

Tandem CN/CO/CC palladium catalyzed synthesis of 3-substituted 1(2*H*)isoquinolone

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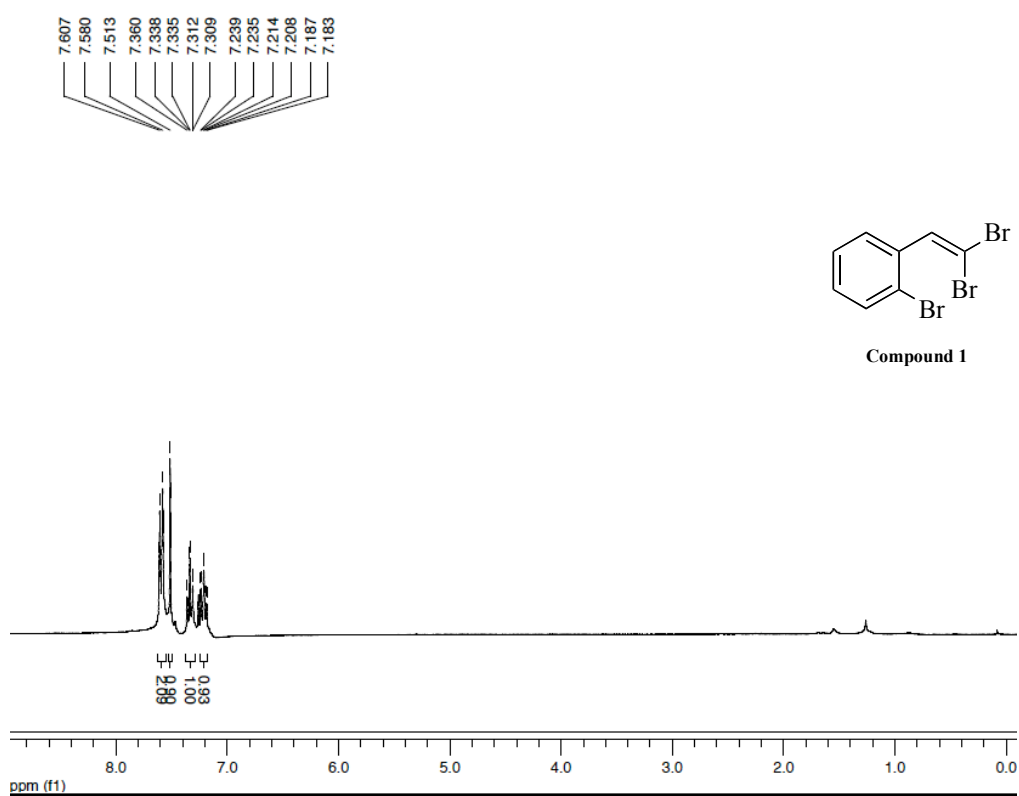
jean-claude.florent@curie.fr

Supporting material

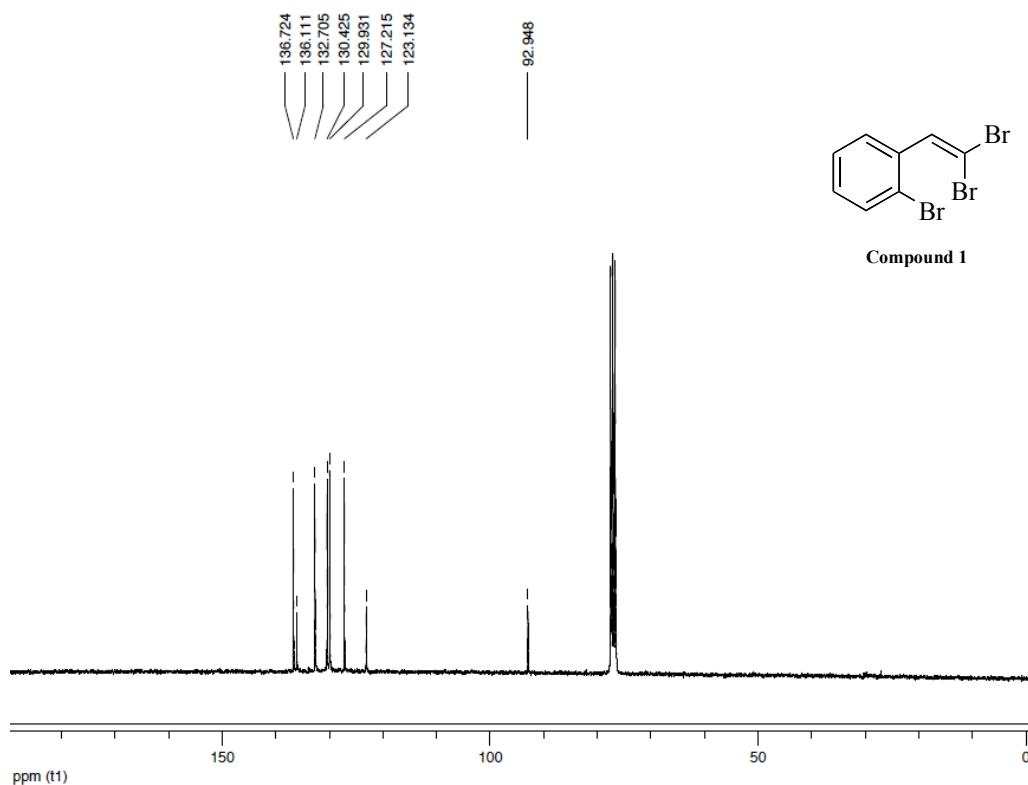
¹H and ¹³C NMR spectra's for compounds **1-15**, **17-25**.

For compound **16**, see ref. 42.

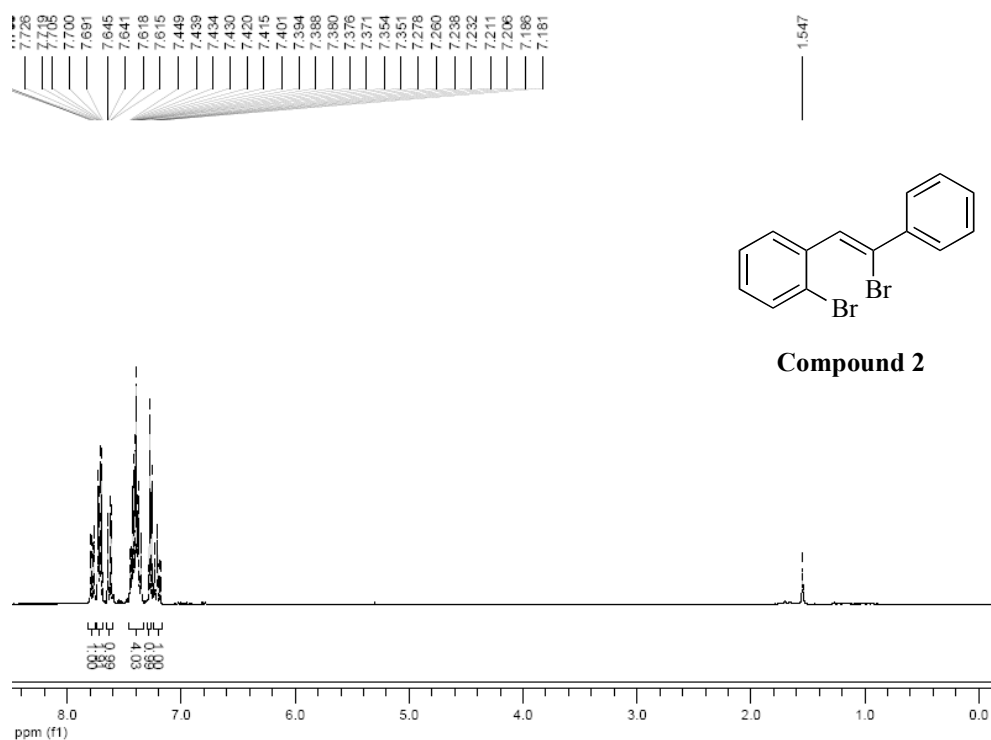
^1H NMR (CDCl_3), 300 MHz: compound 1



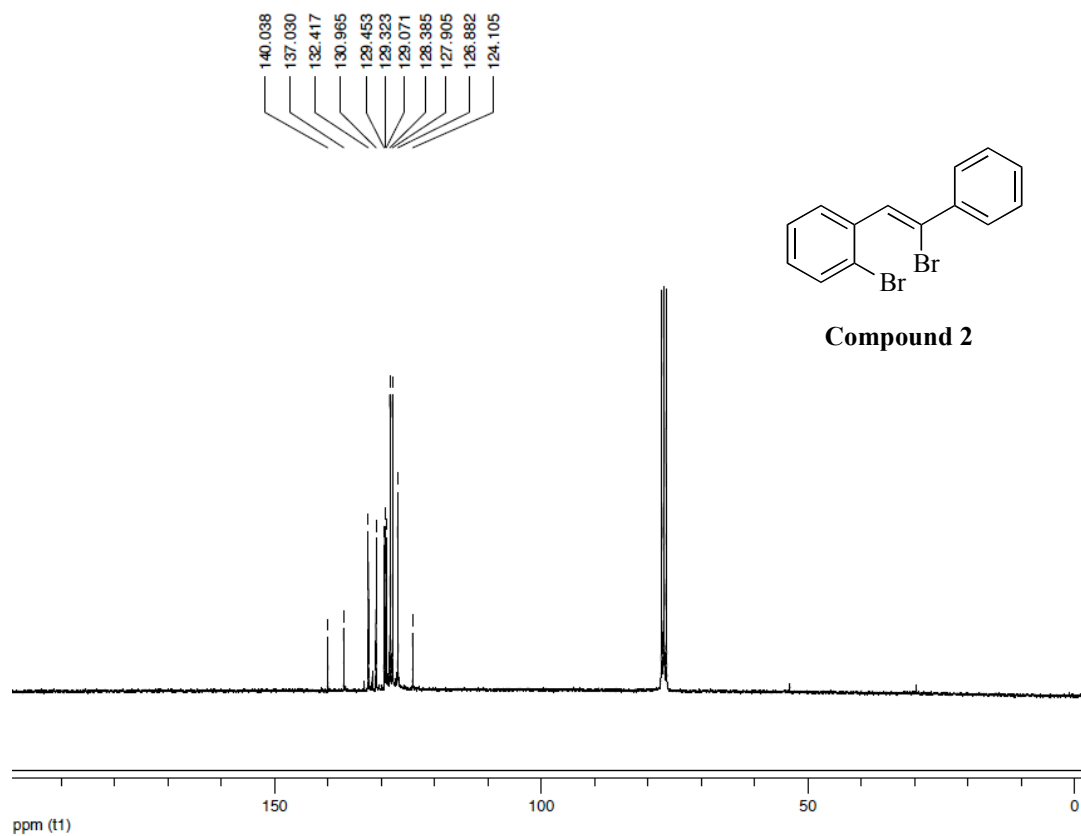
^{13}C NMR ($(\text{CD}_3)_2\text{CO}$), 75 MHz: compound 1



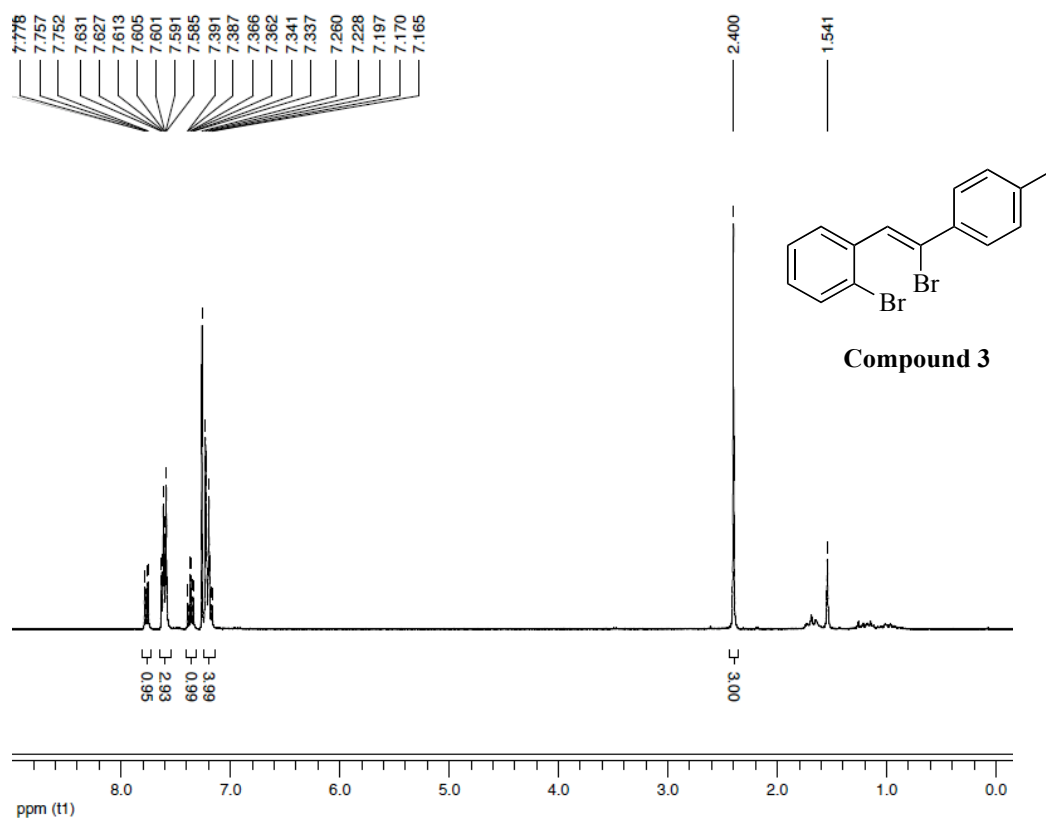
^1H NMR (CDCl_3), 300 MHz: compound 2a



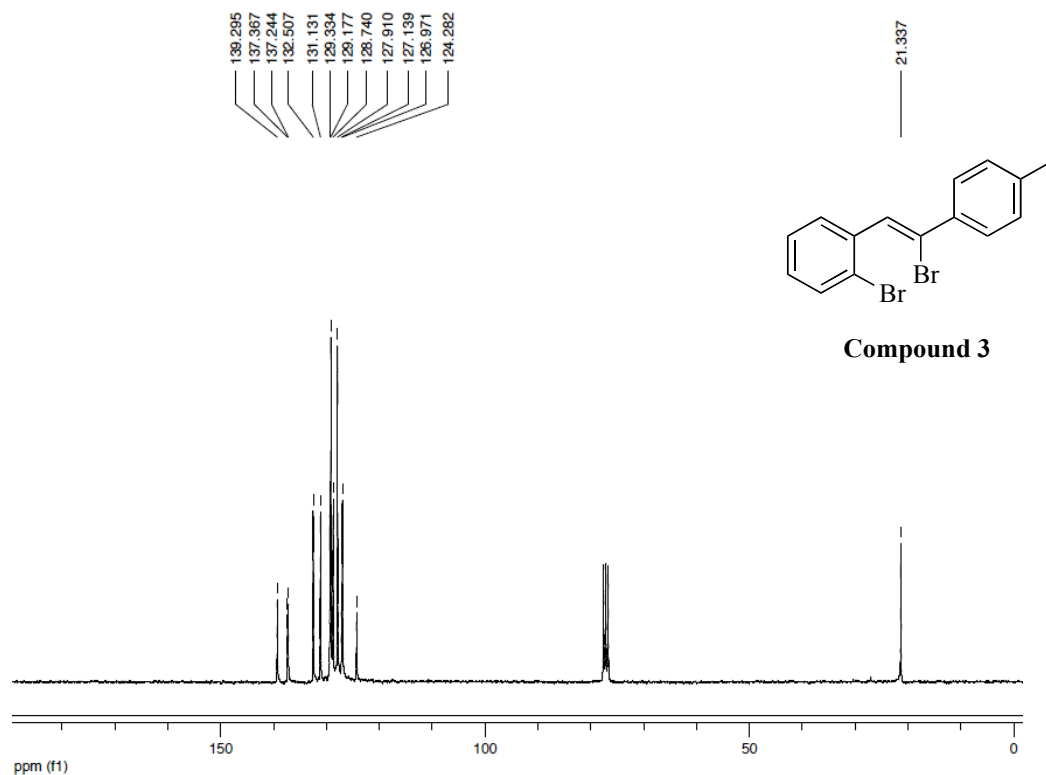
^{13}C NMR (CDCl_3), 75 MHz: compound 2a



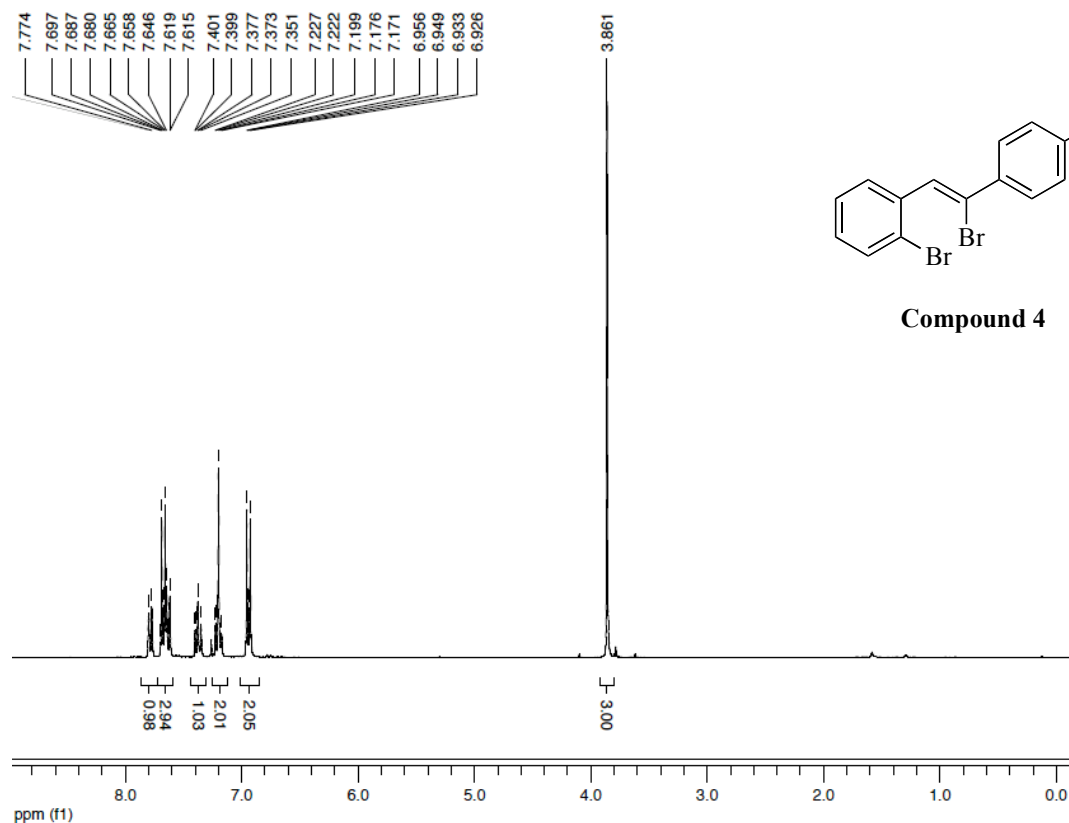
^1H NMR (CDCl_3), 300 MHz): compound 3



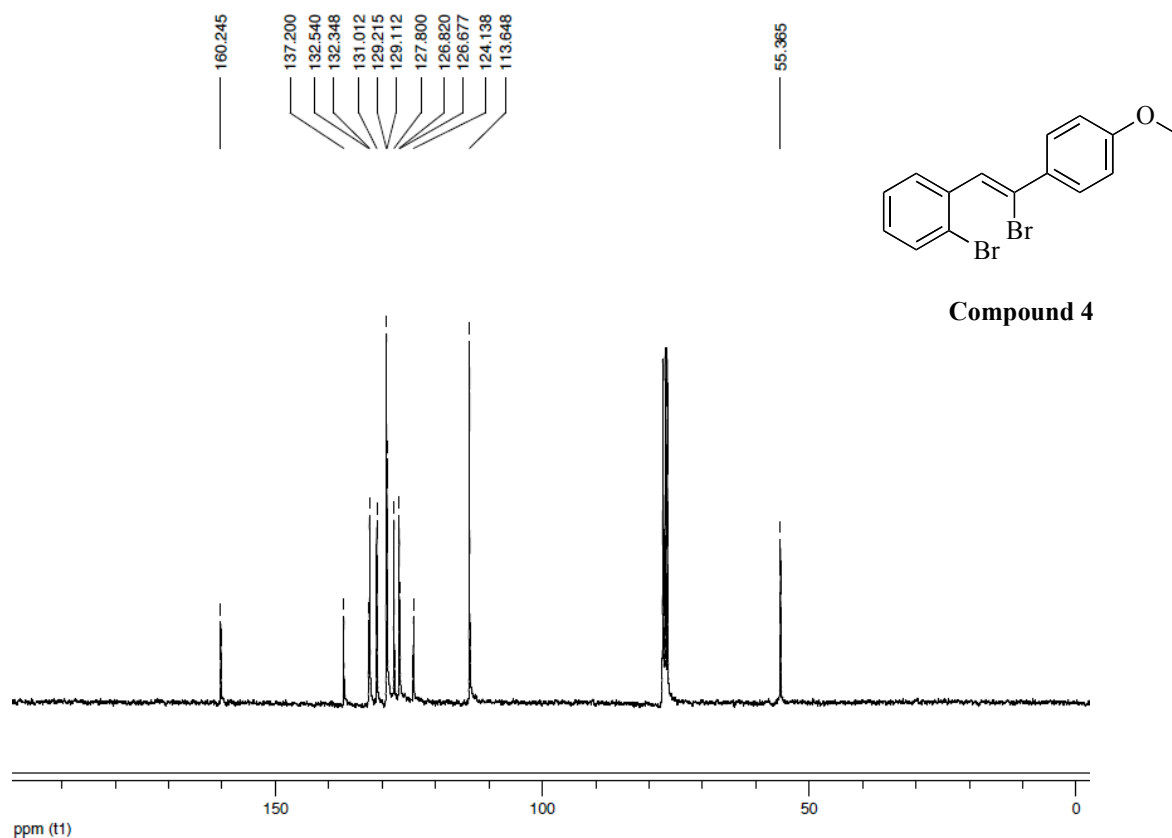
^{13}C NMR (CDCl_3), 75 MHz): compound 3



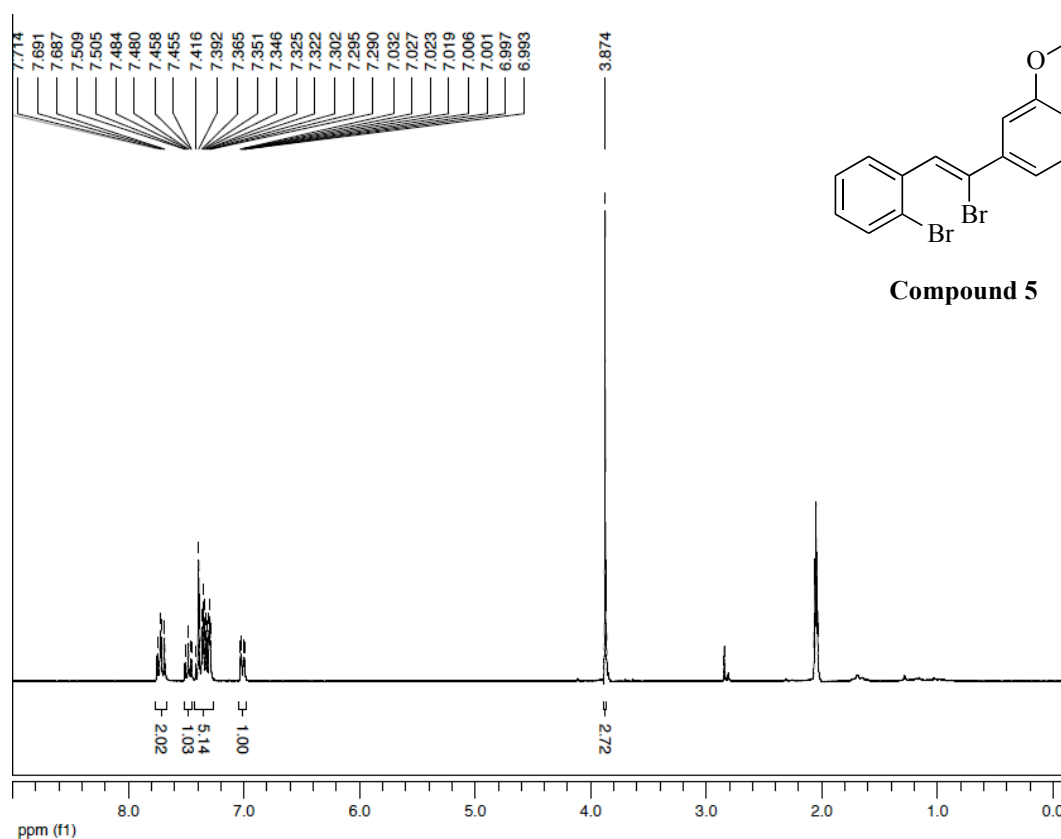
^1H NMR (CDCl_3 , 300 MHz): compound 4



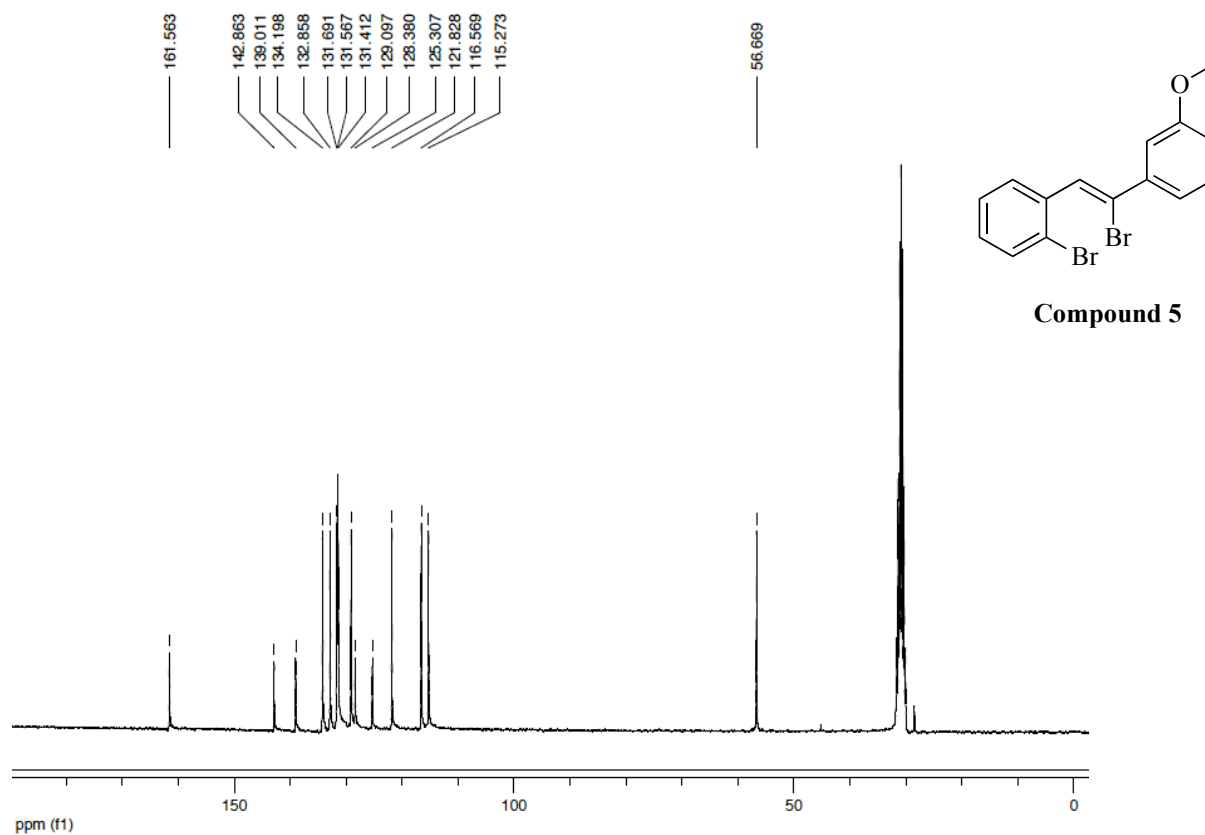
^{13}C NMR (CDCl_3 , 75 MHz): compound 4



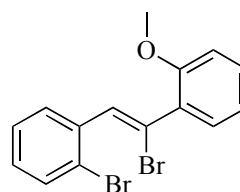
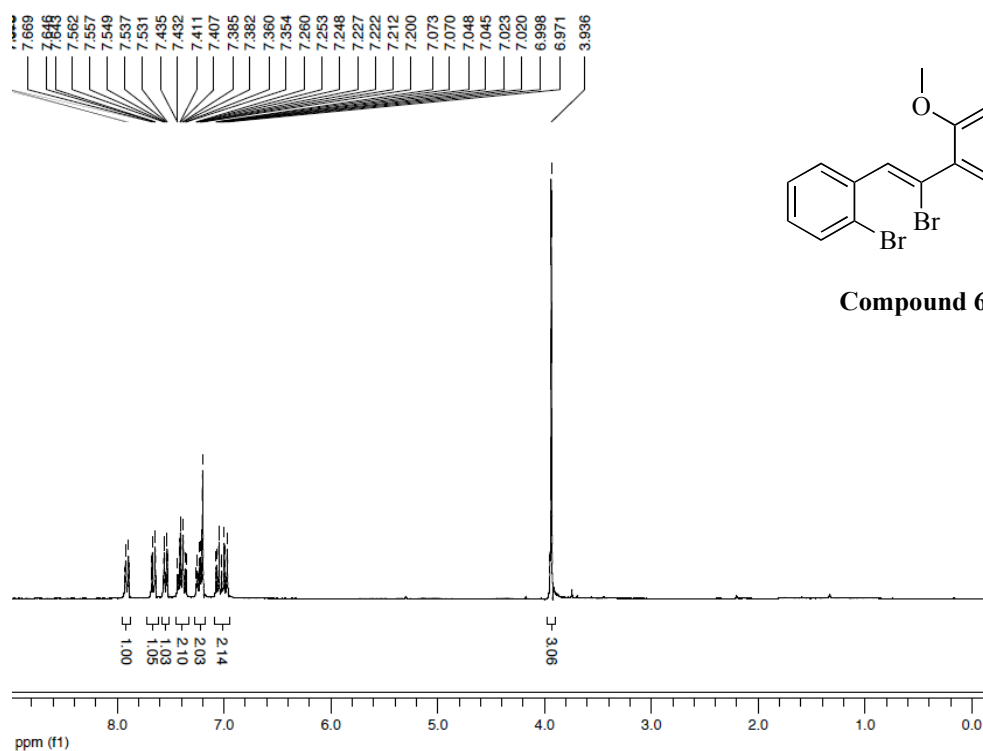
^1H NMR ($(\text{CD}_3)_2\text{CO}$, 300 MHz): compound 5



^{13}C NMR ($(\text{CD}_3)_2\text{CO}$, 75 MHz): compound 5

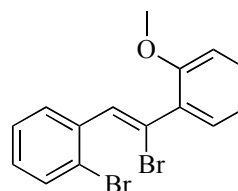
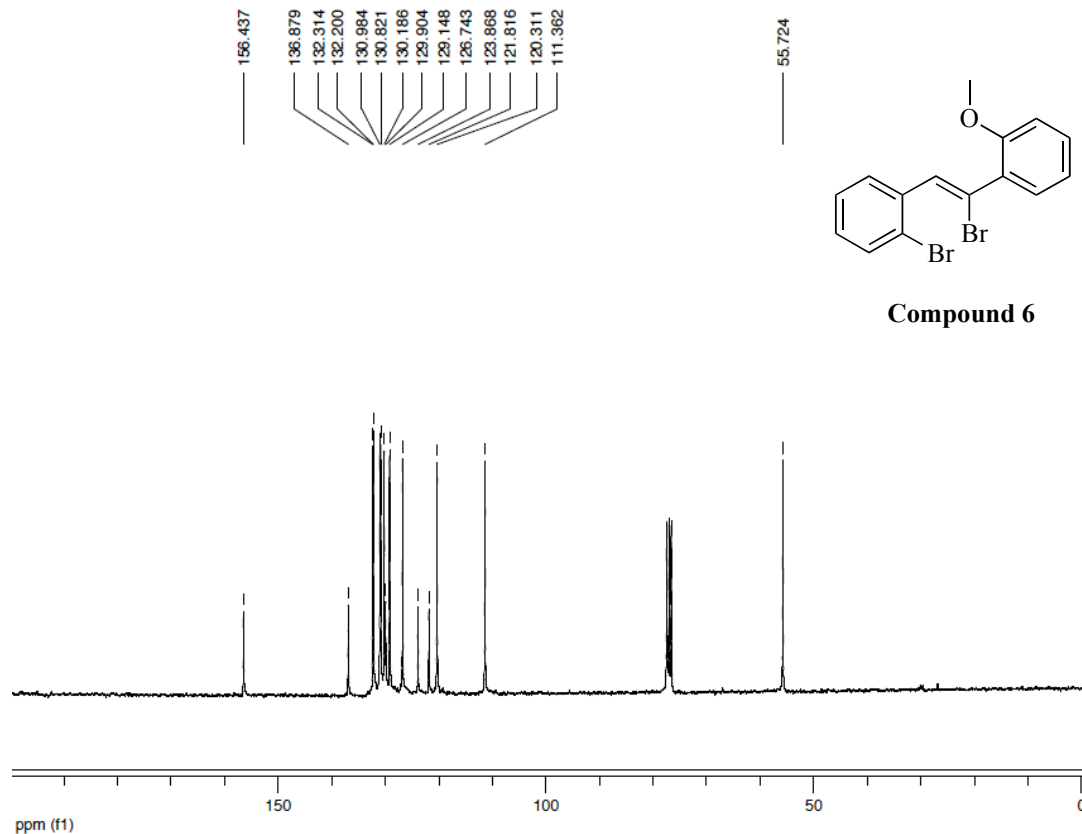


^1H NMR ($(\text{CD}_3)_2\text{CO}$), 300 MHz): compound 6



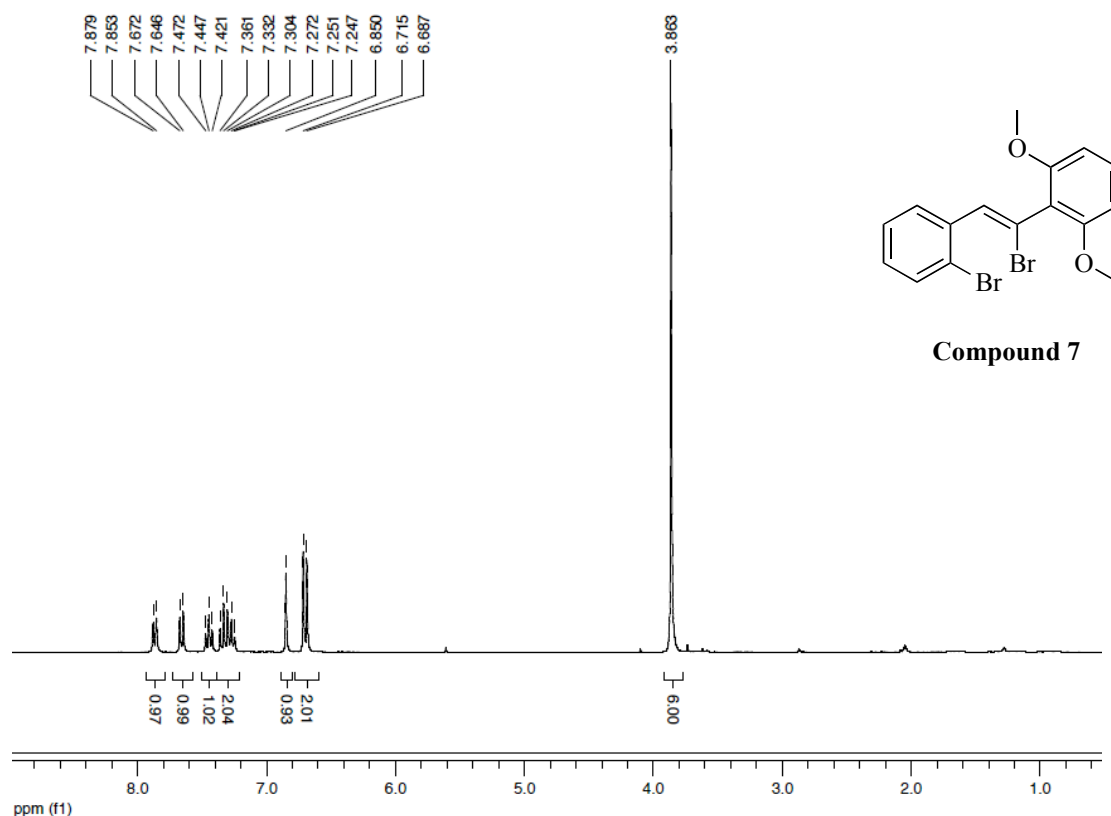
Compound 6

^{13}C NMR ($(\text{CD}_3)_2\text{CO}$), 75 MHz): compound 6

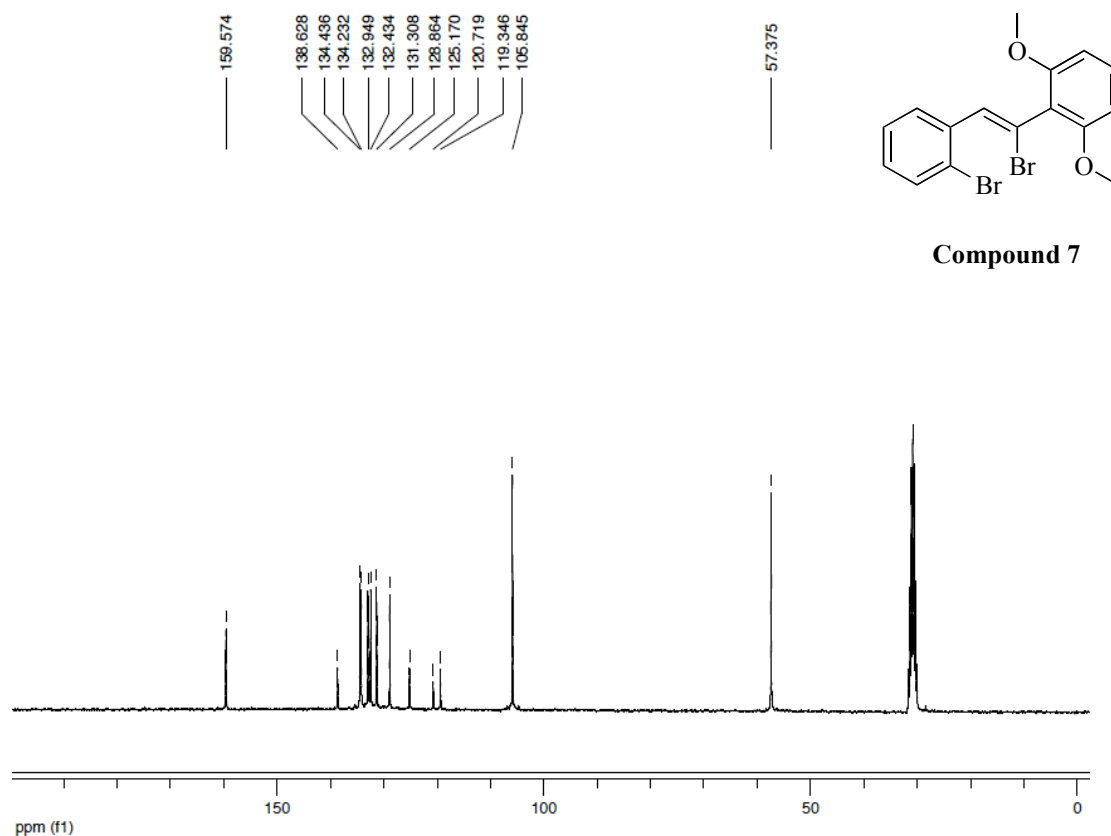


Compound 6

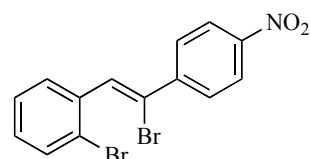
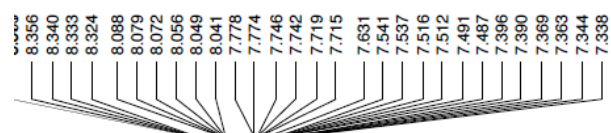
^1H NMR ($(\text{CD}_3)_2\text{CO}$, 300 MHz): compound 7



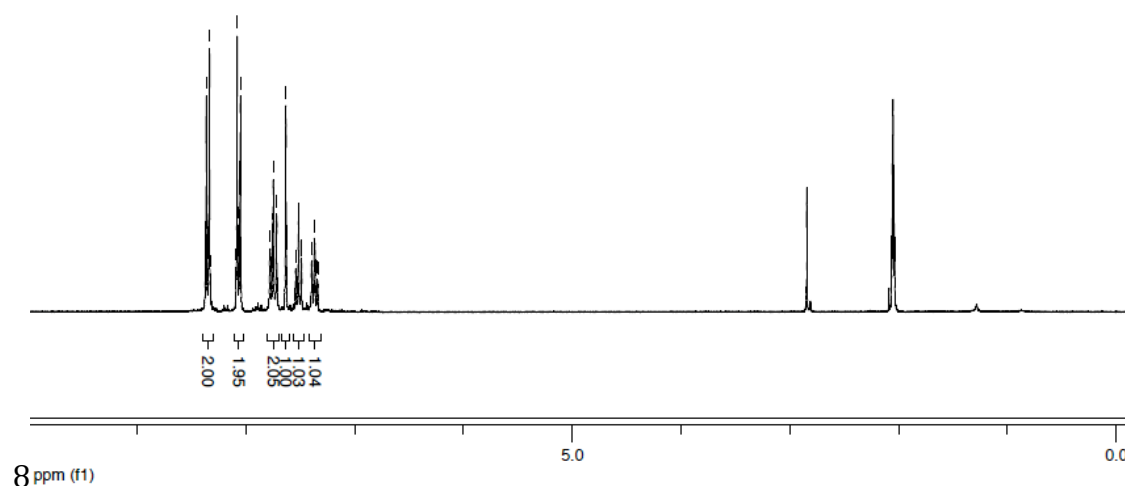
^{13}C NMR ($(\text{CD}_3)_2\text{CO}$, 75 MHz): compound 7



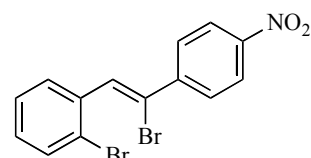
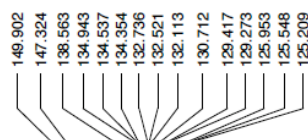
^1H NMR ($(\text{CD}_3)_2\text{CO}$, 300 MHz): compound



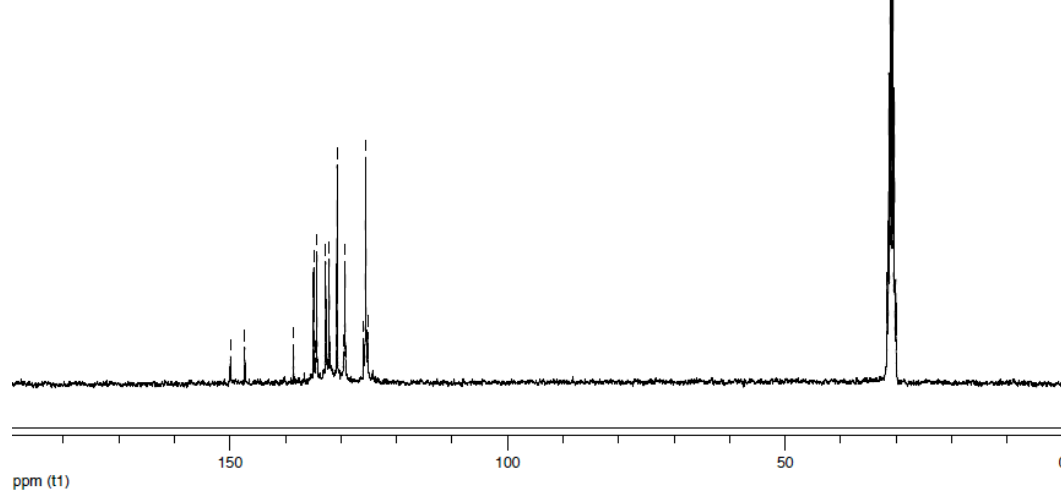
Compound 8



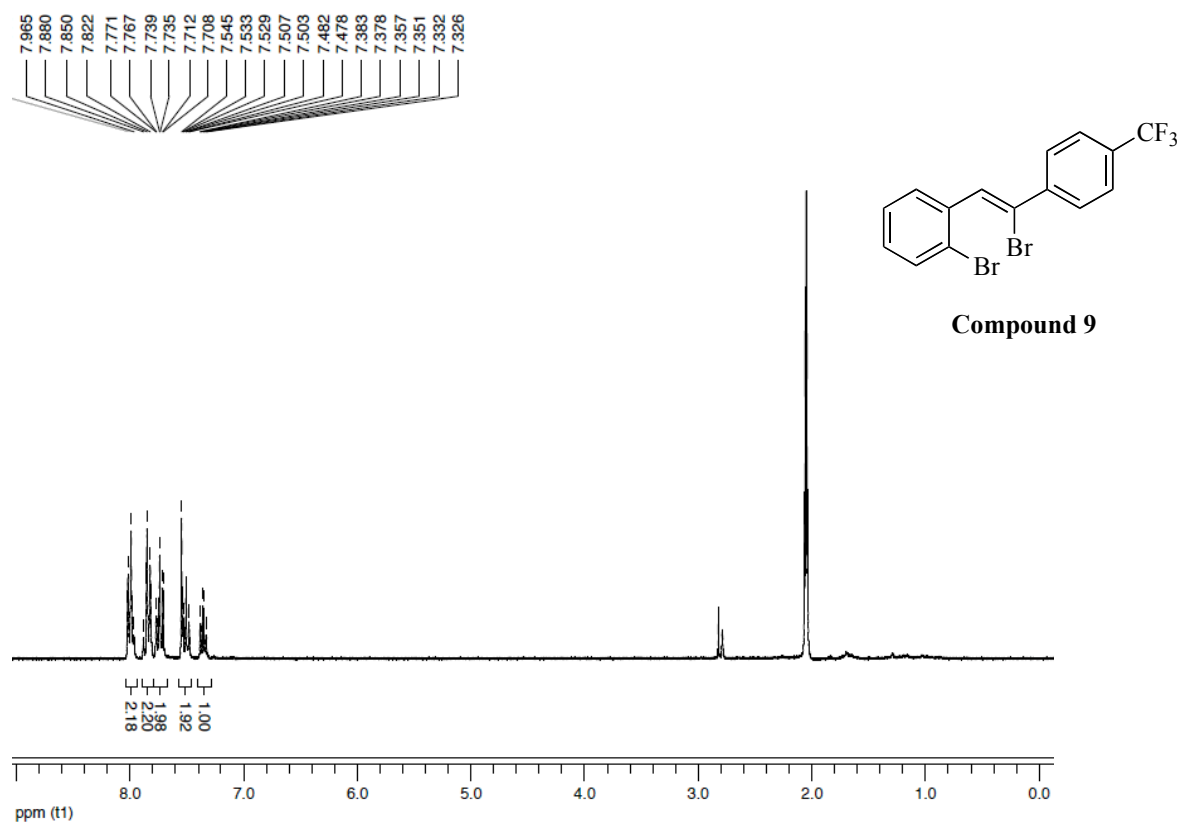
^{13}C NMR ($(\text{CD}_3)_2\text{CO}$, 75 MHz): compound 8



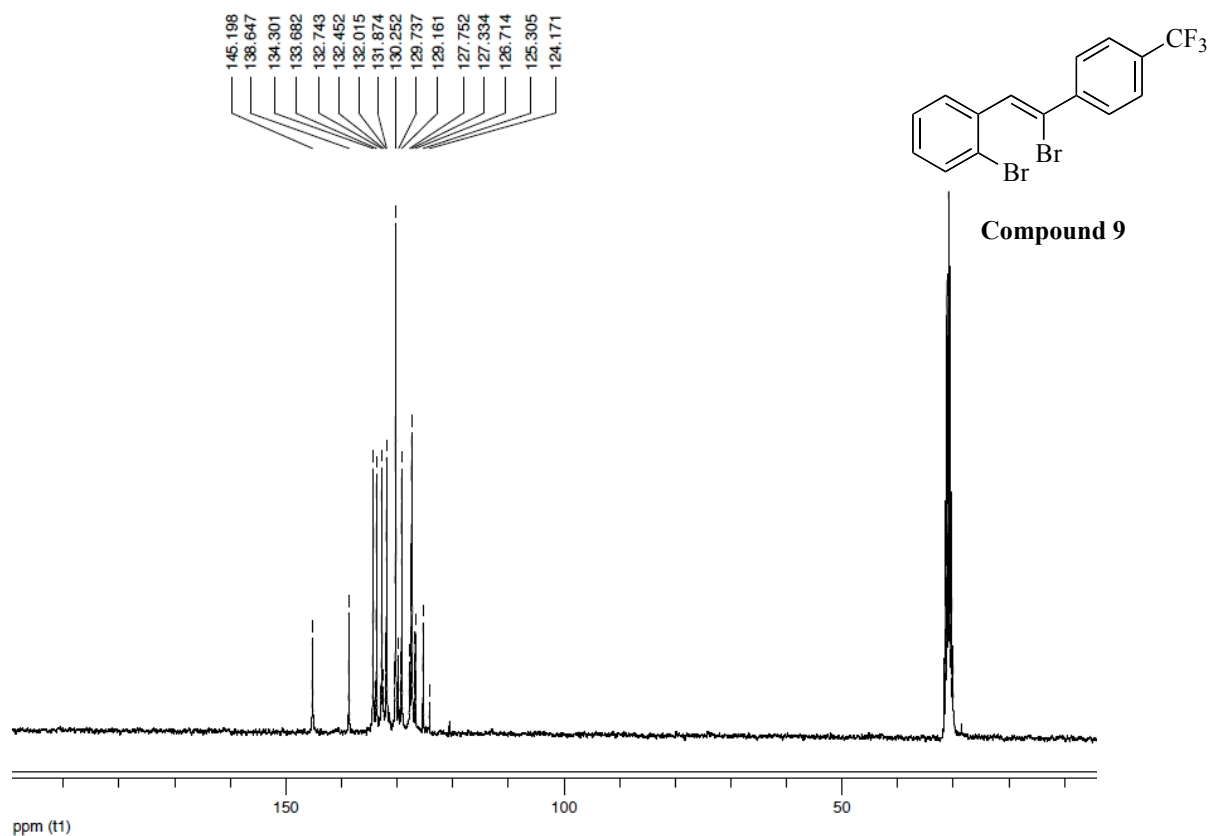
Compound 8



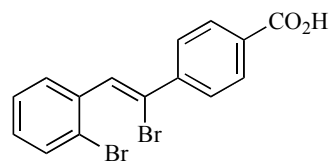
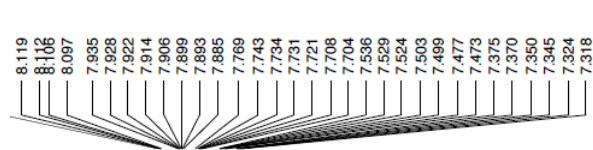
^1H NMR ($(\text{CD}_3)_2\text{CO}$, 300 MHz): compound 9



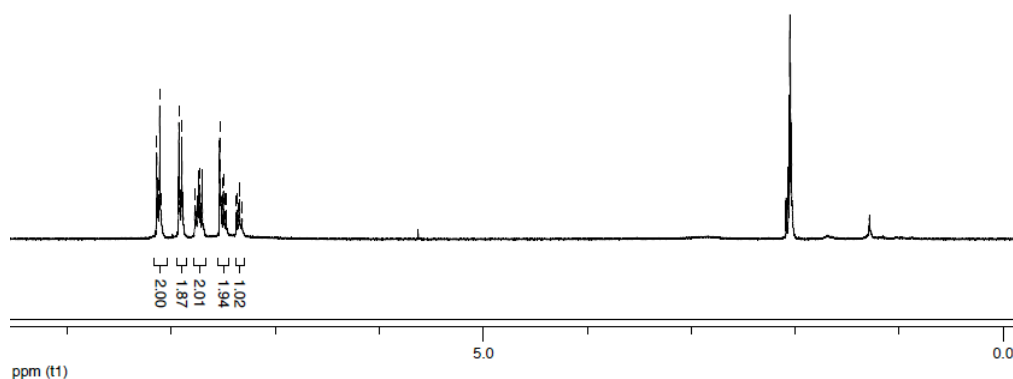
^{13}C $\{^1\text{H}\}$ NMR ($(\text{CD}_3)_2\text{CO}$, 75 MHz): compound 9



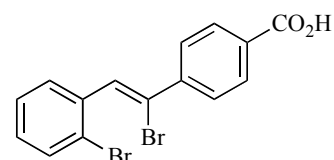
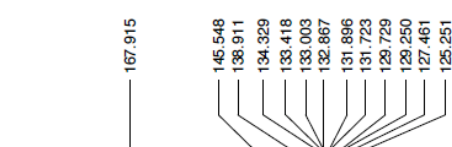
^1H NMR ($(\text{CD}_3)_2\text{CO}$, 300 MHz): compound 10



Compound 10



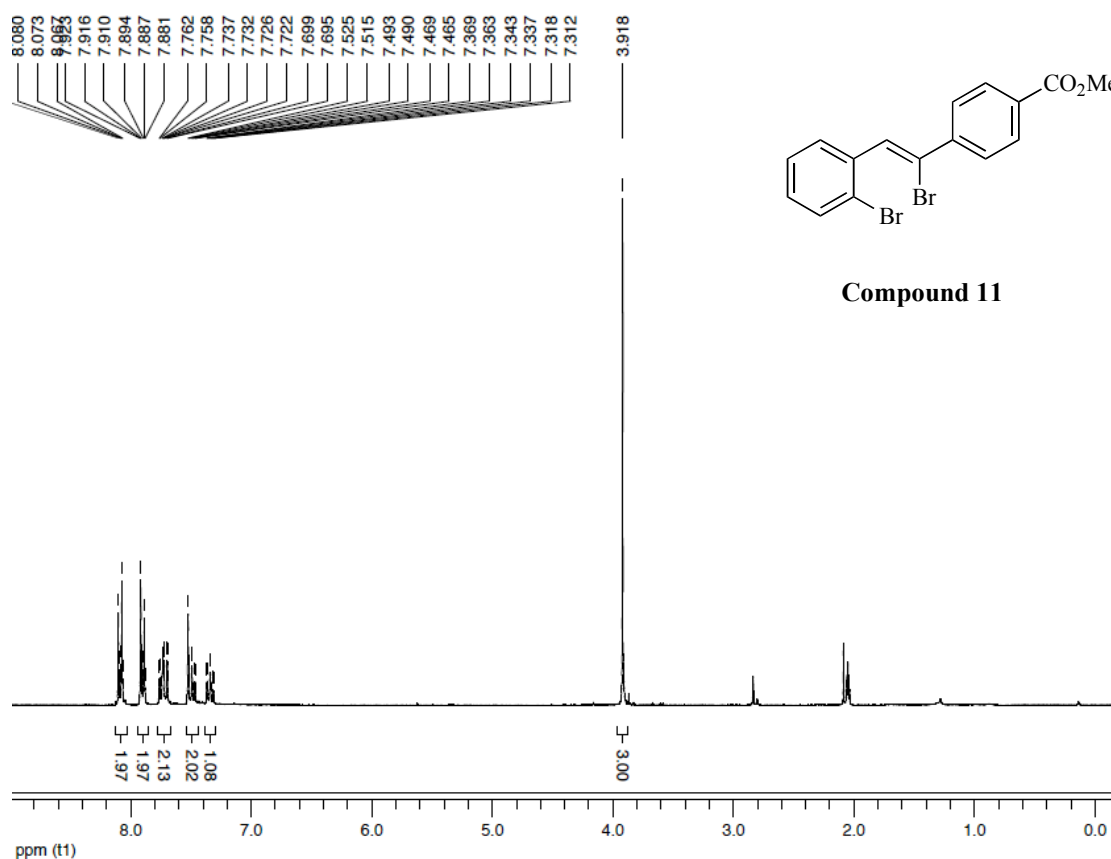
^{13}C $\{^1\text{H}\}$ NMR ($(\text{CD}_3)_2\text{CO}$, 75 MHz): compound 10



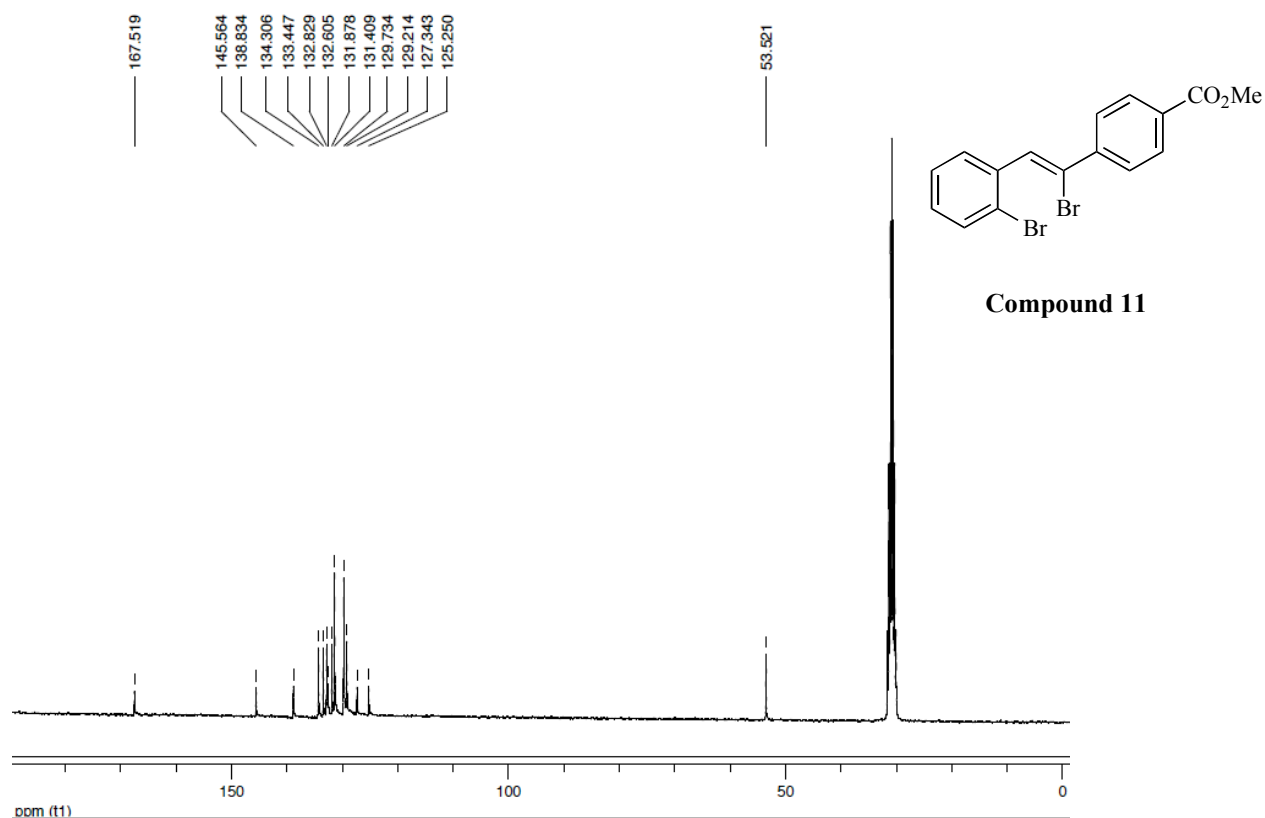
Compound 10

ppm (f1)

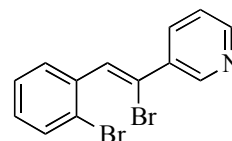
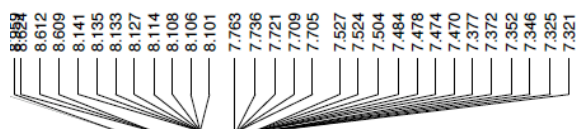
^1H NMR $((\text{CD}_3)_2\text{CO})$, 300 MHz): compound 11



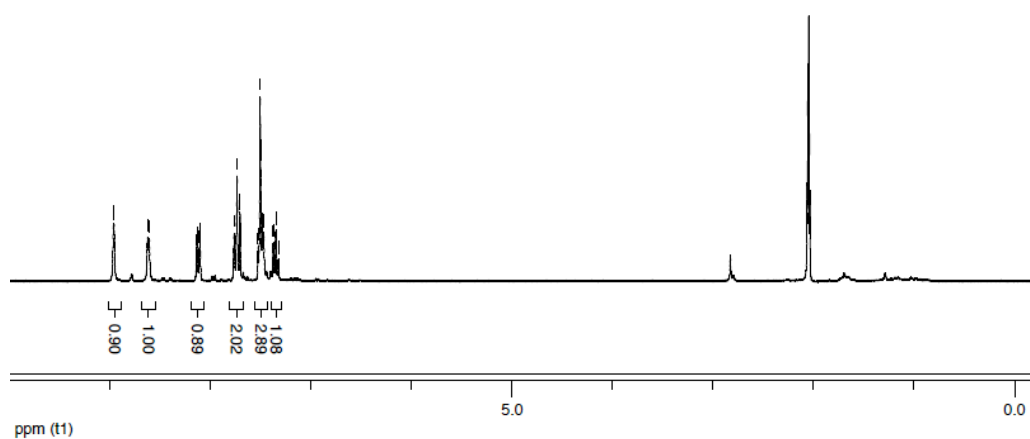
^{13}C $\{^1\text{H}\}$ NMR $((\text{CD}_3)_2\text{CO})$, 75 MHz): compound 11



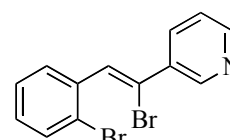
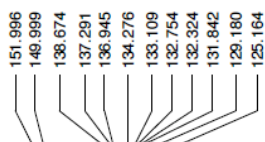
^1H NMR ($(\text{CD}_3)_2\text{CO}$), 300 MHz): compound 12



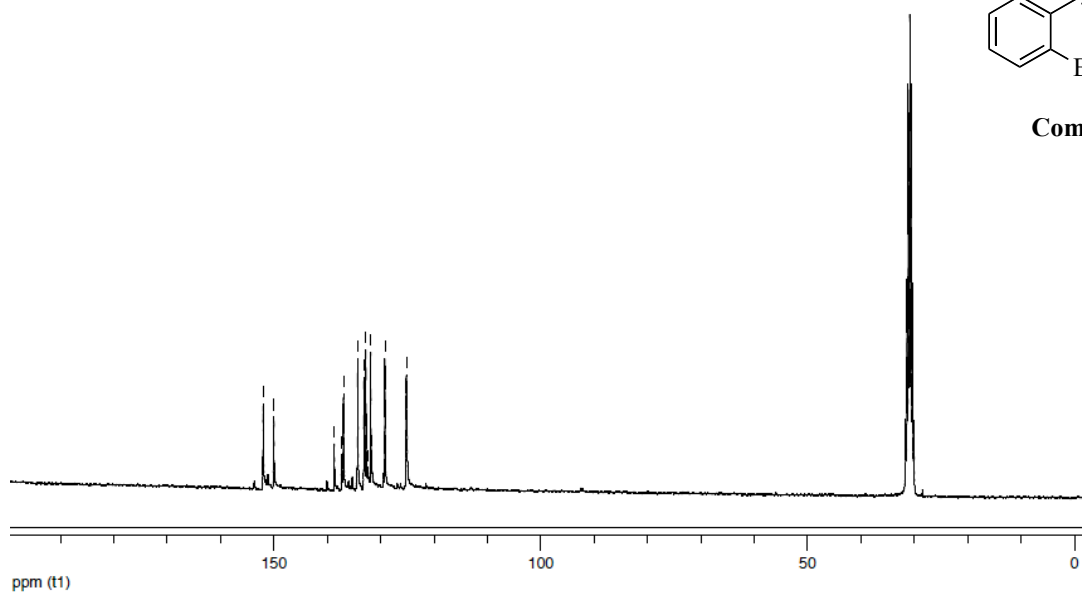
Compound 12



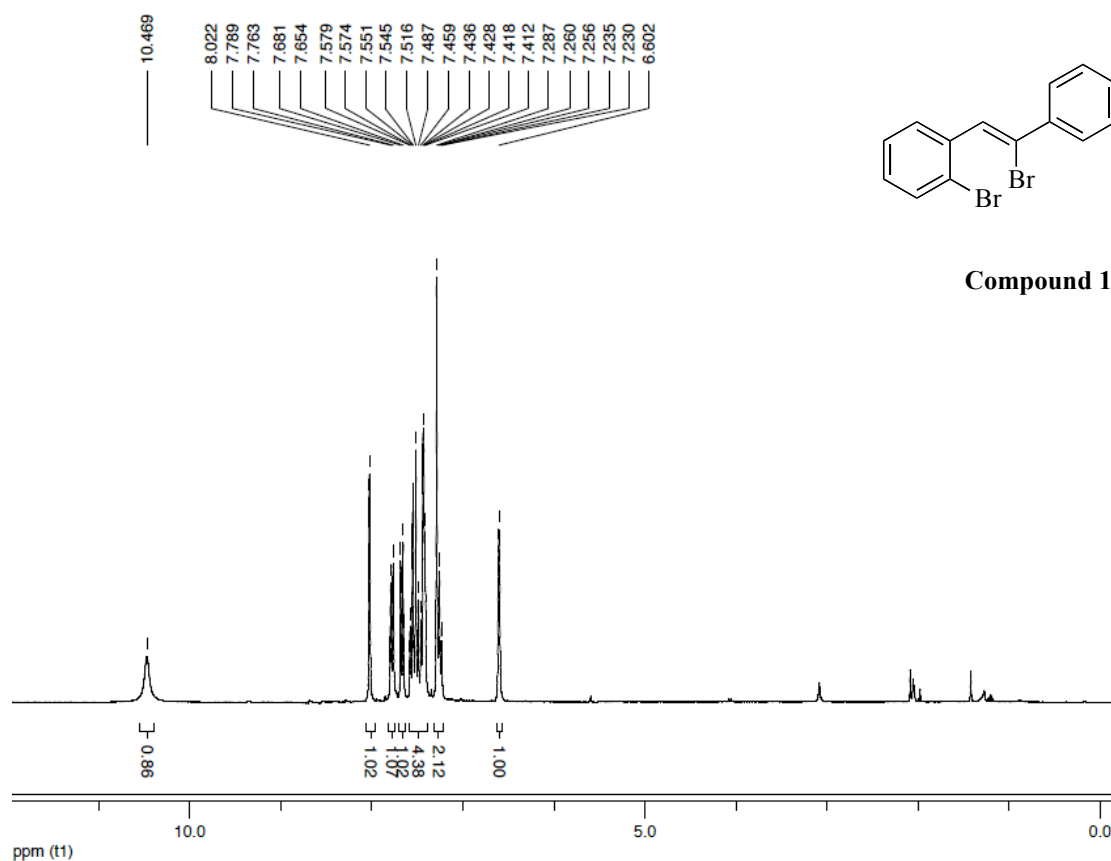
^{13}C $\{^1\text{H}\}$ NMR ($(\text{CD}_3)_2\text{CO}$), 75 MHz): compound 12



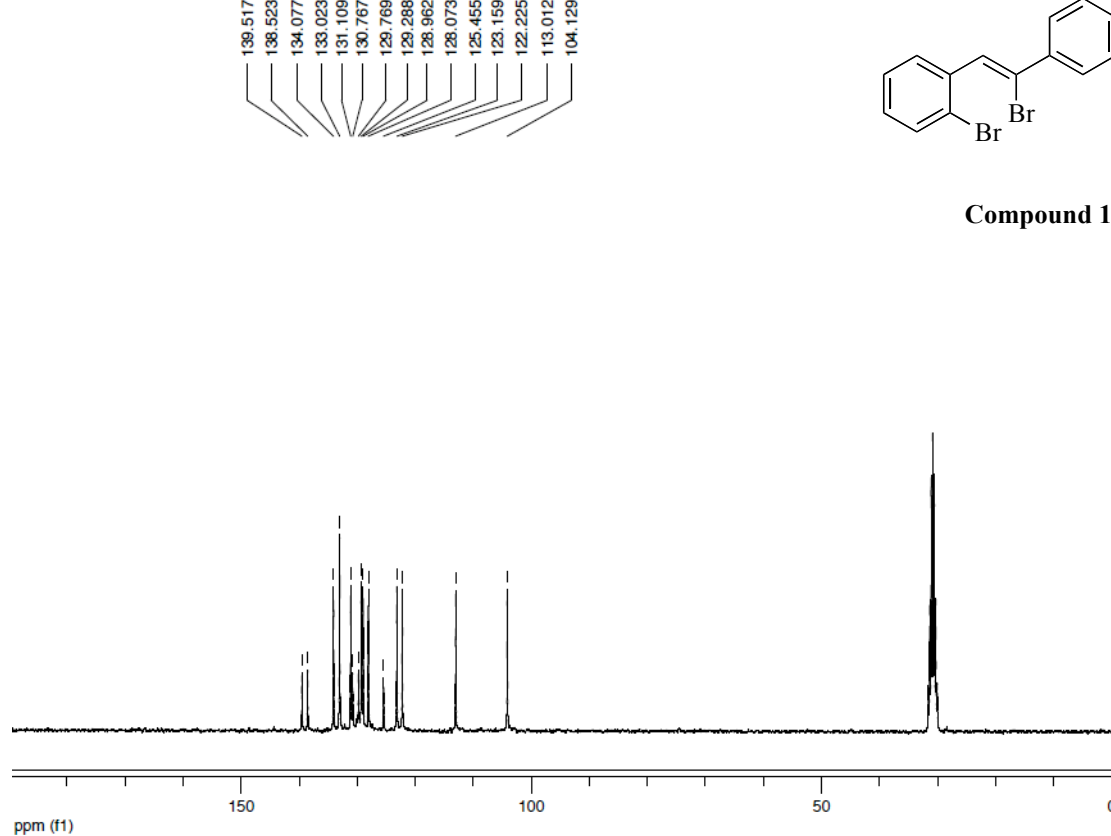
Compound 12



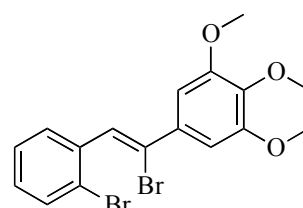
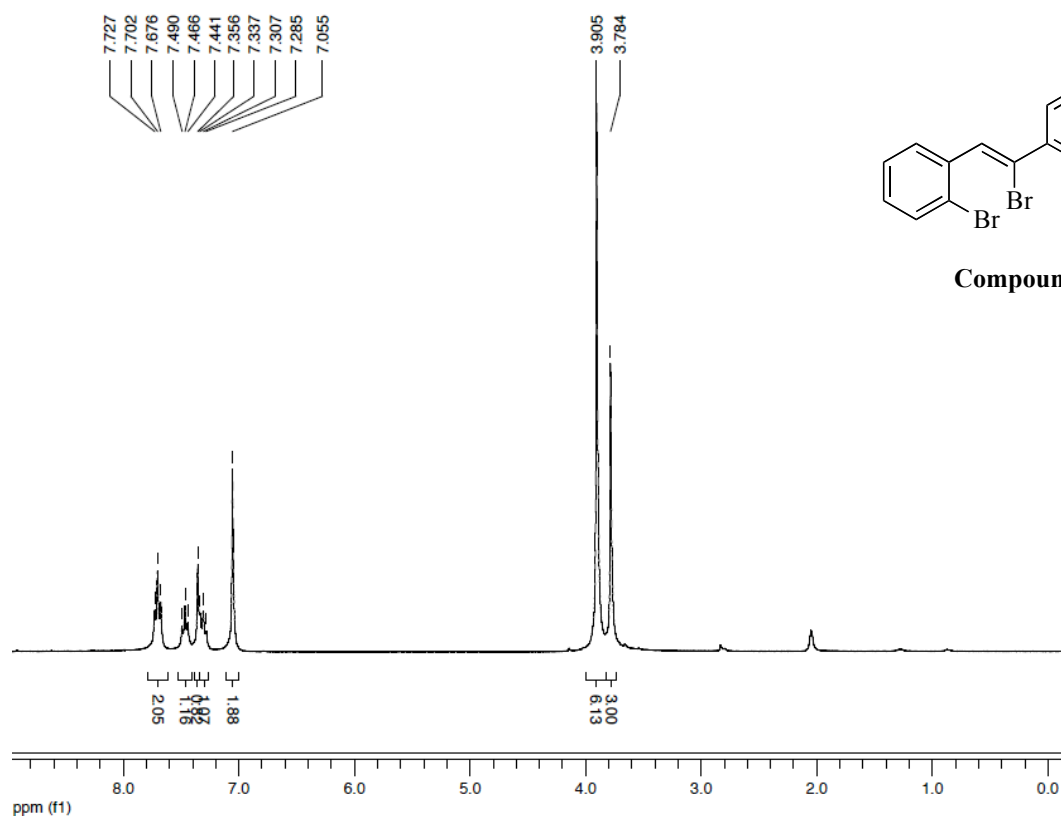
^1H NMR ($(\text{CD}_3)_2\text{CO}$, 300 MHz): compound 13



^{13}C NMR ($(\text{CD}_3)_2\text{CO}$, 75 MHz): compound 13

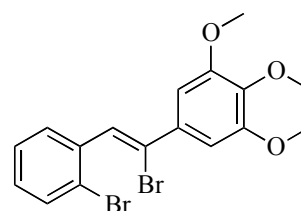
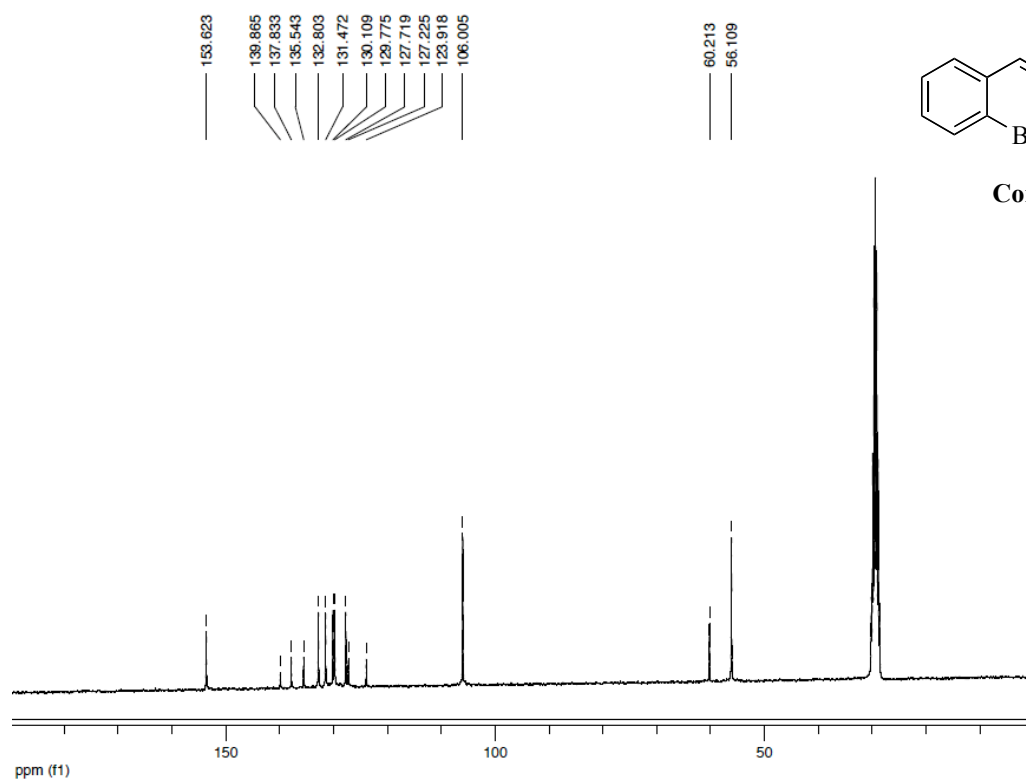


^1H NMR (CDCl_3)₂, 300 MHz): compound 14



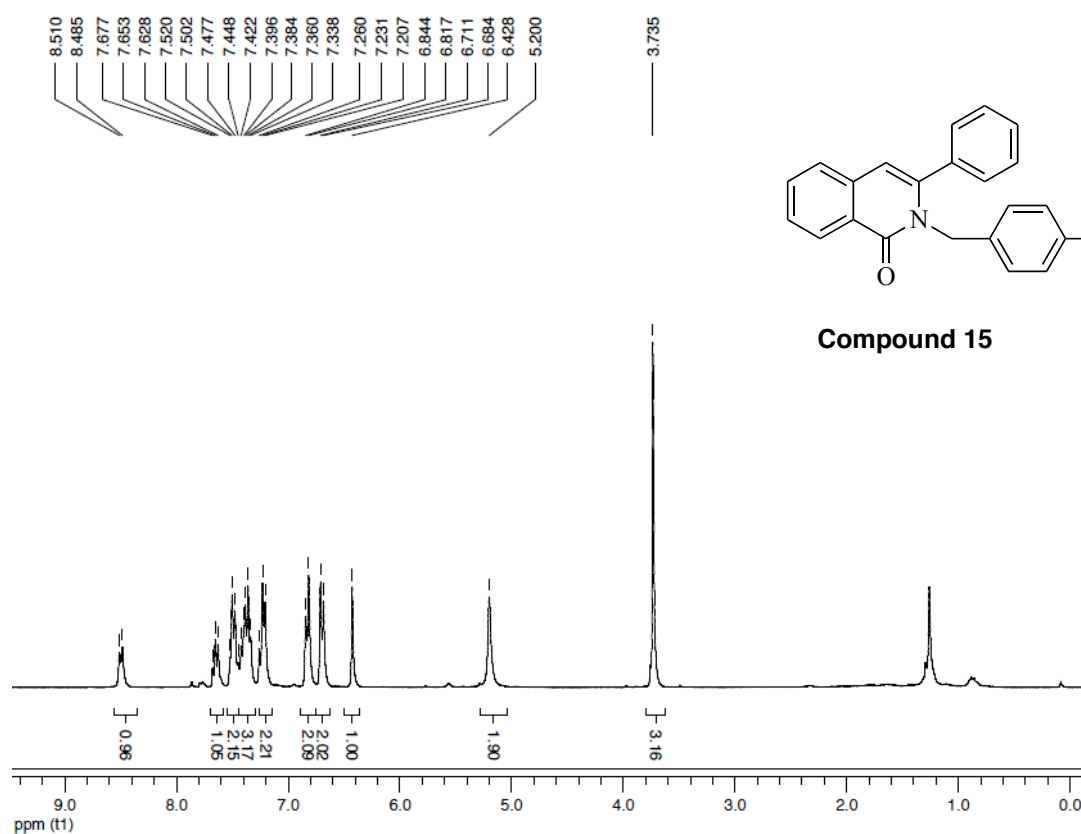
Compound 14

^{13}C $\{^1\text{H}\}$ NMR (CDCl_3 , 75 MHz): compound 14

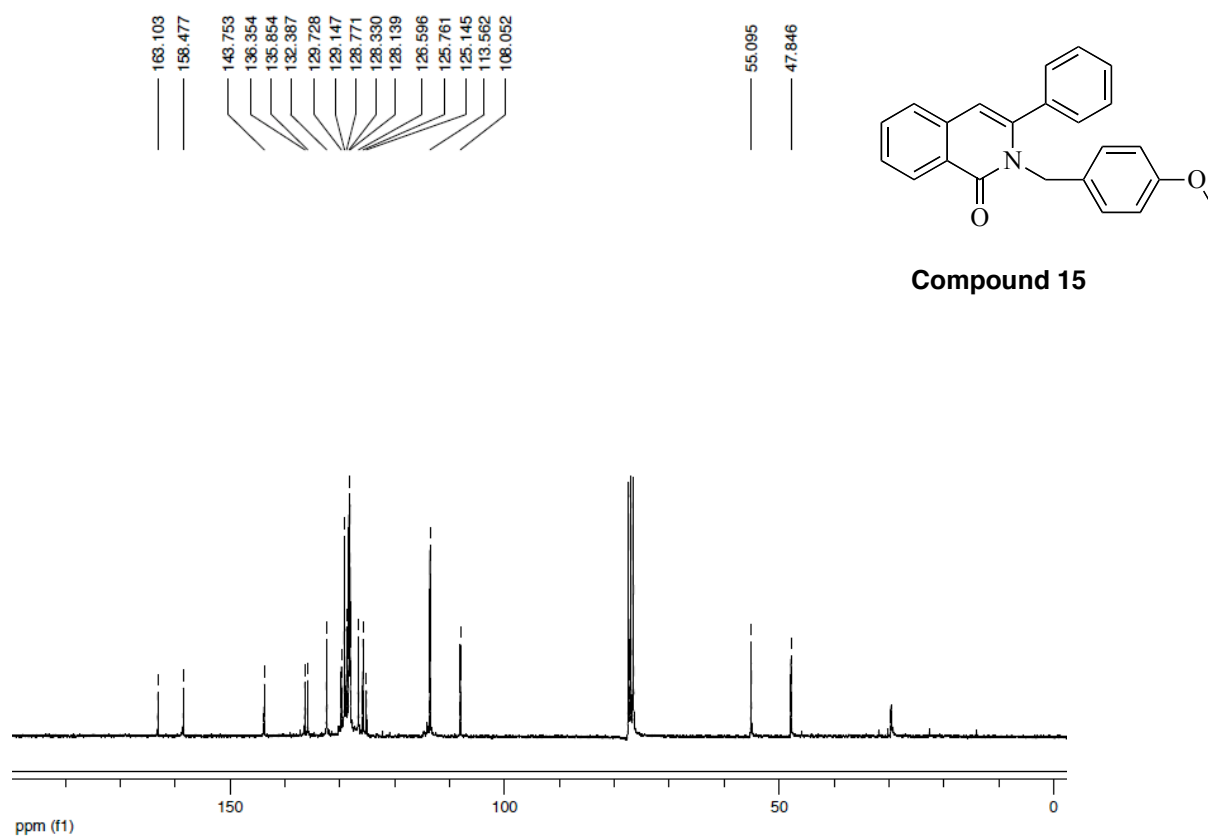


Compound 14

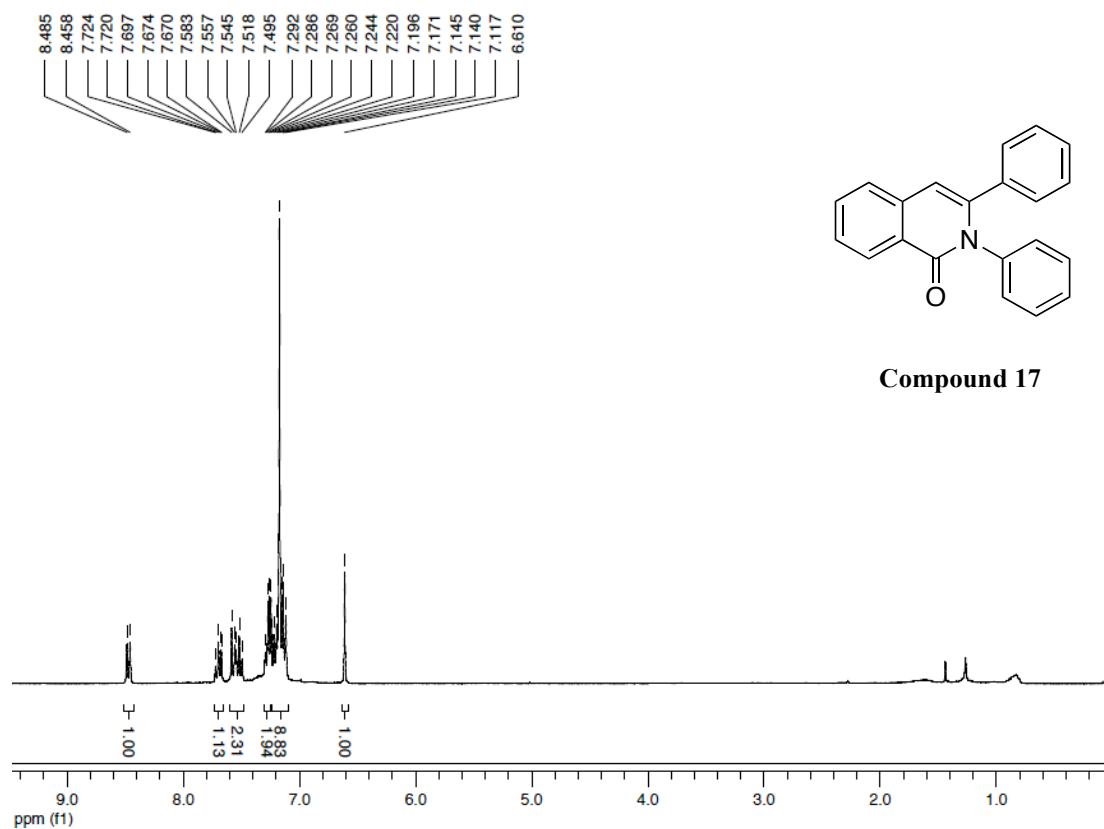
^1H NMR (CDCl_3 , 300 MHz): compound 15



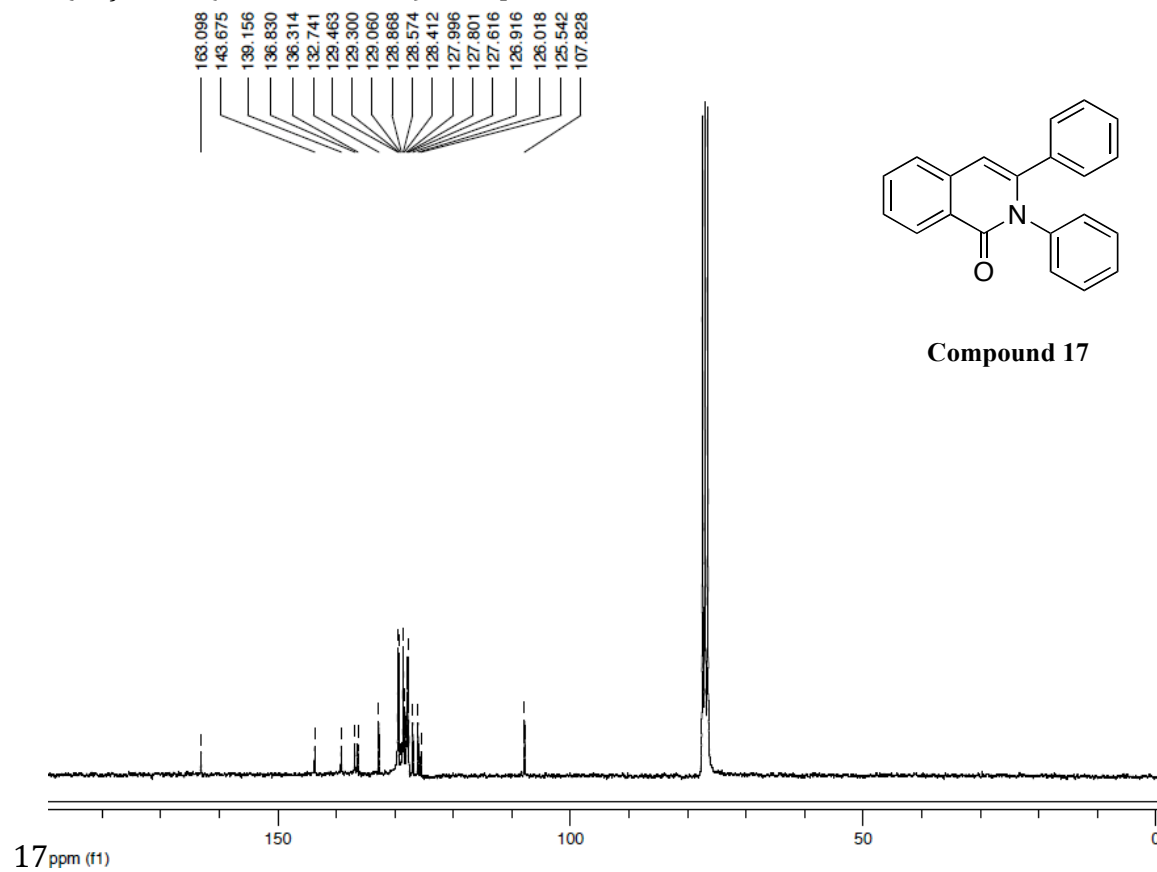
^{13}C $\{^1\text{H}\}$ NMR (CDCl_3 , 75 MHz): compound 15



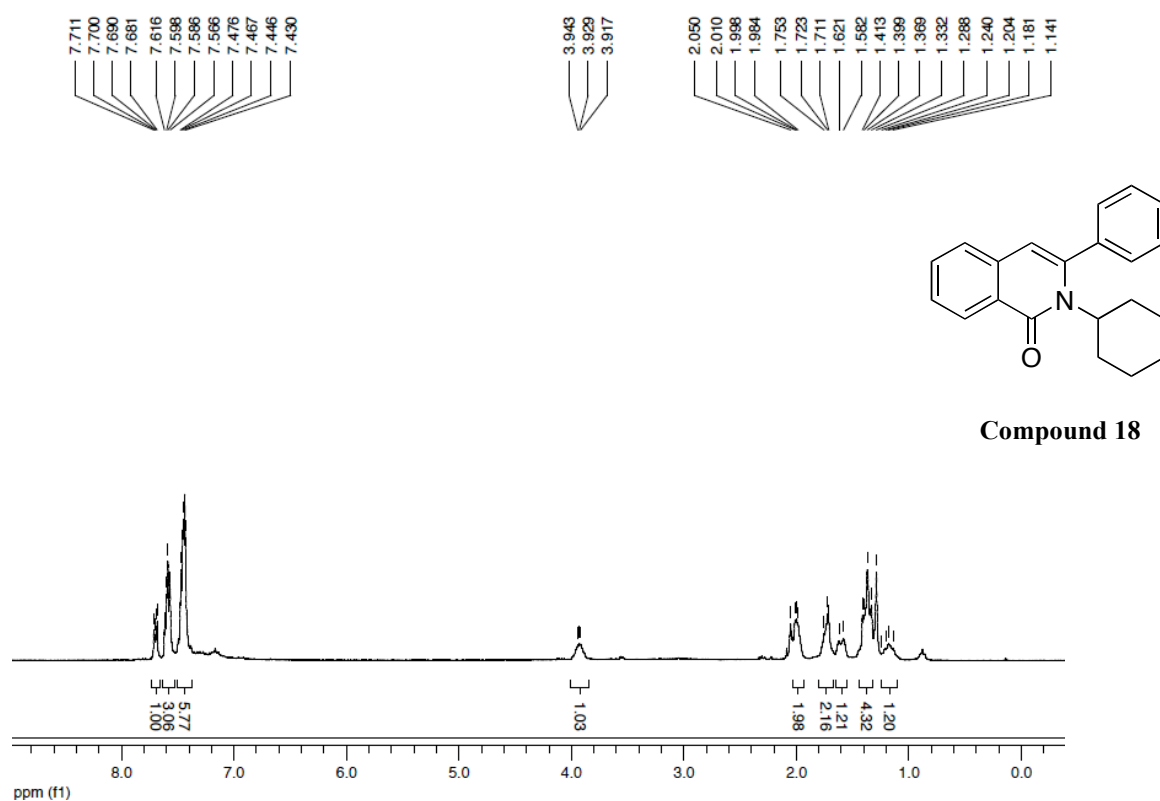
^1H NMR (CDCl_3 , 300 MHz): compound 17



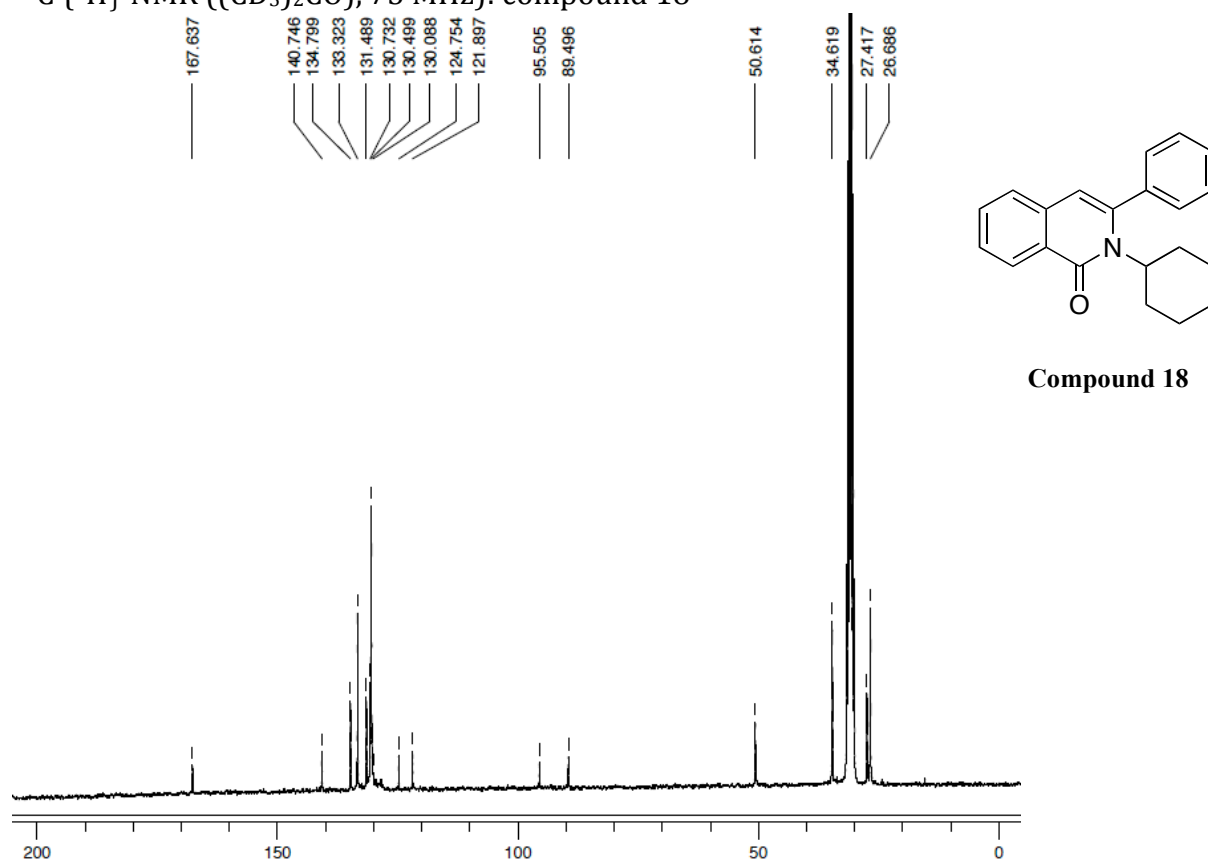
^{13}C $\{^1\text{H}\}$ NMR (CDCl_3 , 75 MHz): compound



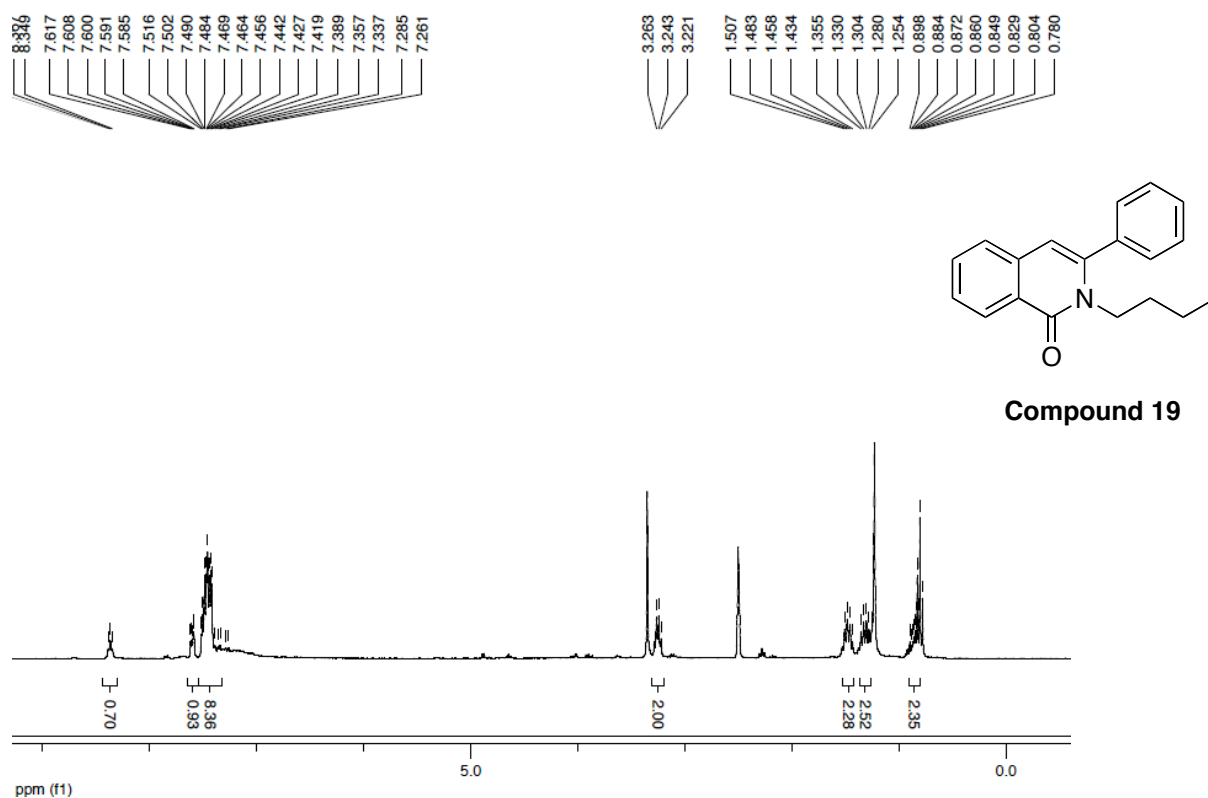
^1H NMR ($(\text{CD}_3)_2\text{CO}$, 300 MHz): compound 18



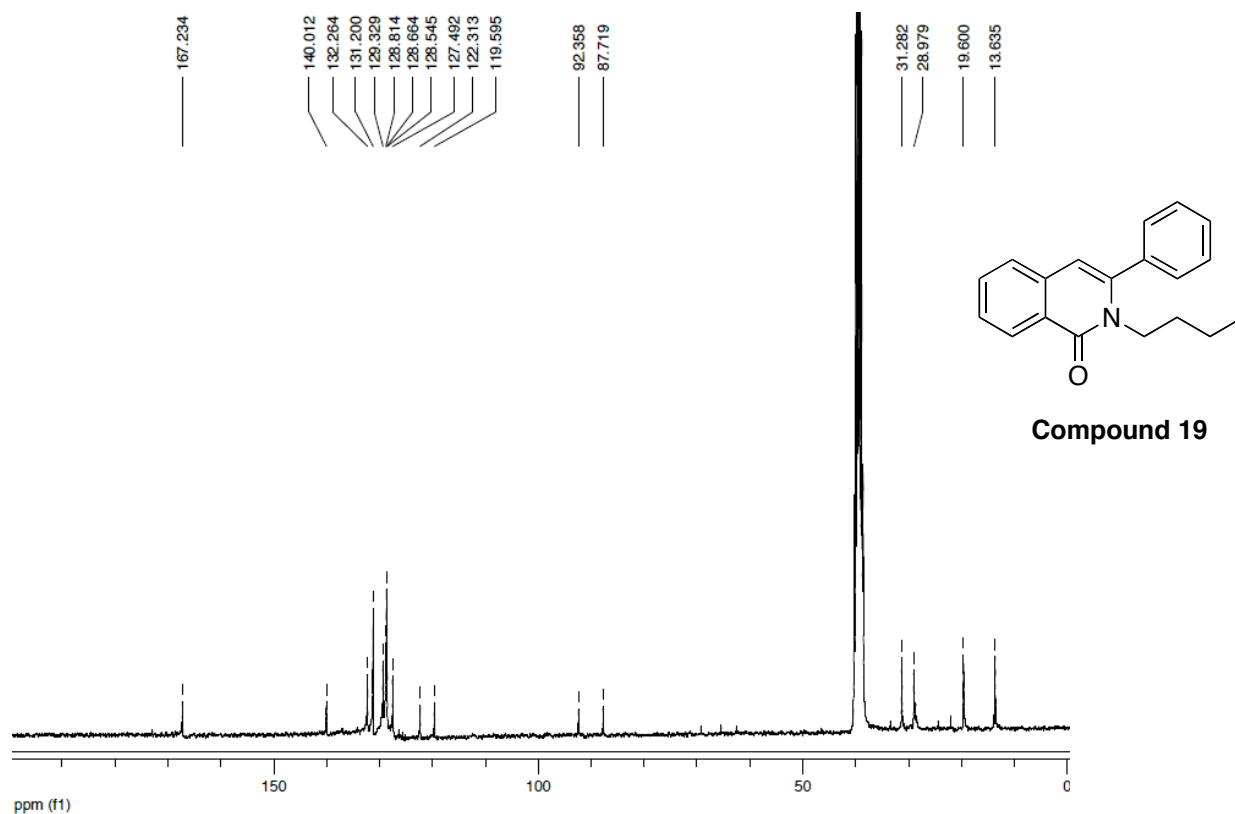
^{13}C $\{^1\text{H}\}$ NMR ($(\text{CD}_3)_2\text{CO}$, 75 MHz): compound 18



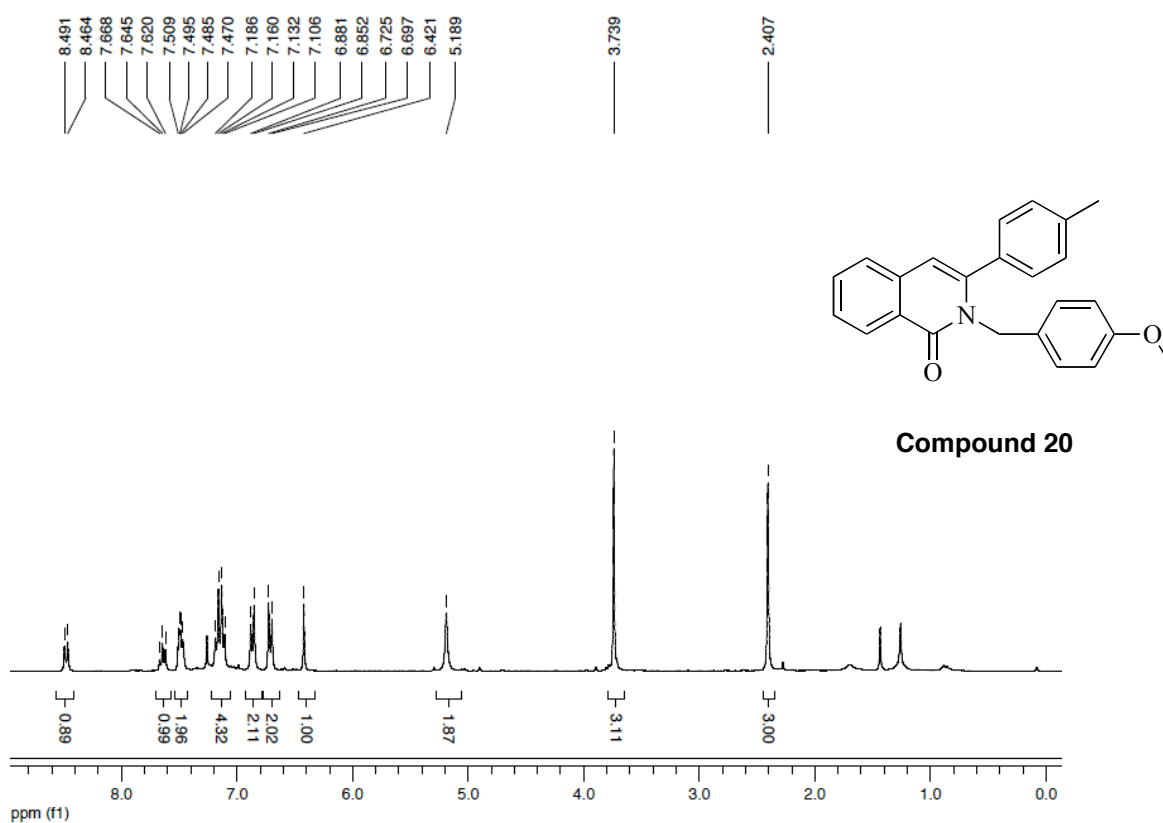
^1H NMR (DMSO d_6 , 300 MHz): compound 19



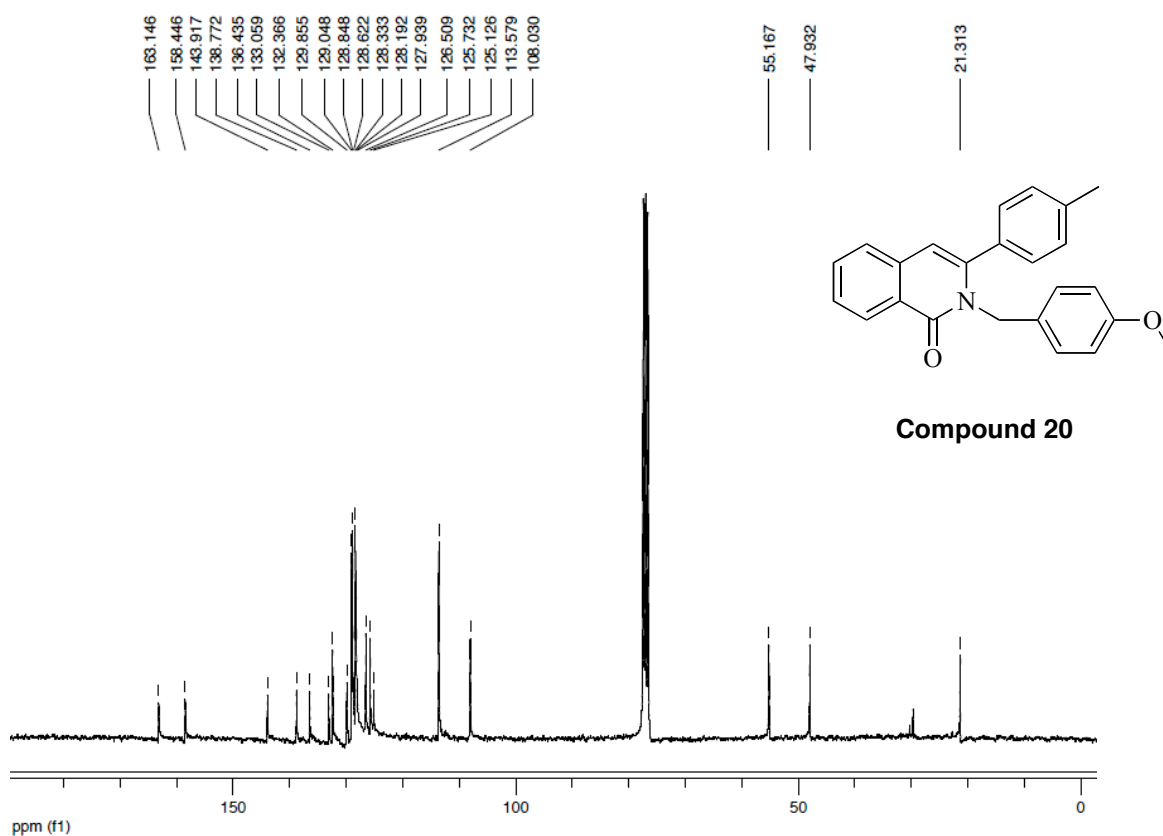
^{13}C { ^1H } NMR (DMSO d_6 , 75 MHz): compound 19



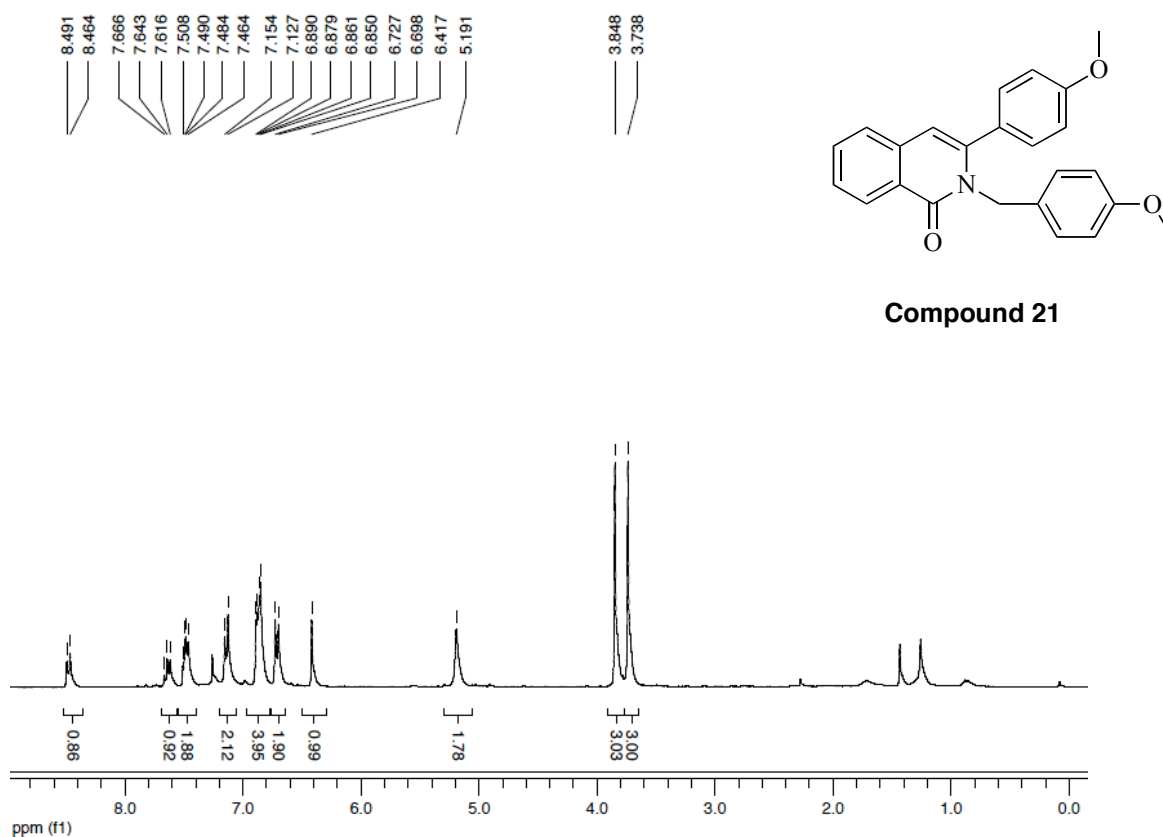
^1H NMR (CDCl_3 , 300 MHz): compound 20



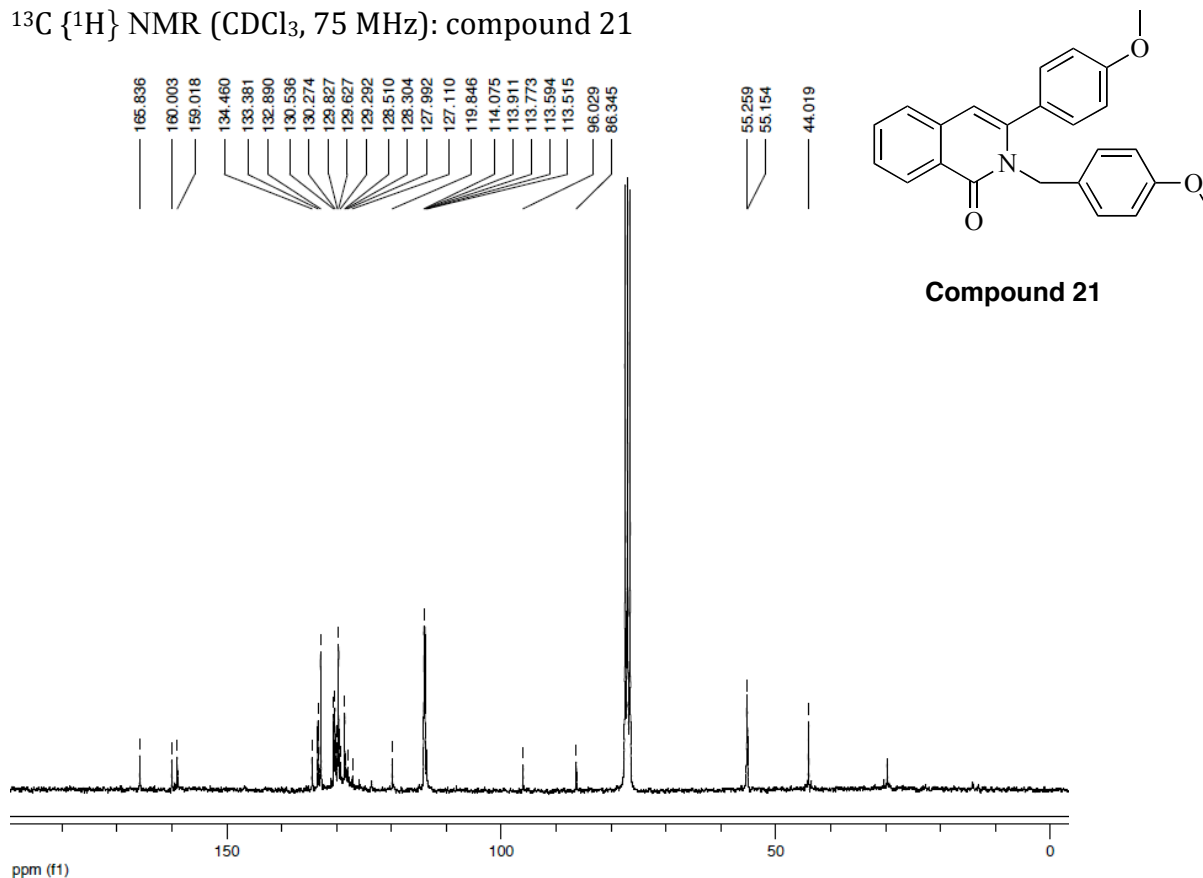
^{13}C $\{^1\text{H}\}$ NMR (CDCl_3 , 75 MHz): compound 20



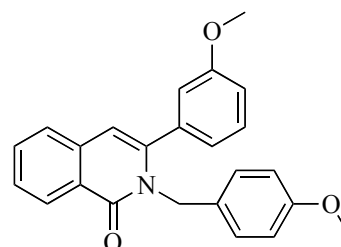
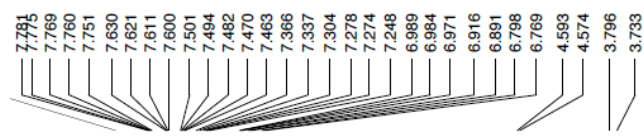
^1H NMR (CDCl_3 , 300 MHz): compound 21



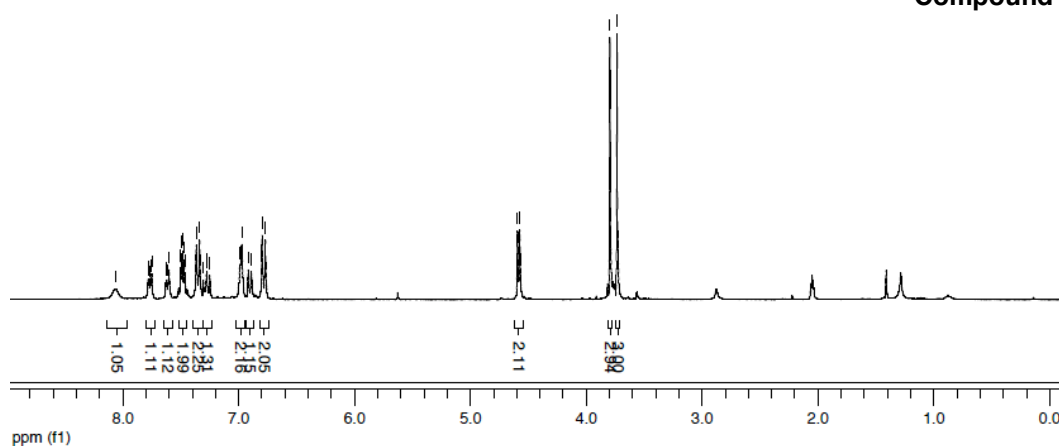
^{13}C { ^1H } NMR (CDCl_3 , 75 MHz): compound 21



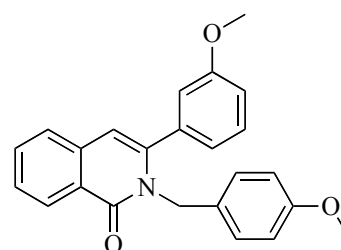
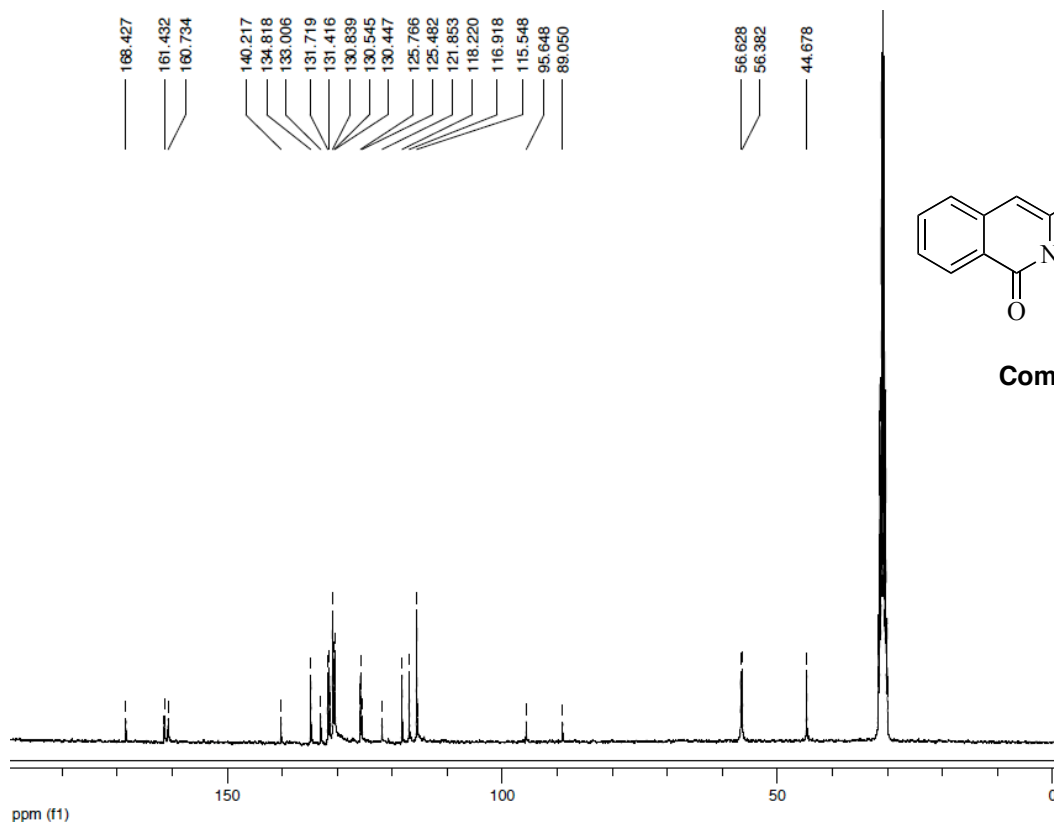
^1H NMR (CDCl_3 , 300 MHz): compound 22



Compound 22

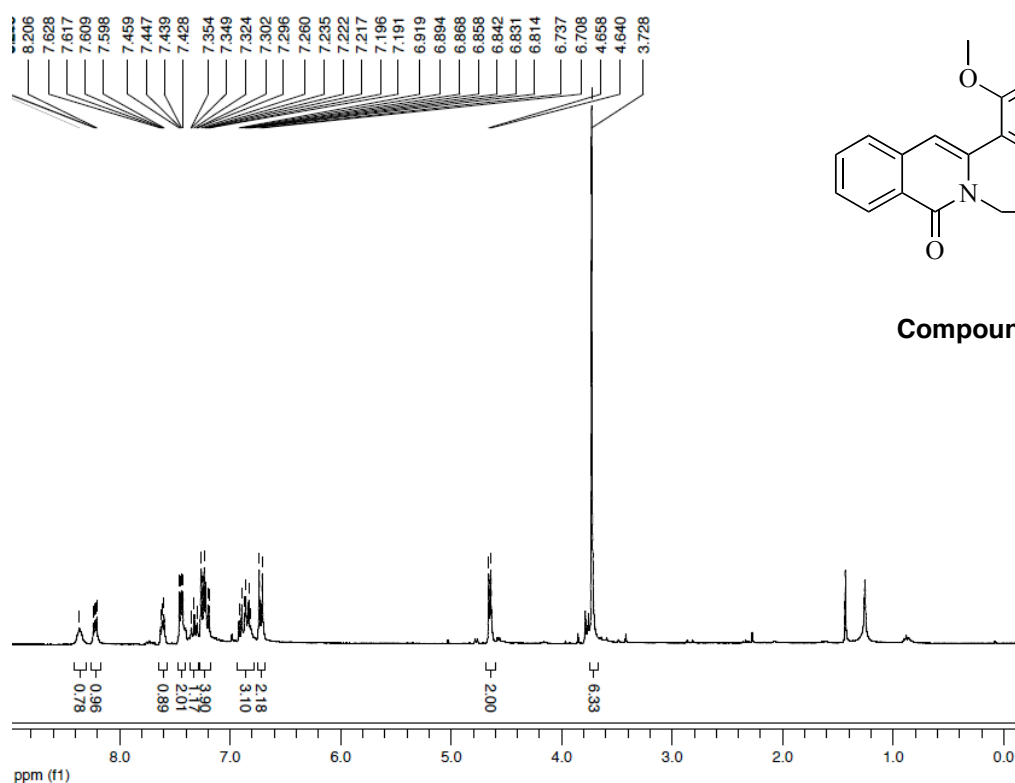


^{13}C $\{^1\text{H}\}$ NMR (CDCl_3 , 75 MHz): compound 22

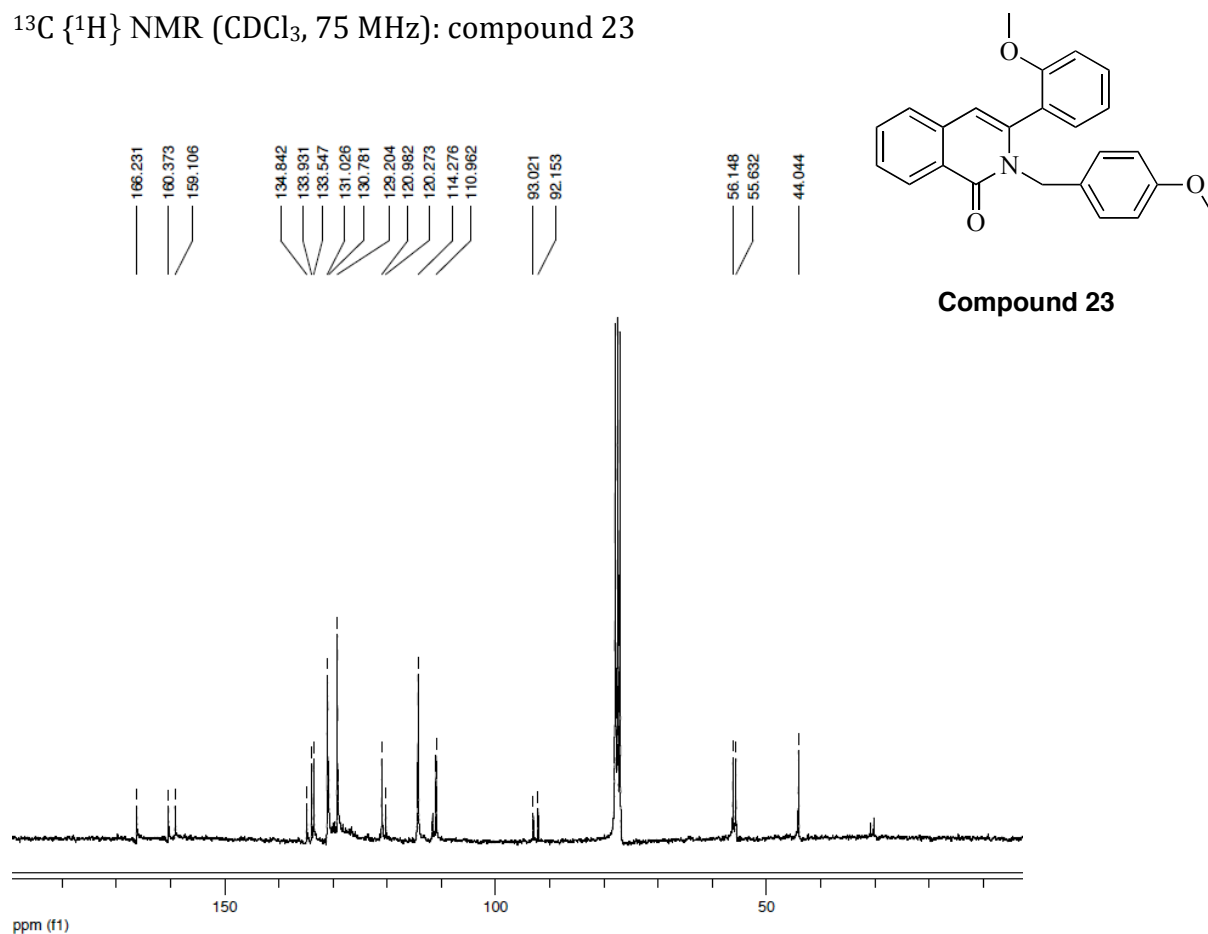


Compound 22

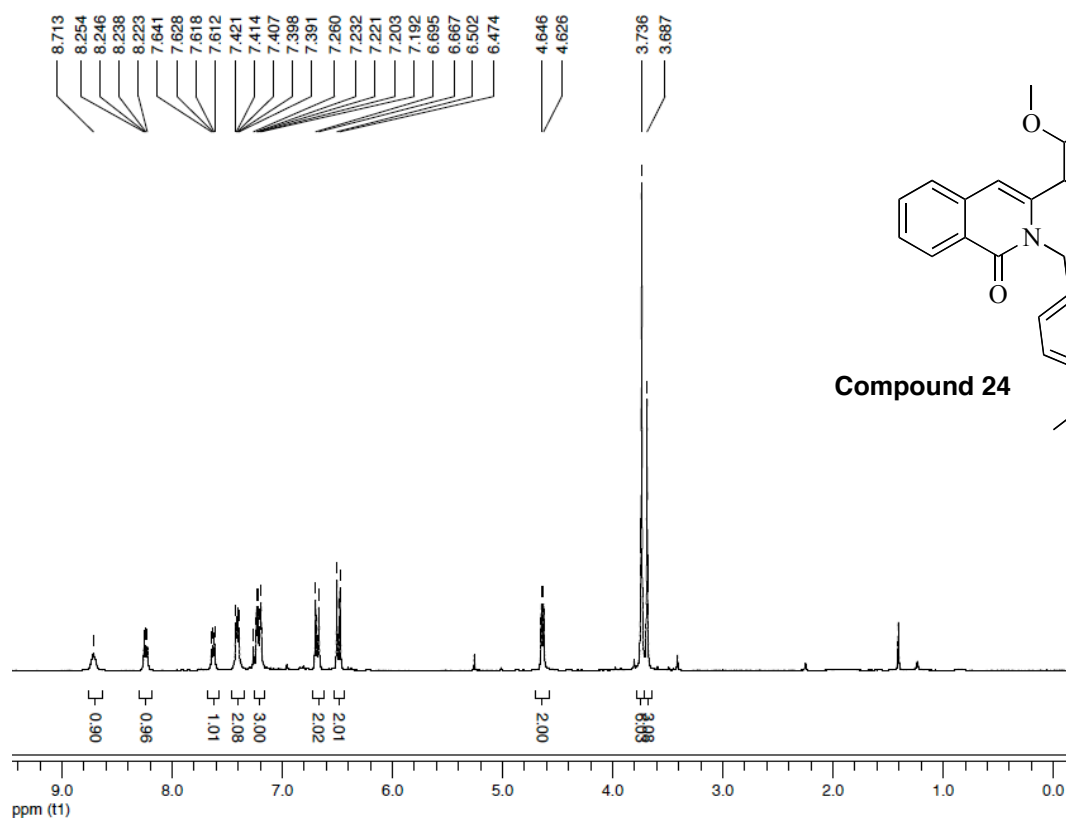
^1H NMR (CDCl_3 , 300 MHz): compound 23



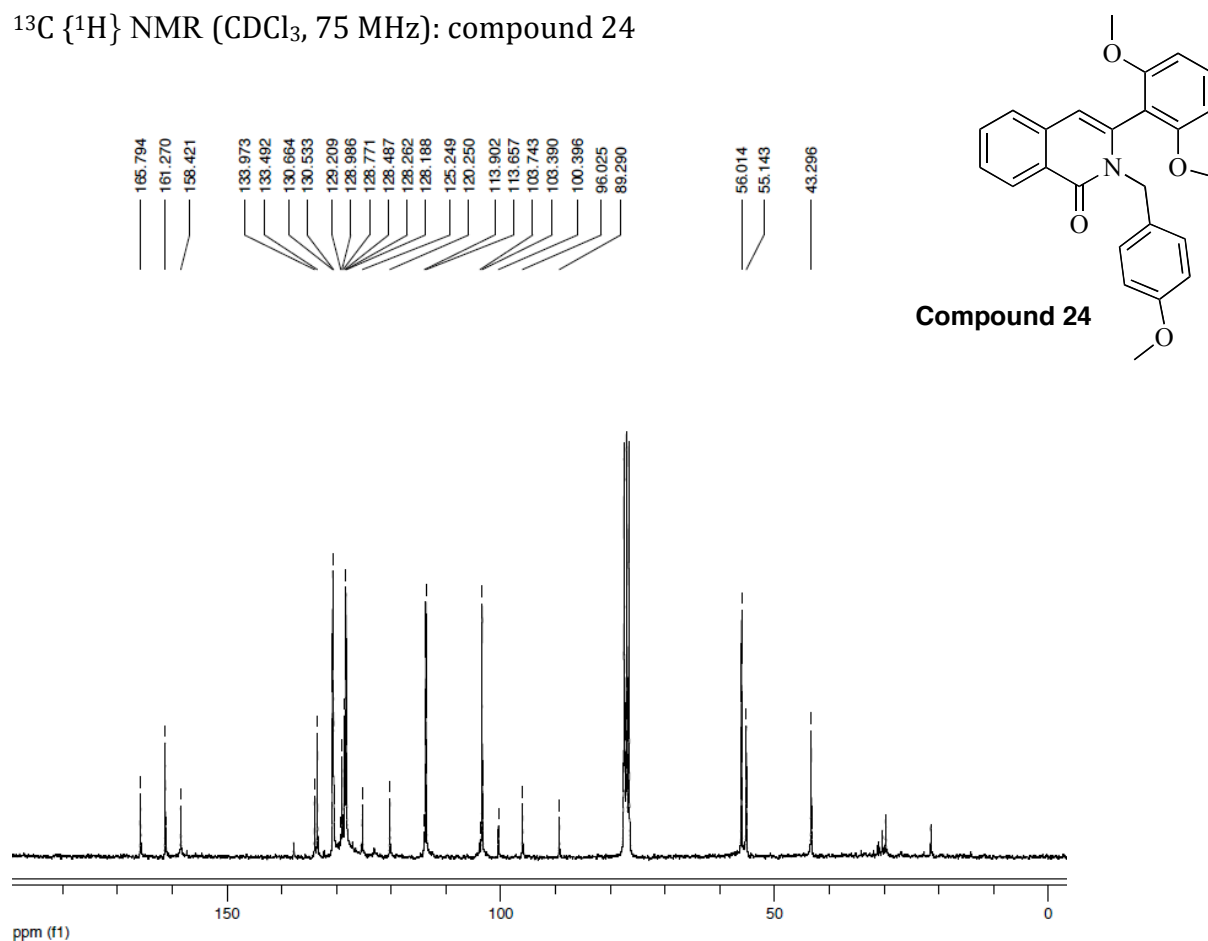
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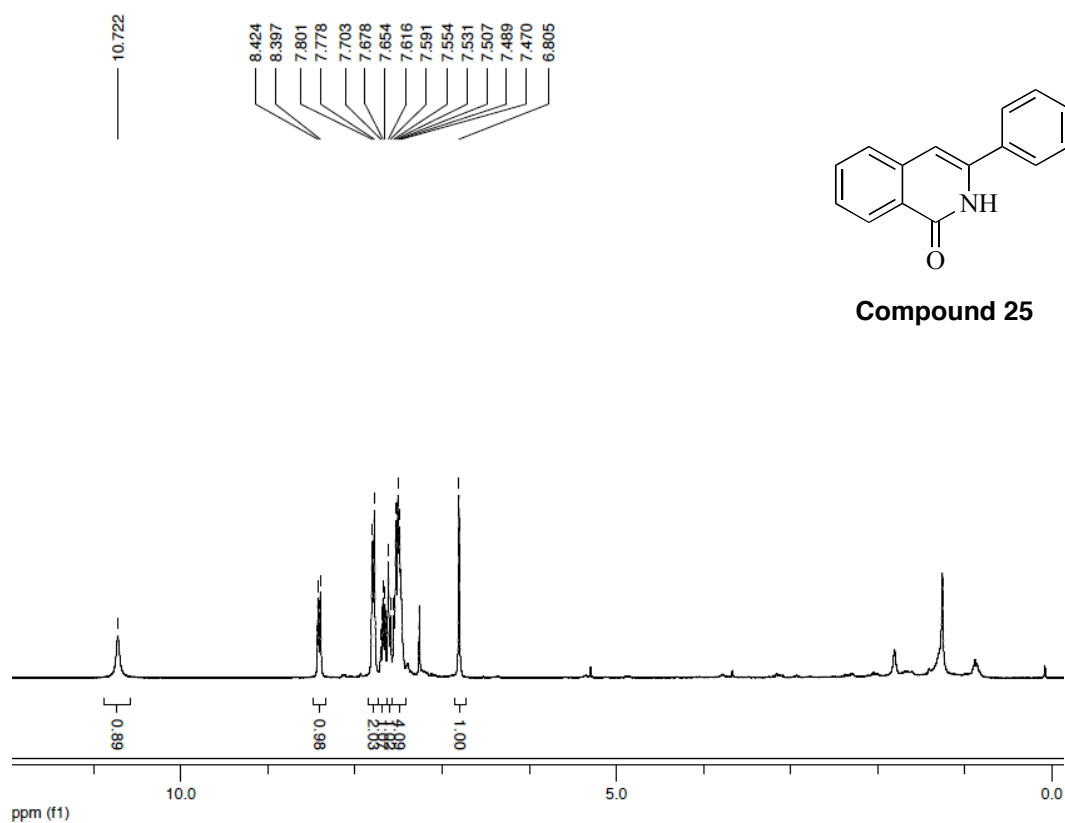
^1H NMR (CDCl_3 , 300 MHz): compound 24



^{13}C $\{^1\text{H}\}$ NMR (CDCl_3 , 75 MHz): compound 24



¹H NMR (CDCl₃, 300 MHz): compound 25



¹³C {¹H} NMR (CDCl₃, 75 MHz): compound 25

