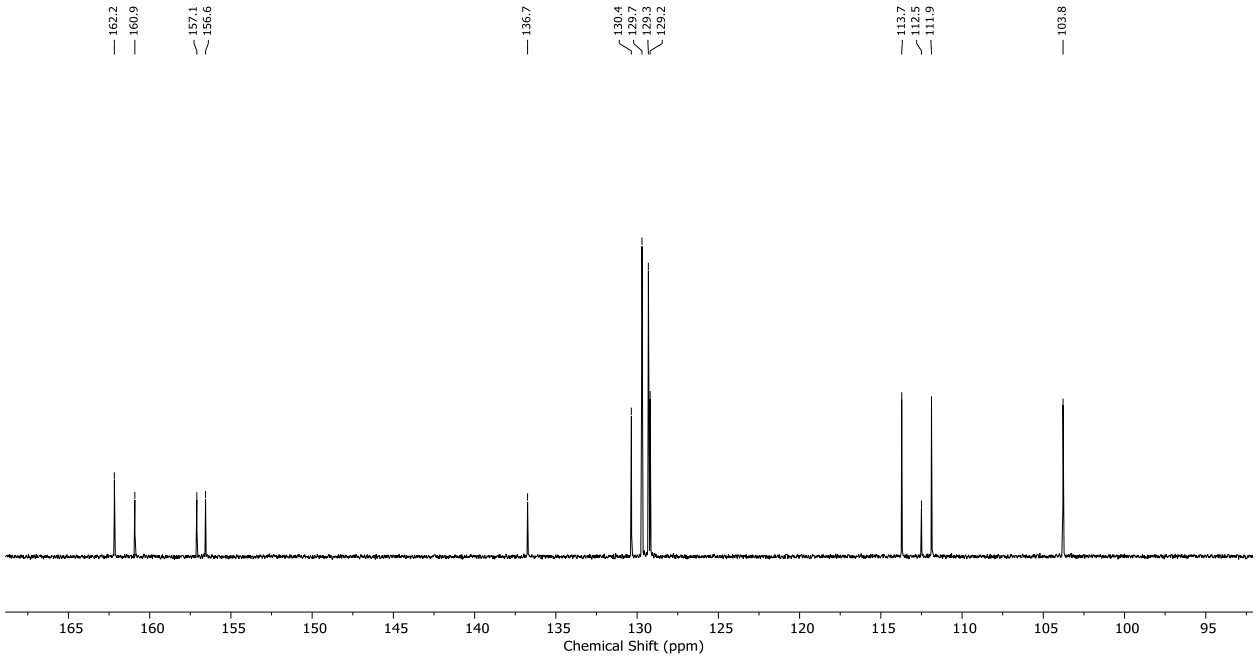

Figure 7. ^{1}H NMR (500 MHz, chloroform-d) spectrum of neoflavone **10.**

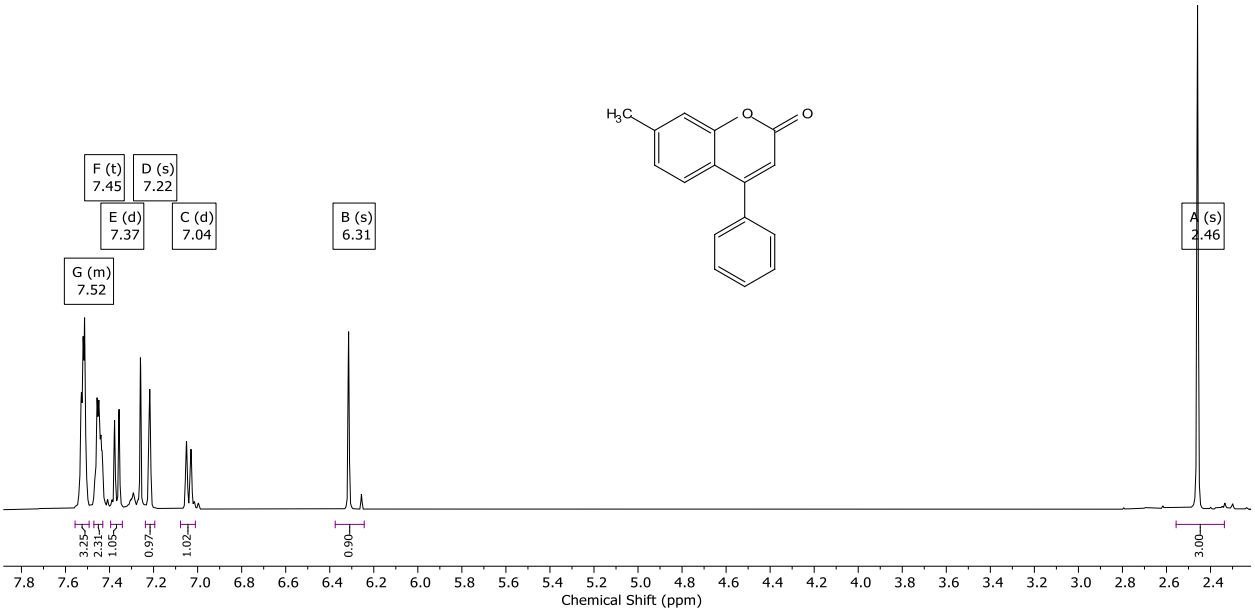

Figure 8. ^{13}C NMR (125 MHz, chloroform-d) spectrum of flavone **10.**

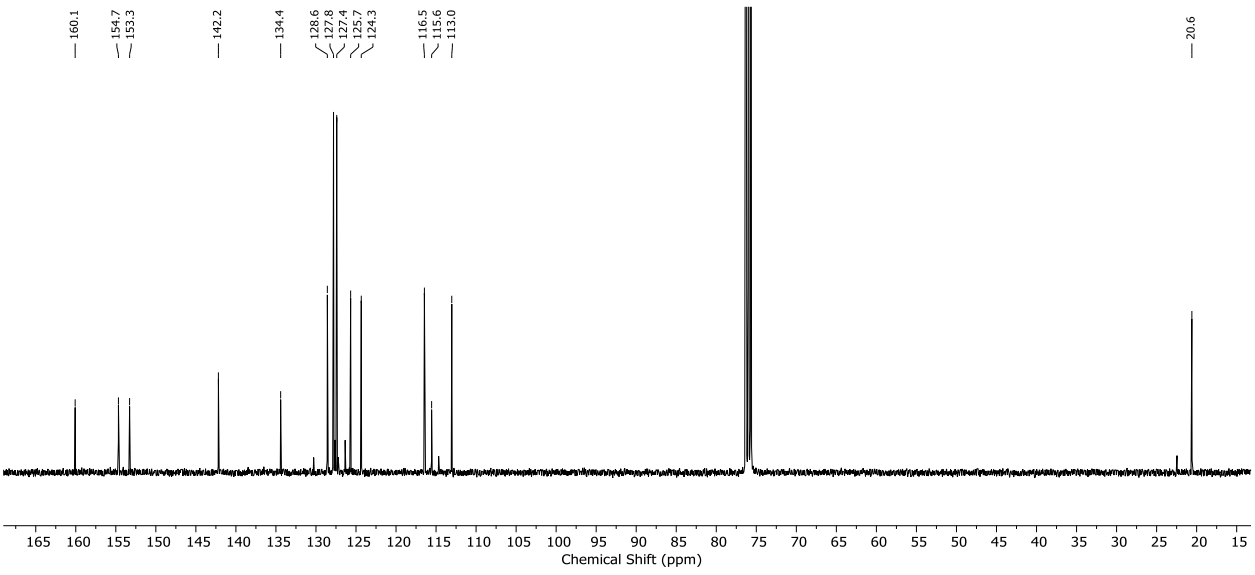

Figure 9. ^{1}H NMR (500 MHz, chloroform-d) spectrum of neoflavone **11.**

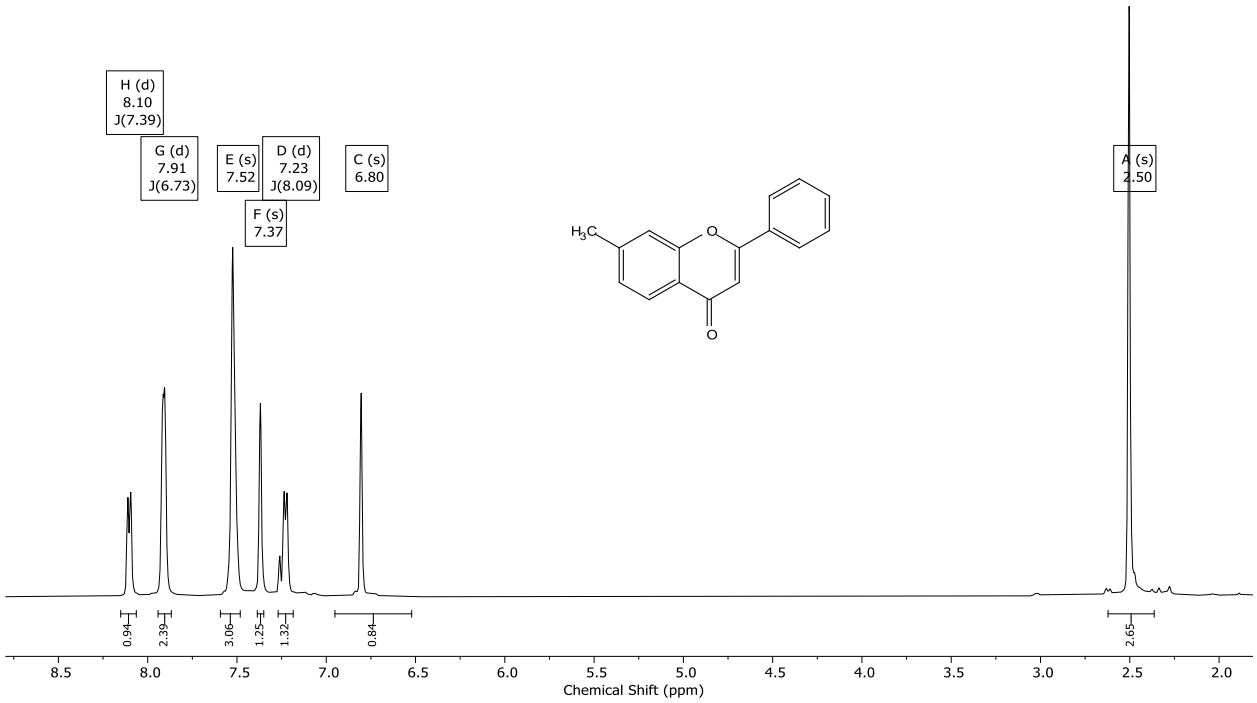

Figure 10. ^{13}C NMR (125 MHz, chloroform-d) spectrum of flavone **11.**

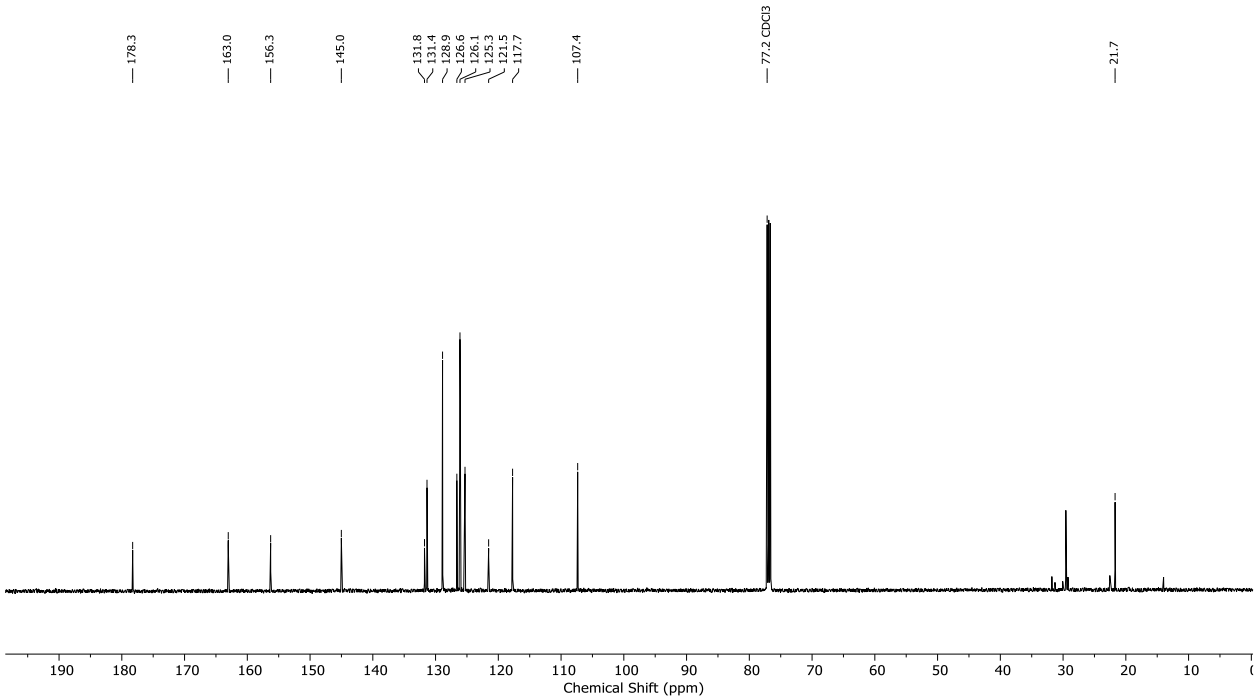

Figure 11. ^{1}H NMR (500 MHz, chloroform-d) spectrum of flavone **12.**

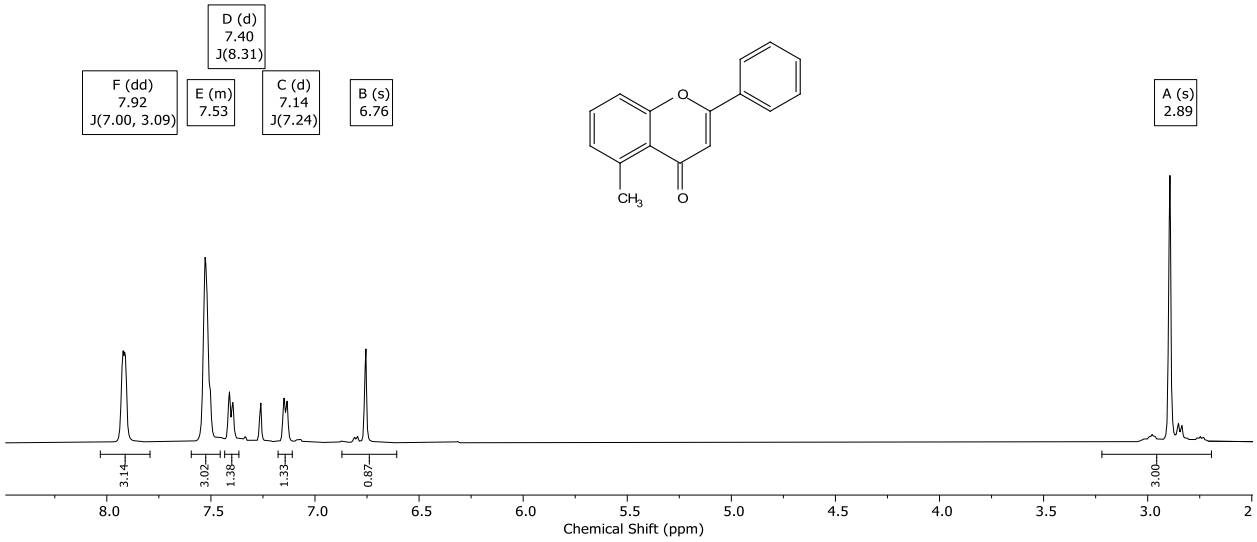

Figure 12. ^{13}C NMR (125 MHz, chloroform-d) spectrum of flavone **12.**

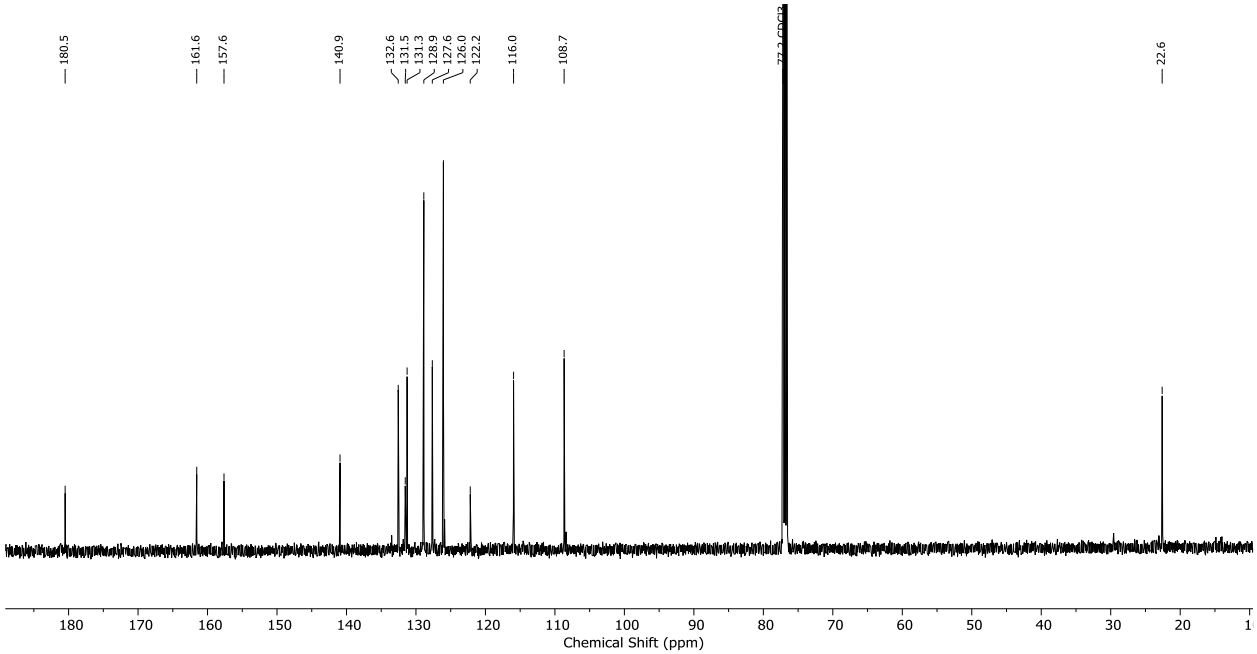

Figure 13. ^{1}H NMR (500 MHz, chloroform-d) spectrum of neoflavone **14.**

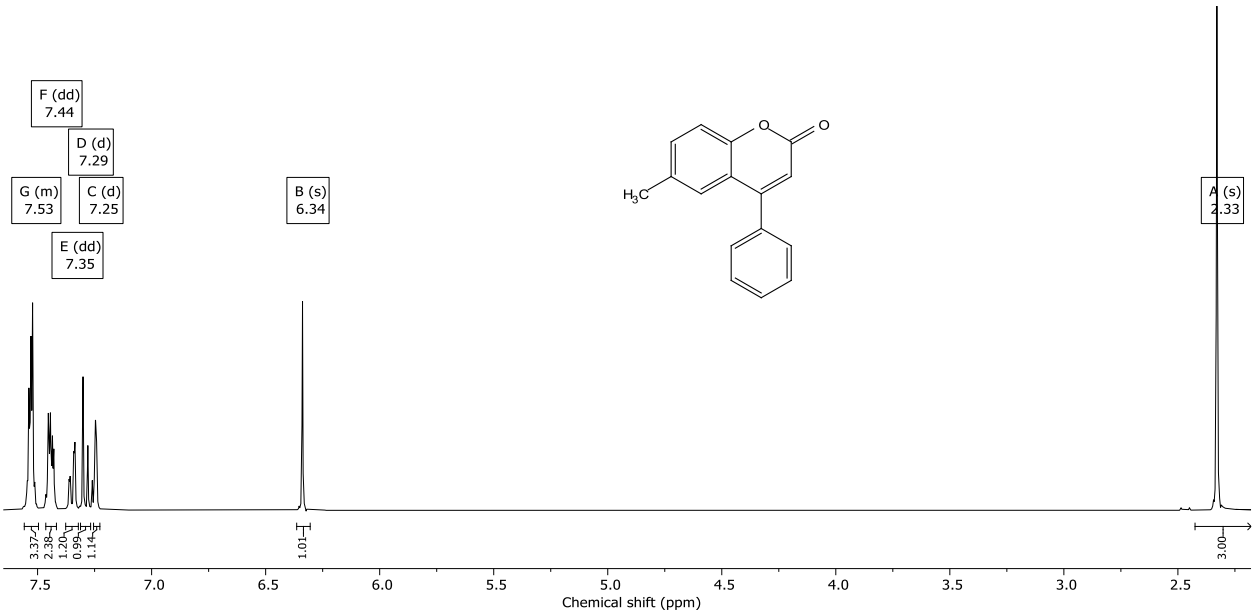

Figure 14. ^{13}C NMR (125 MHz, chloroform-d) spectrum of neoflavone **14.**

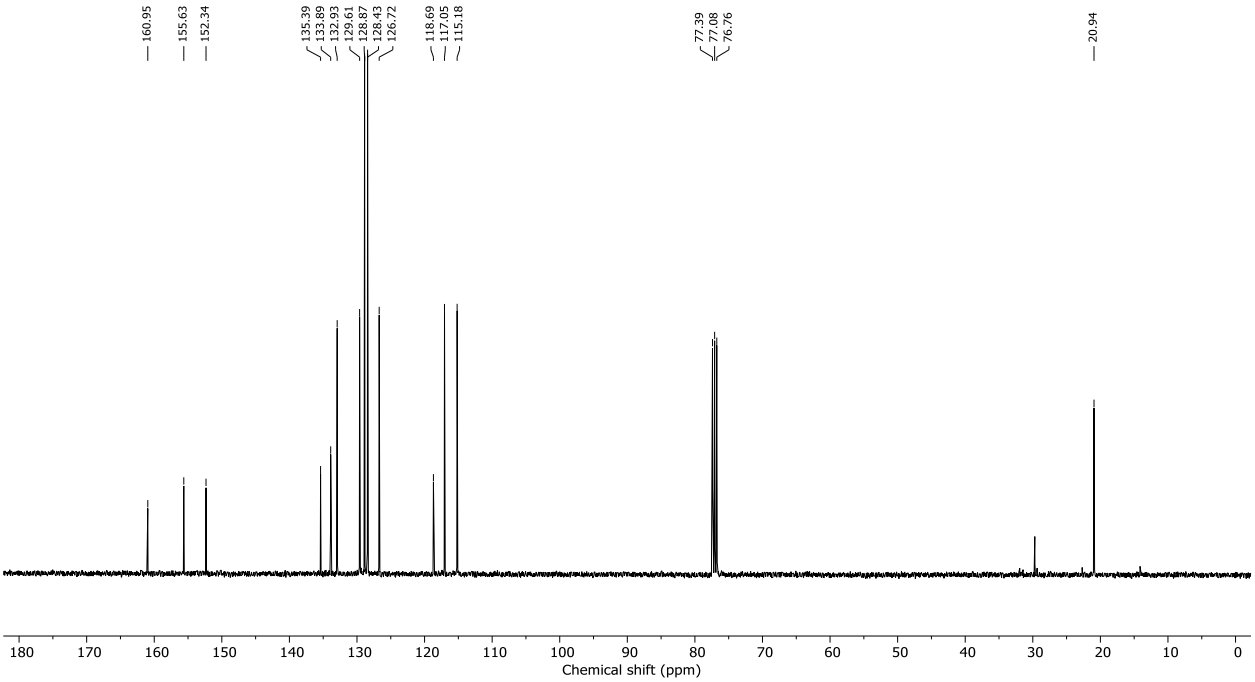

Figure 15. ^{1}H NMR (500 MHz, chloroform-d) spectrum of flavone **15.**

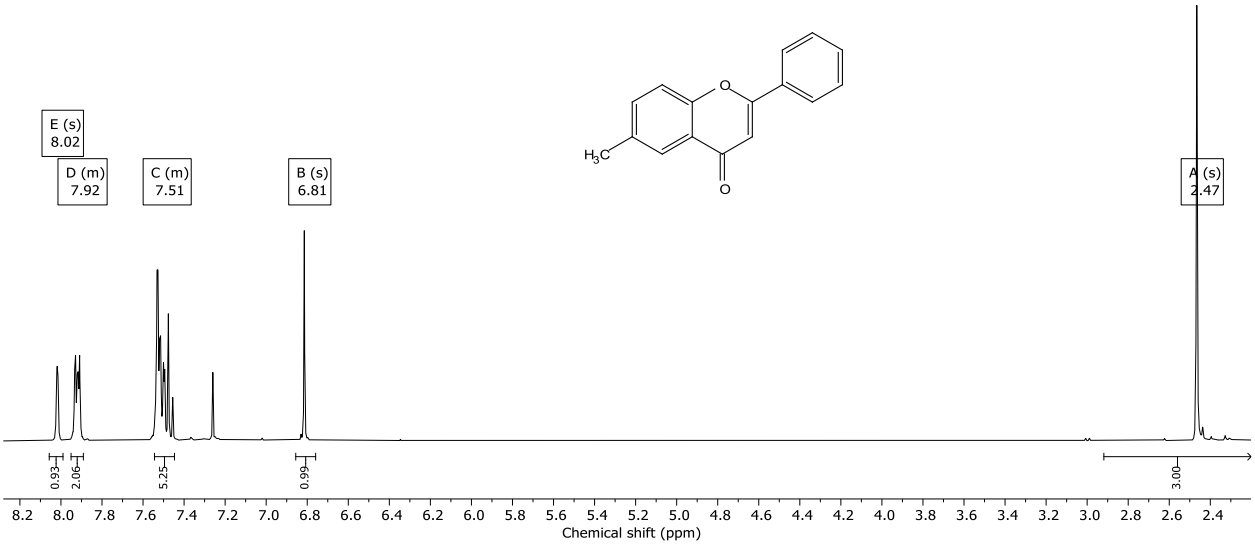

Figure 16. ^{13}C NMR (125 MHz, chloroform-d) spectrum of flavone **15.**

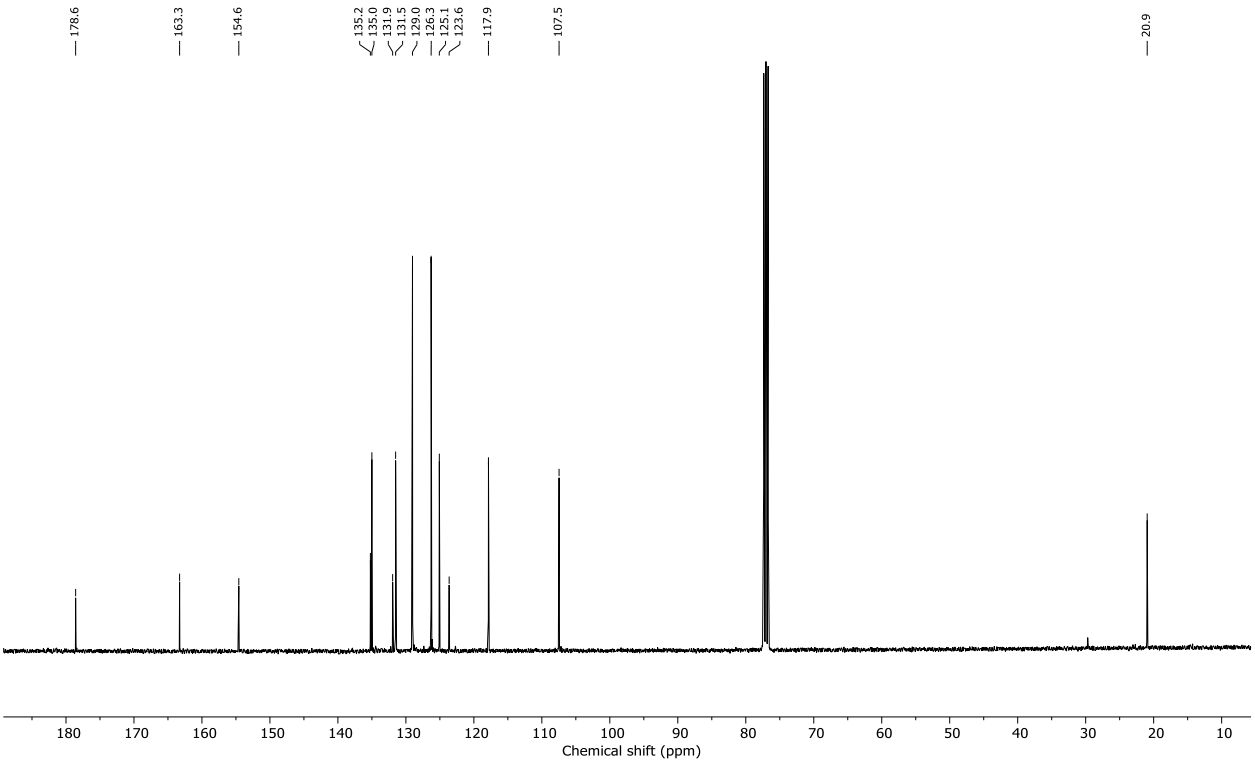

Figure 17. ^{1}H NMR (500 MHz, chloroform-d) spectrum of neoflavone **17.**

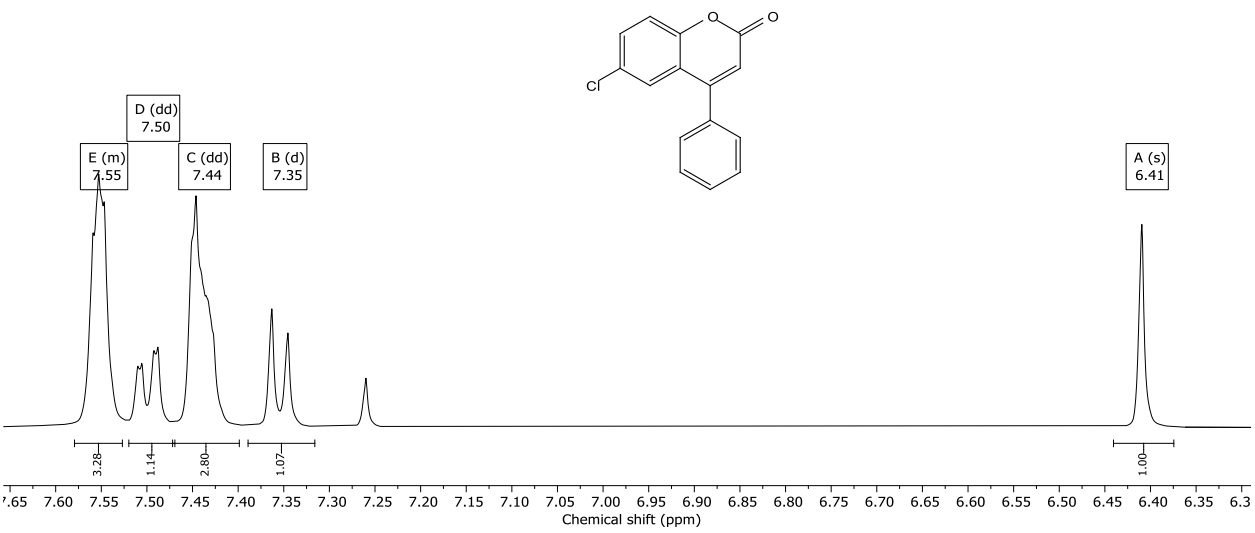

Figure 18. ^{13}C NMR (125 MHz, chloroform-d) spectrum of neoflavone **17.**

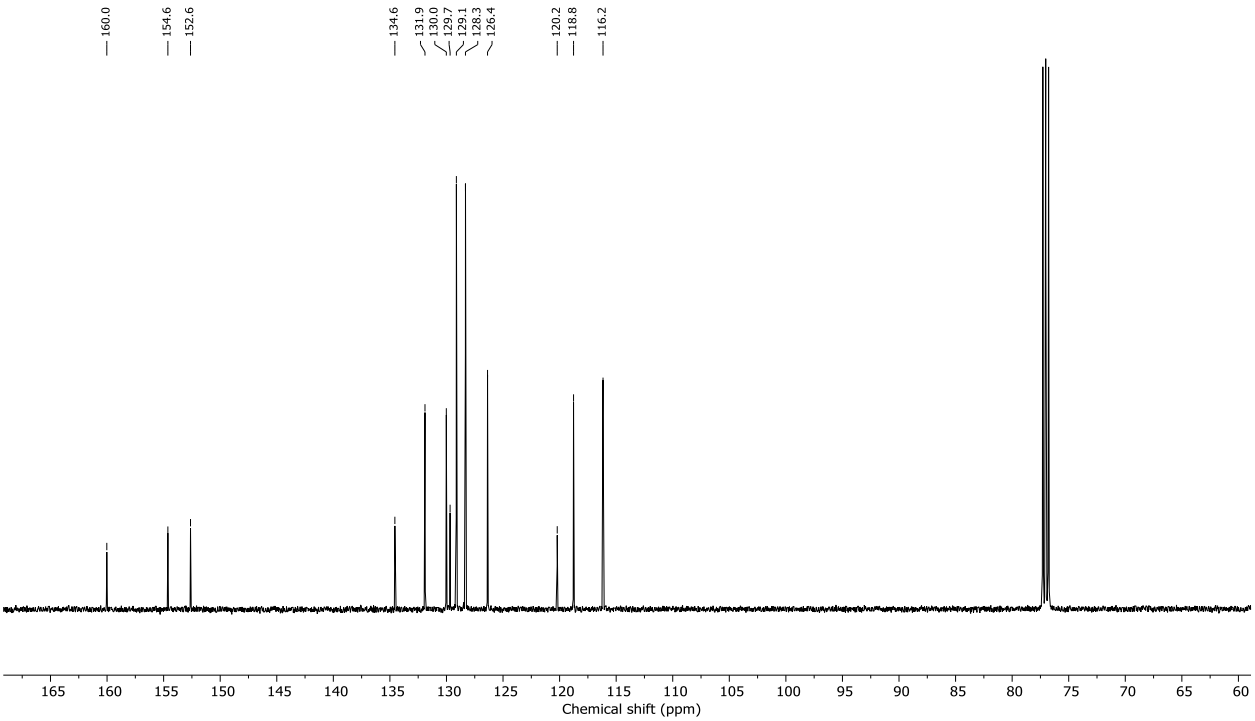

Figure 19. ^{1}H NMR (500 MHz, chloroform-d) spectrum of flavone **18.**

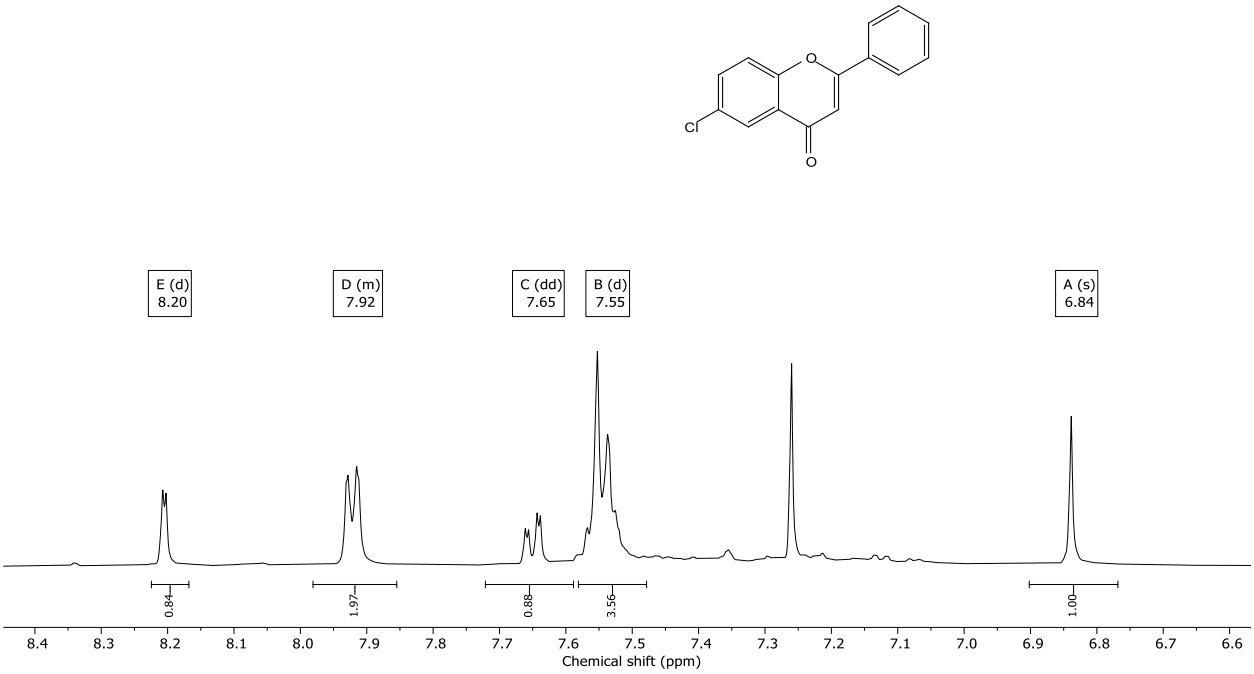

Figure 20. ^{13}C NMR (125 MHz, chloroform-d) spectrum of flavone **18.**