

Supplementary Information

Design and discovery of tyrosinase inhibitors based on the coumarin scaffold

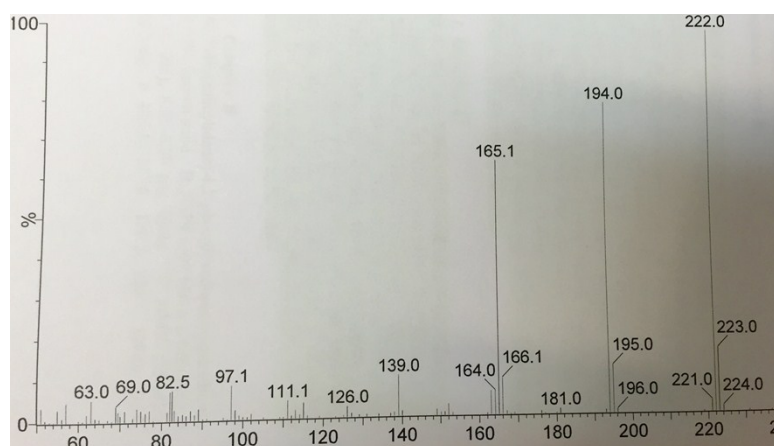
M. J. Matos, C. Varela, S. Vilar, G. Hripcsak, F. Borges, L. Santana, E.
Uriarte, A. Fais, A. Di Petrillo, F. Pintus and B. Era

Experimental section: Mass, ^1H NMR and ^{13}C NMR spectra of the studied
compounds (**1**, **2b-6b**, **7** and **8b-15b**).

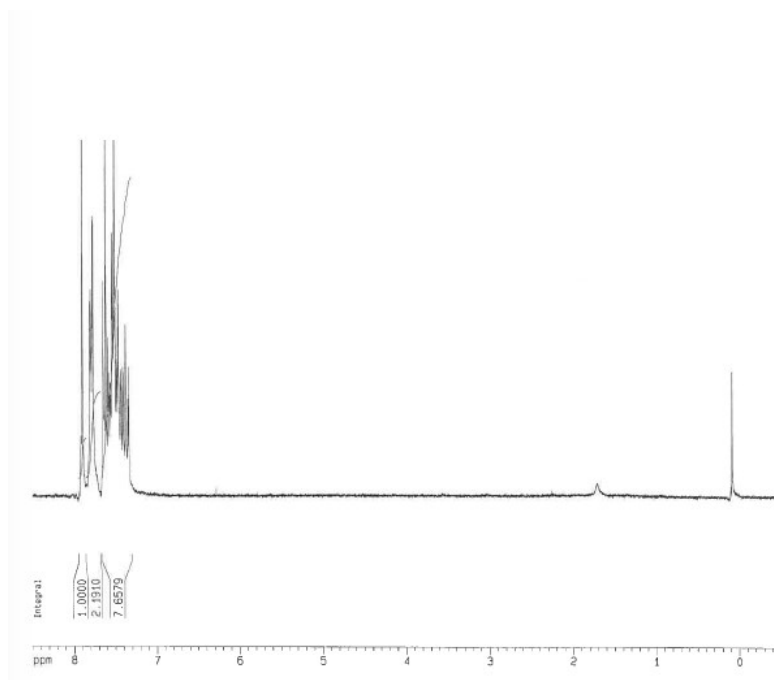
Data regarding the two equilibrium constants of compound **15b**.

Compound 1

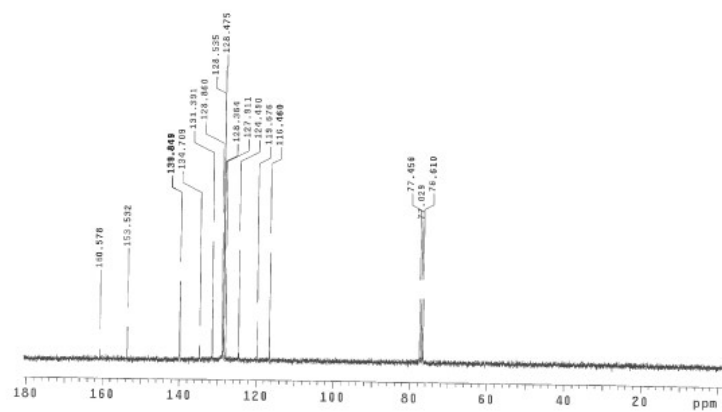
Mass



^1H NMR

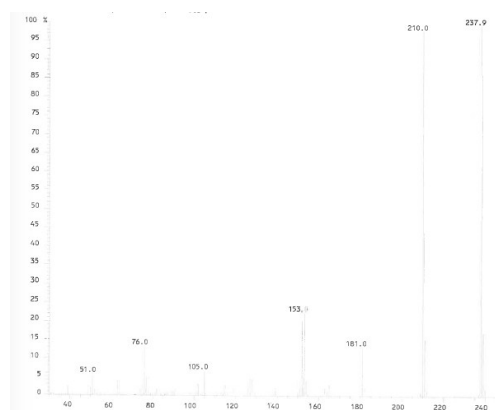


^{13}C NMR

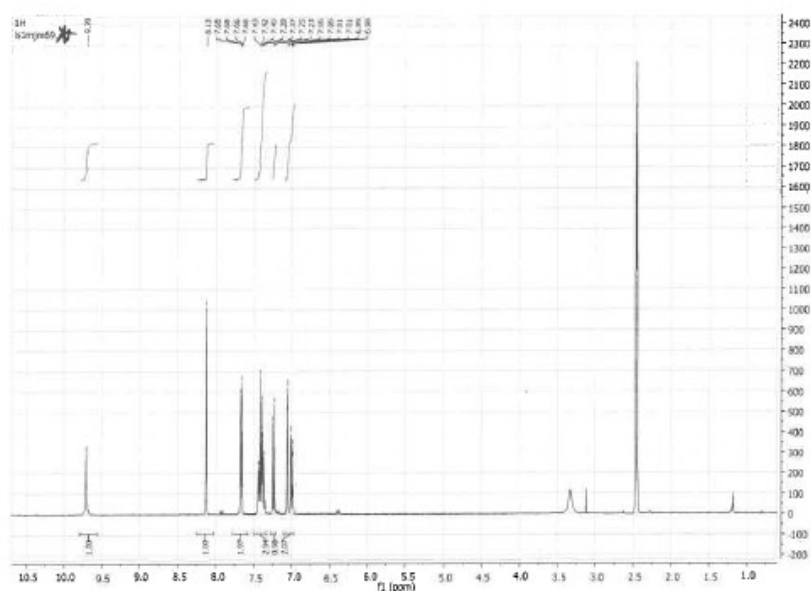


Compound **2b**

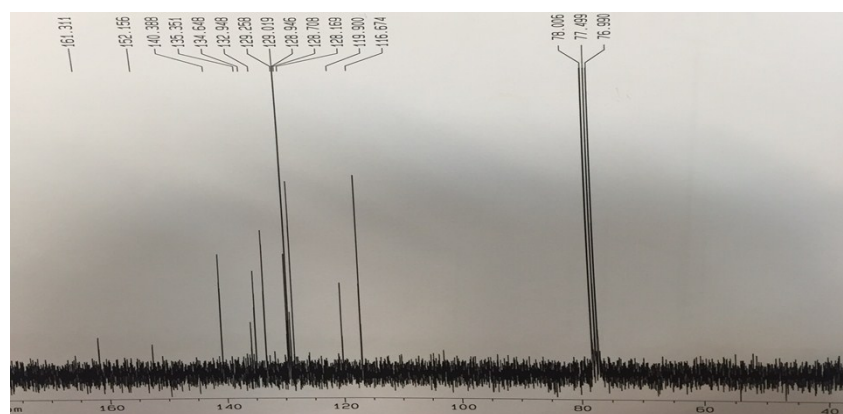
Mass



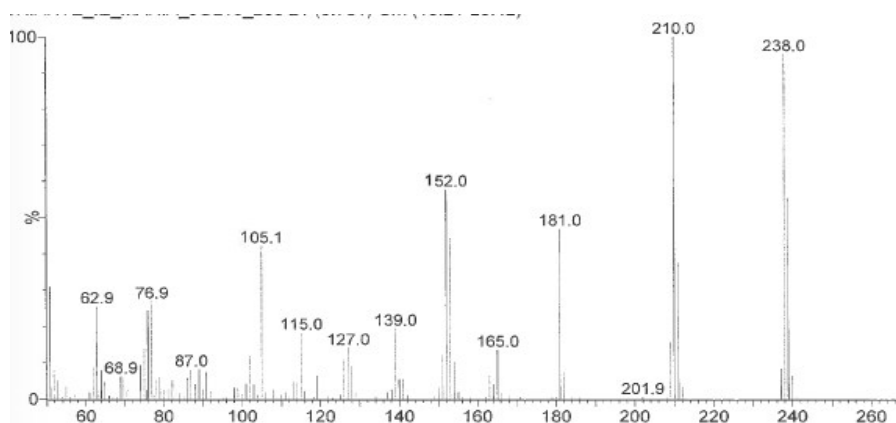
^1H NMR



^{13}C RMN

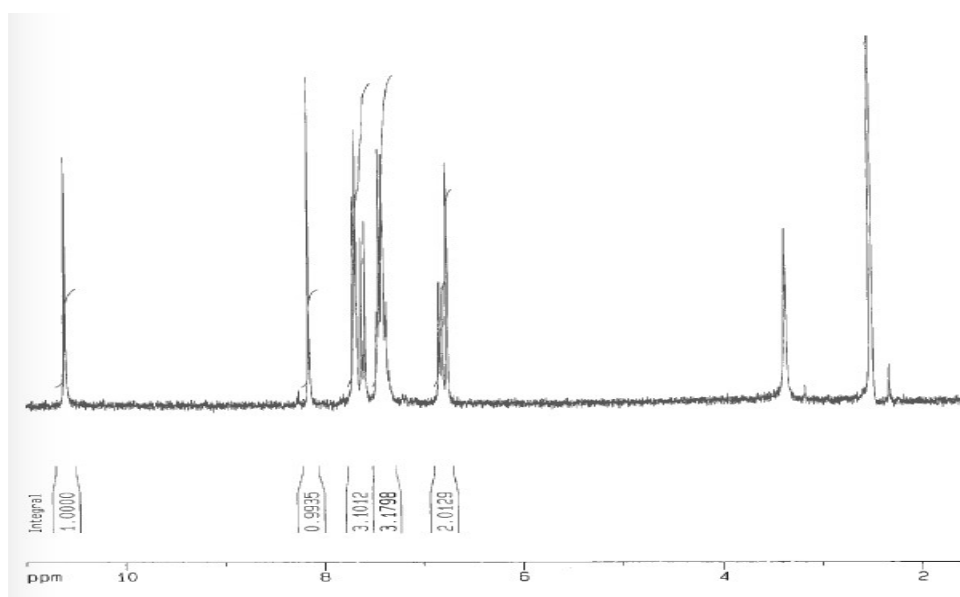


Compound **3b**

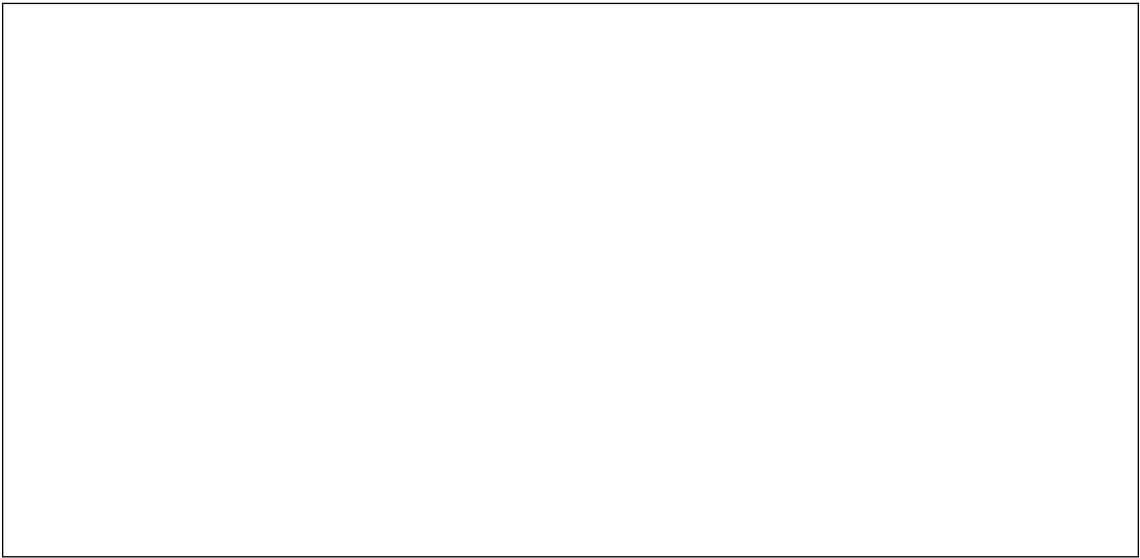


Mass

¹H NMR

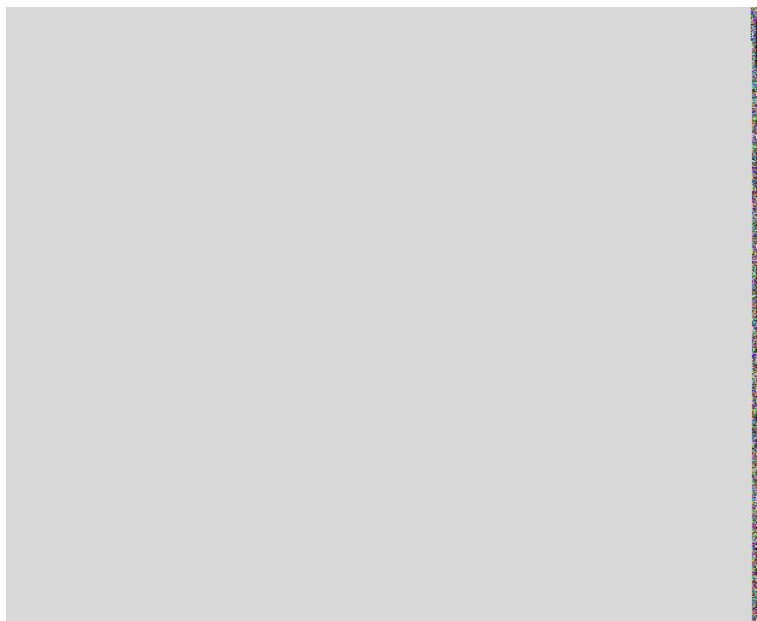


¹³C NMR

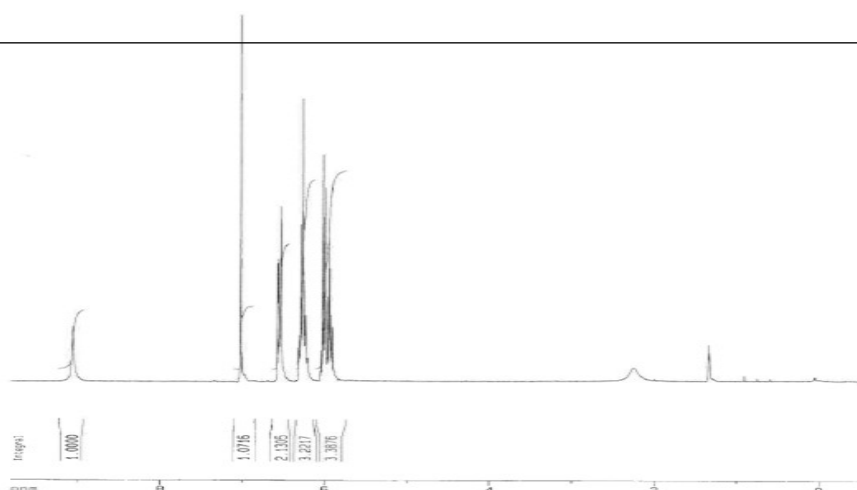


Compound **4b**

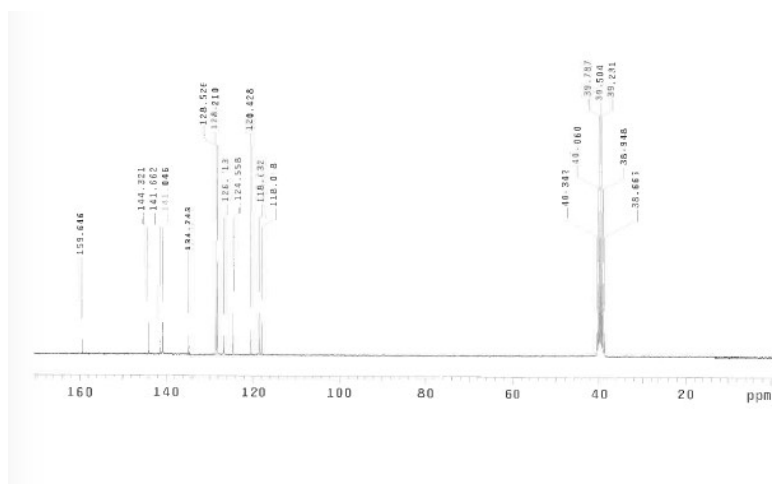
Mass



^1H NMR

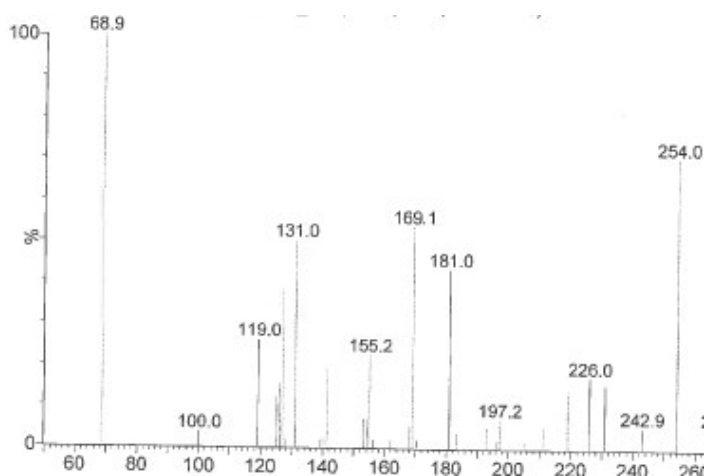


^{13}C NMR

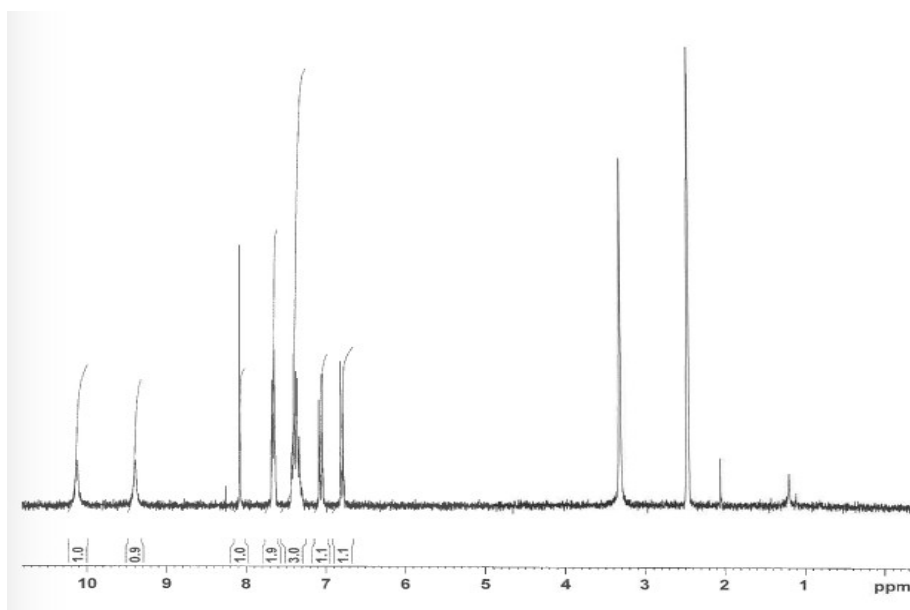


Compound **5b**

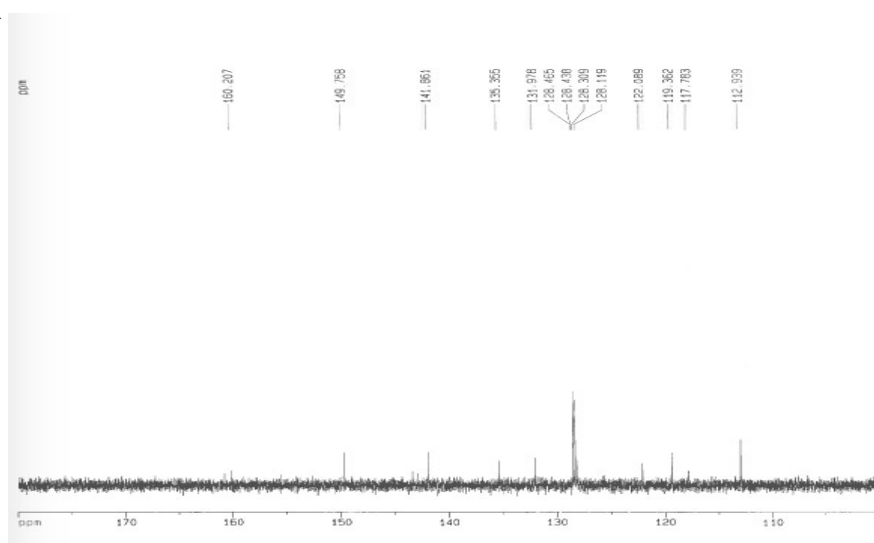
Mass



^1H NMR

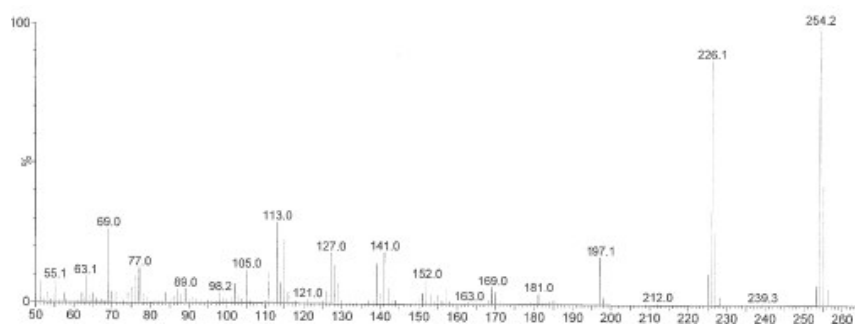


^{13}C NMR

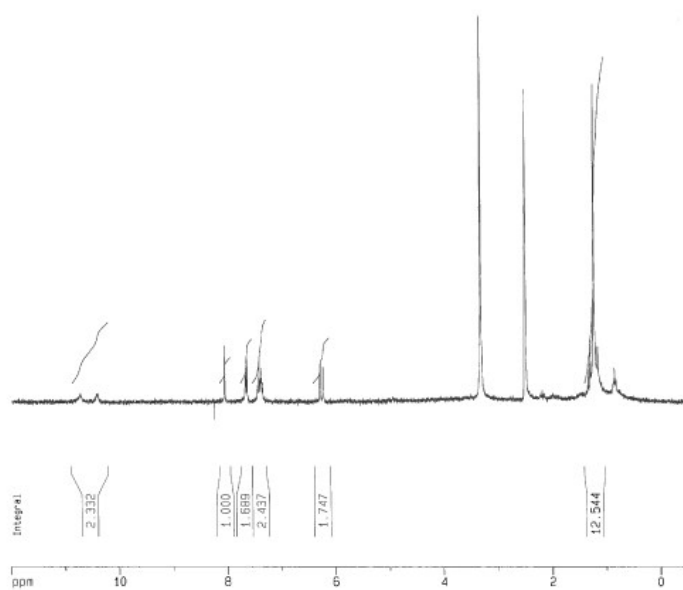


Compound **6b**

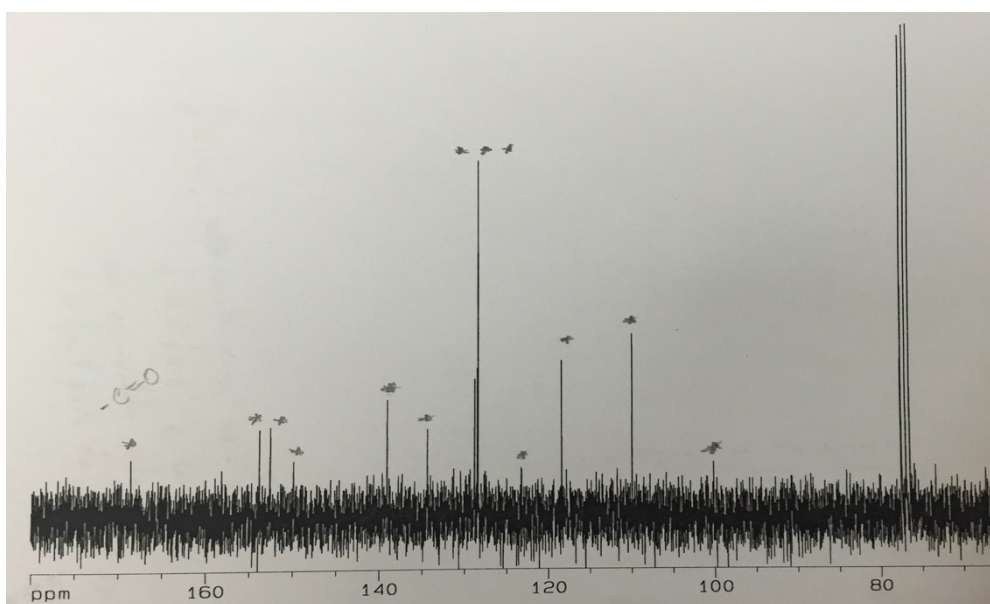
Mass



^1H NMR

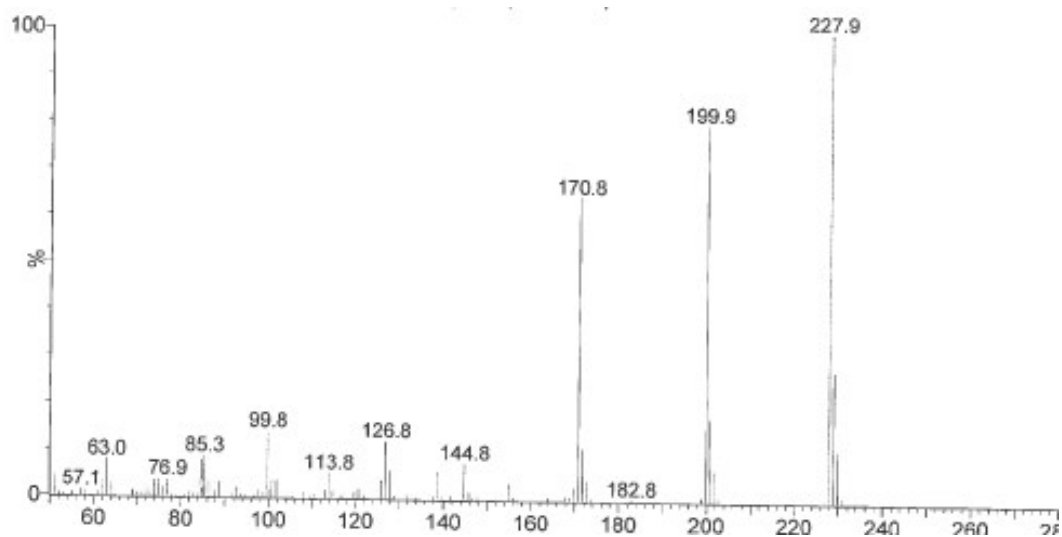


^{13}C NMR

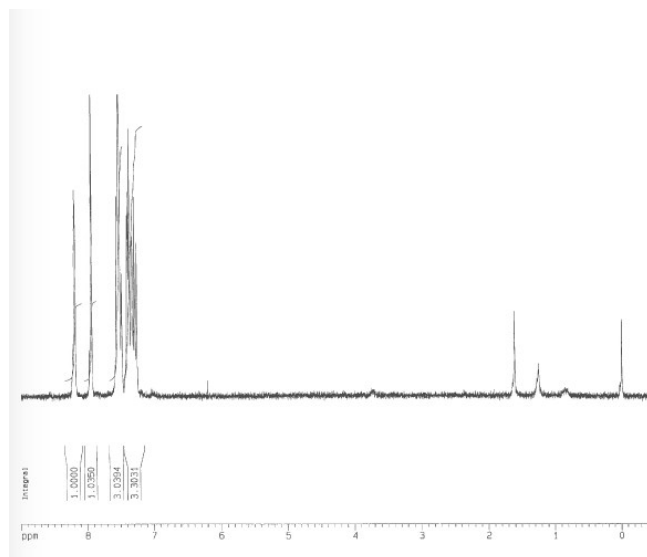


Compound 7

Mass



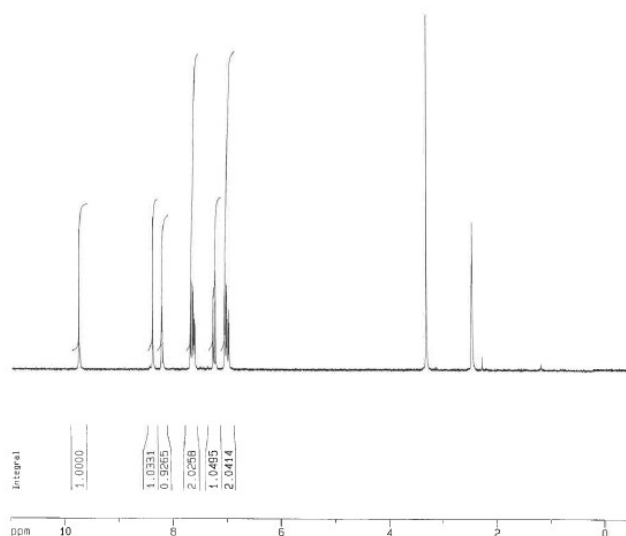
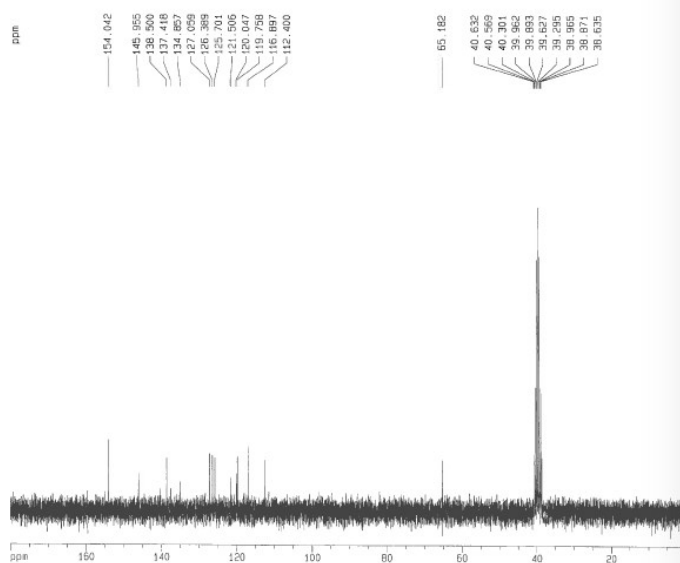
¹H NMR



¹³C NMR

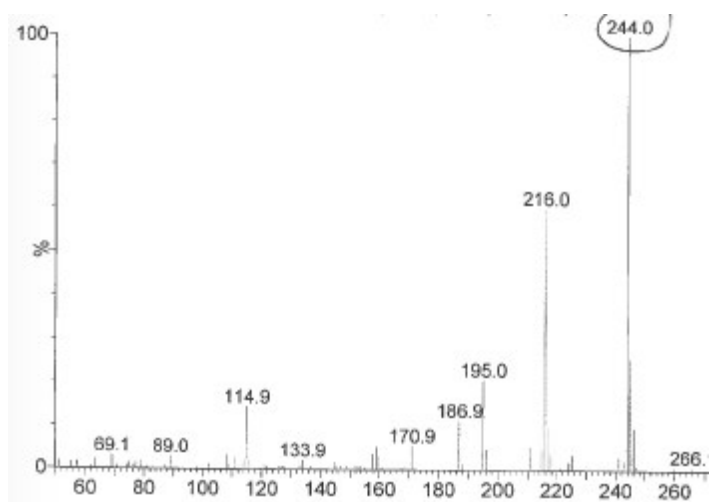


Mass

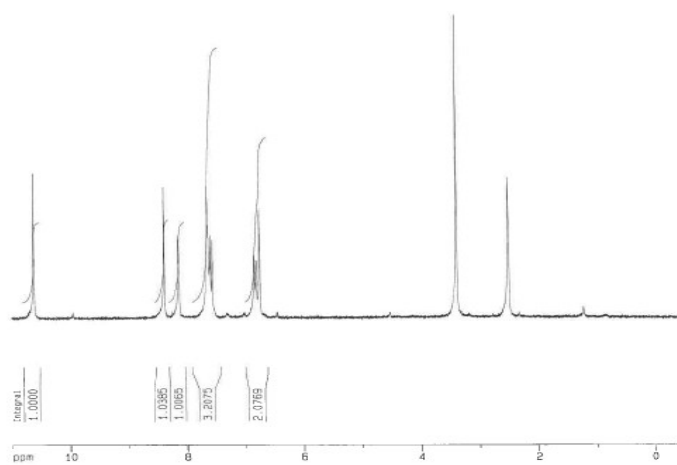
[illegible]¹H NMR¹³C NMR

Compound **9b**

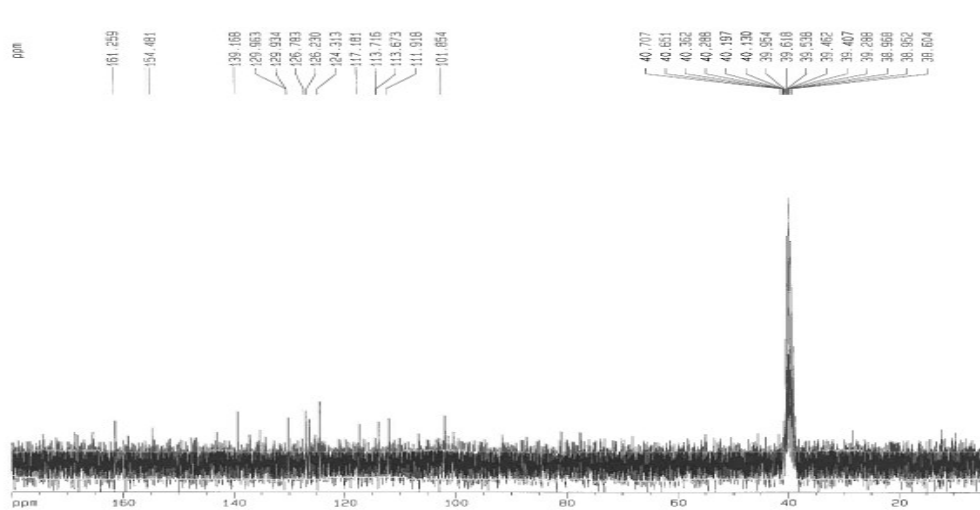
Mass



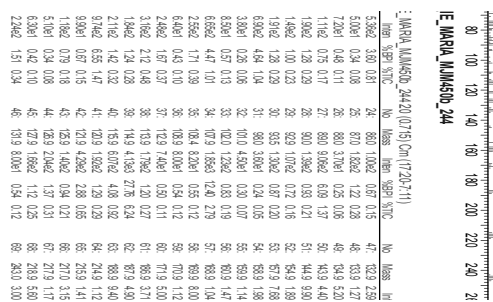
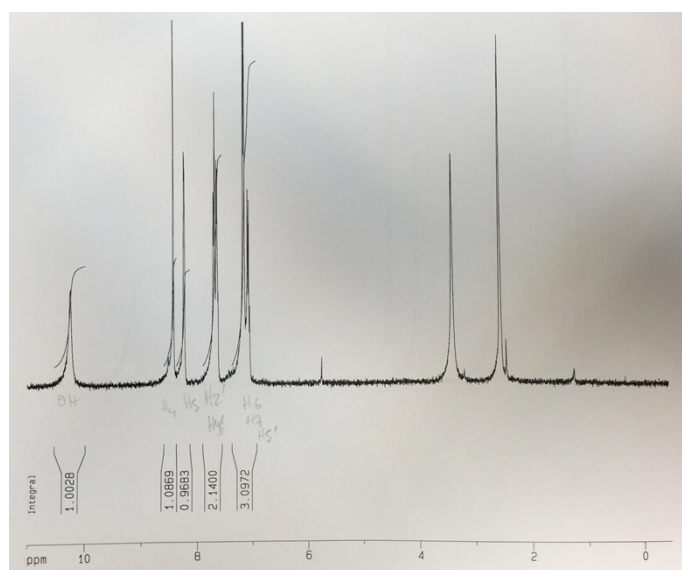
^1H NMR

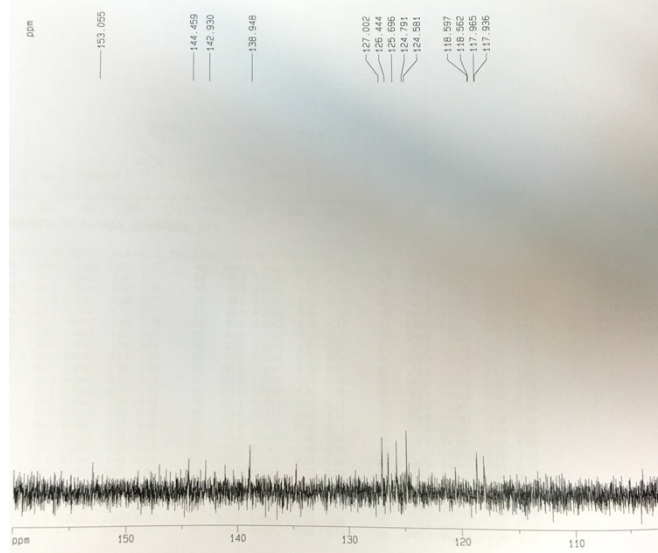


^{13}C NMR



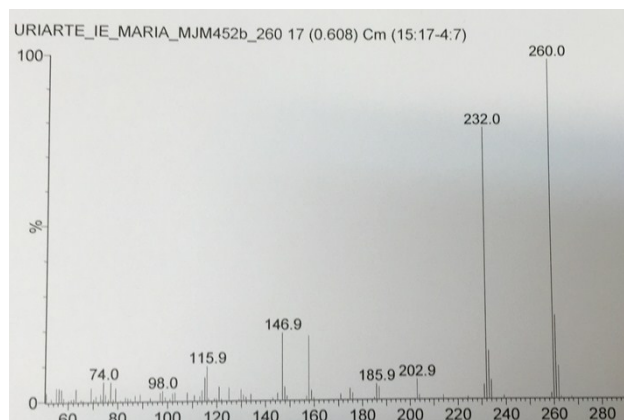
Mass

¹H NMR¹³C NMR

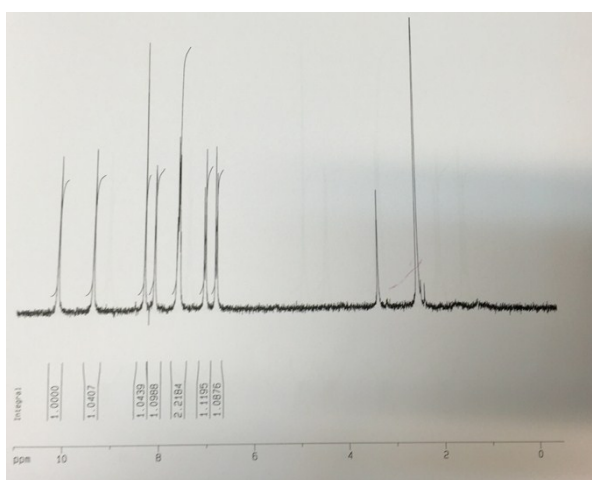


Compound **11b**

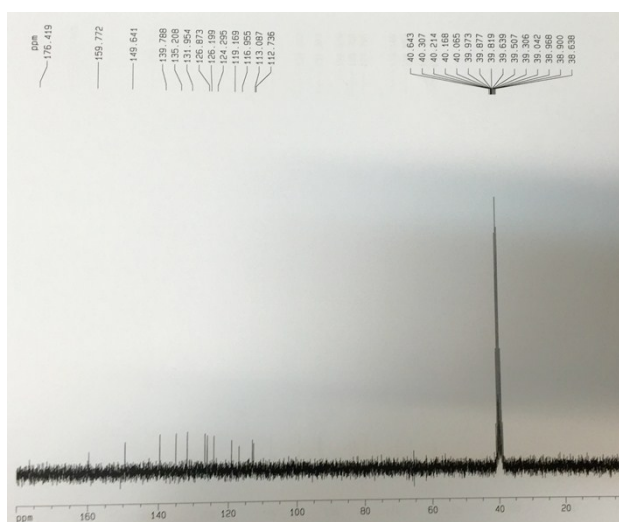
Mass



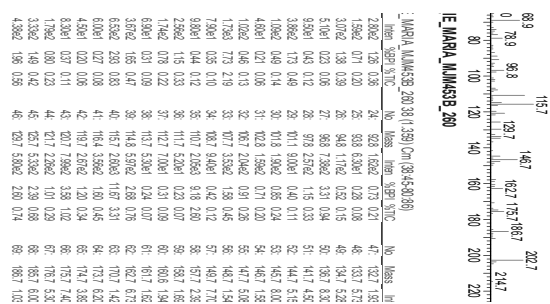
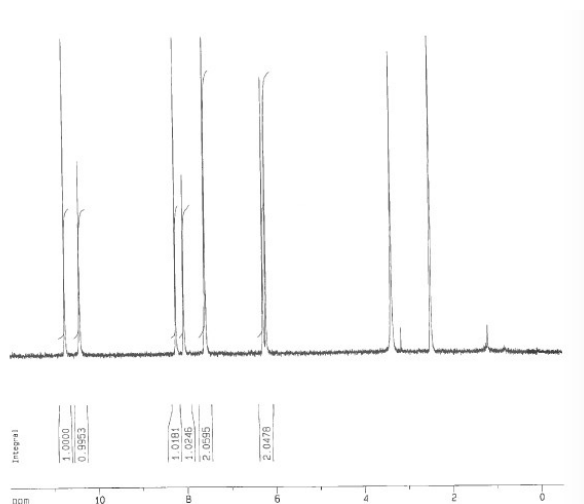
^1H NMR

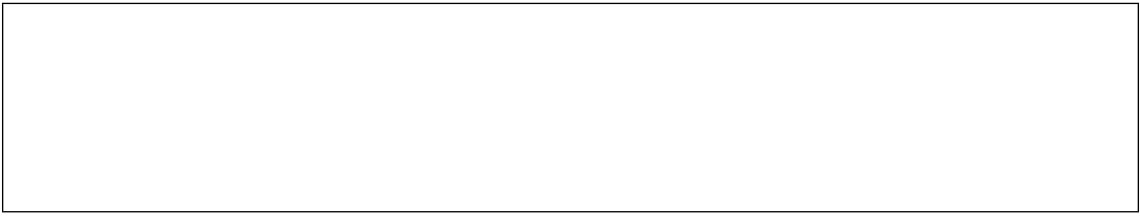


^{13}C NMR



Mass

¹H NMR¹³C NMR



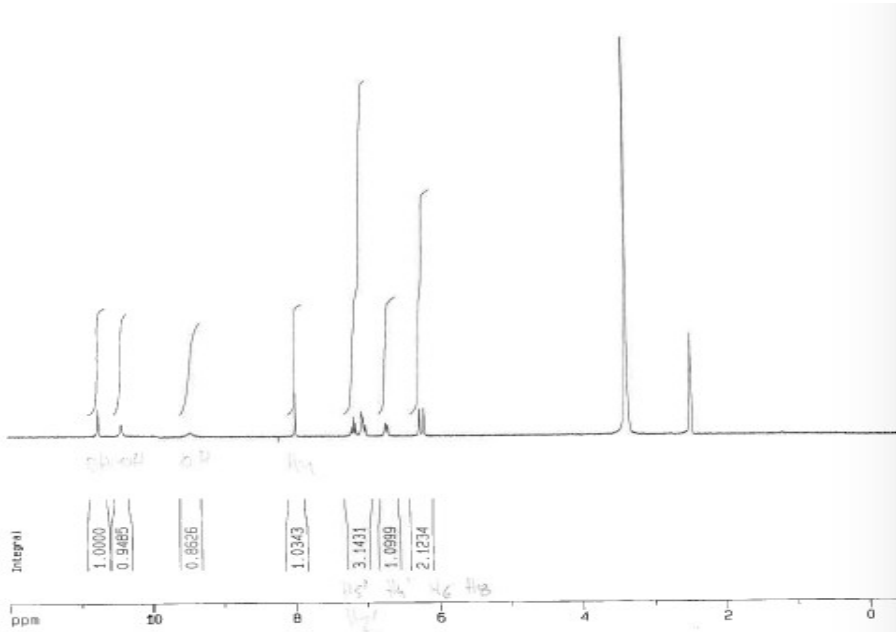
Compound **13b**

1H NMR spectrum (400 MHz, CDCl3) of Compound 13b. The spectrum shows peaks from 0 to 8 ppm. The table below provides the chemical shift (ppm), integration, and assignment for each peak.

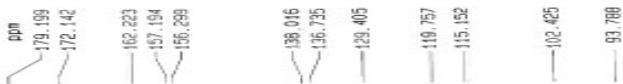
Chemical Shift (ppm)	Integration	Assignment
7.99, 7.97	1.0000	Aromatic H
7.72, 7.70	0.9485	Aromatic H
7.22, 7.20	0.8526	Aromatic H
6.43	1.0343	Aromatic H
6.22, 6.20	3.1431	CH2
6.09, 6.07	1.0989	CH
5.75, 5.73	2.1234	CH2
4.25		CH2
3.79, 3.77		CH2
3.43, 3.41		CH2
3.28, 3.26		CH2
3.08, 3.06		CH2
2.82, 2.80		CH2
2.62, 2.60		CH2
2.42, 2.40		CH2
2.22, 2.20		CH2
2.02, 2.00		CH2
1.82, 1.80		CH2
1.62, 1.60		CH2
1.42, 1.40		CH2
1.22, 1.20		CH2
1.02, 1.00		CH2
0.82, 0.80		CH2
0.62, 0.60		CH2
0.42, 0.40		CH2
0.22, 0.20		CH2
0.02, 0.00		CH2

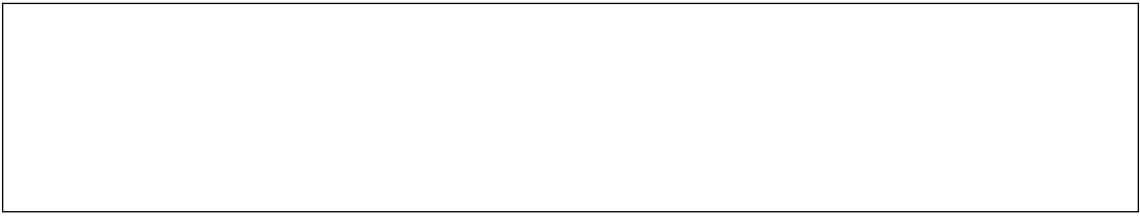
Mass

¹H NMR



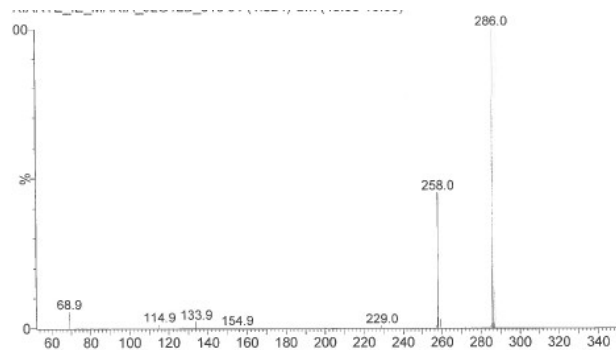
¹³C NMR



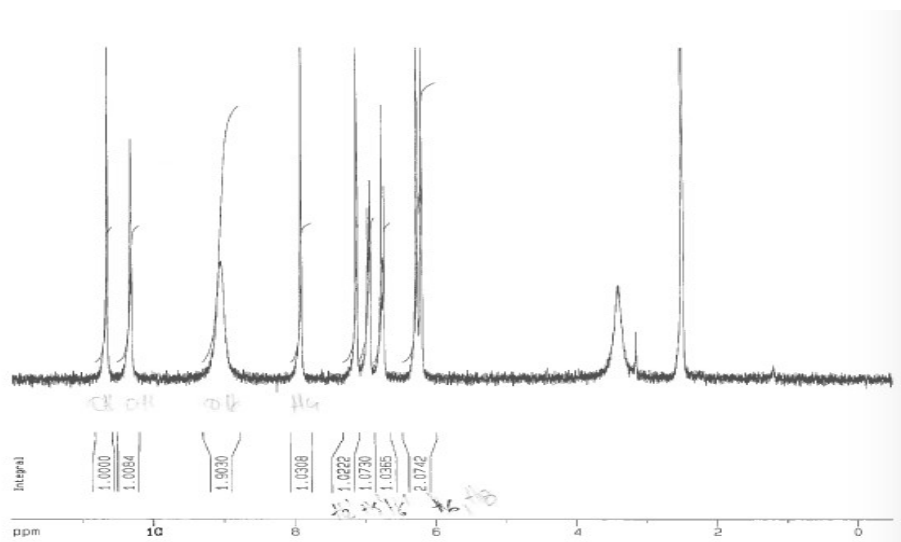


Compound **14b**

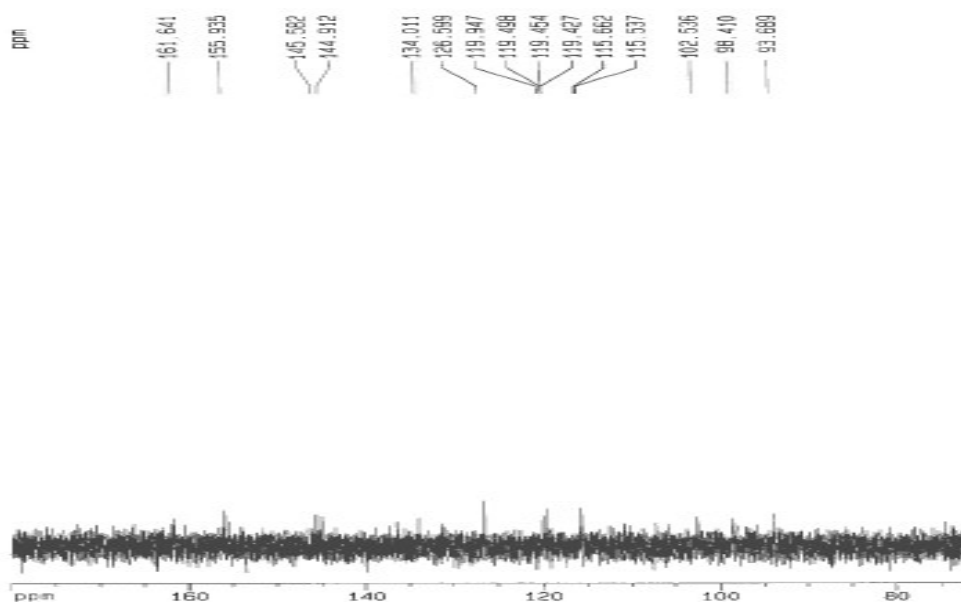
Mass



¹H NMR

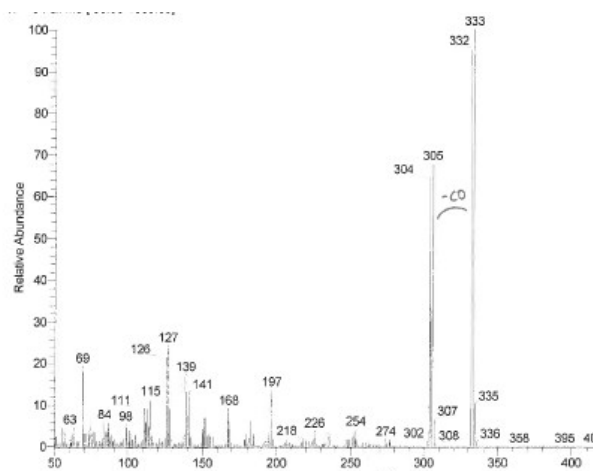


¹³C NMR

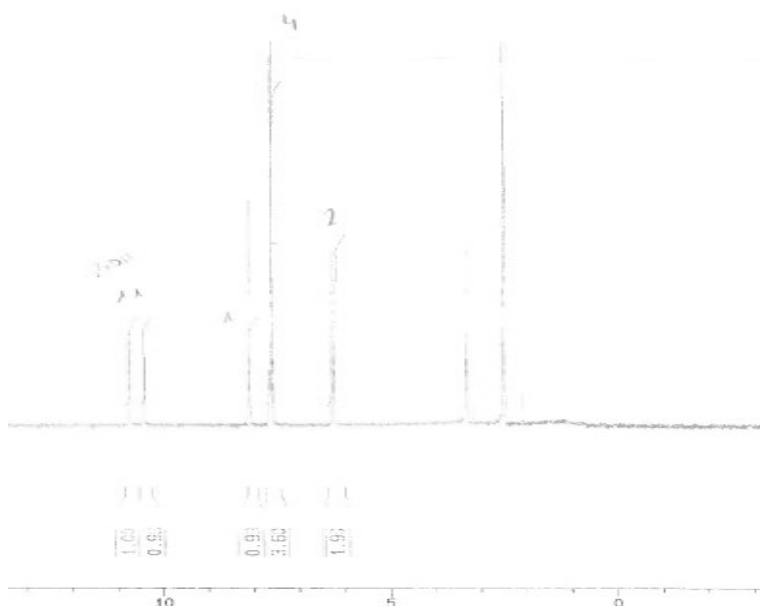


Compound **15b**

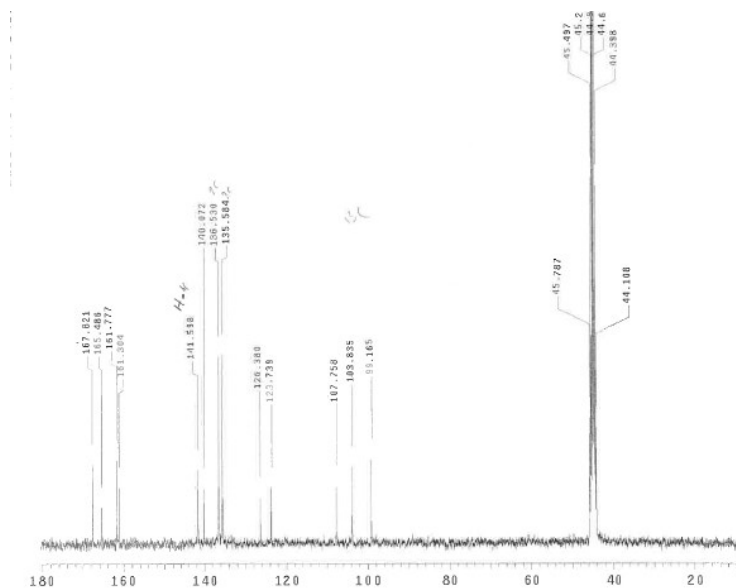
Mass



^1H NMR



^{13}C NMR



Data regarding the two equilibrium constants of compound **15b**:

The secondary plots

