ANNEX

DEDUCCIÓ DE L'EQUACIÓ SIMPLIFICADA DEL MÈTODE EQUIMOLAR

$$S + L \underset{}{\overset{K_1}{\rightleftharpoons}} SL$$

$$SL + L \underset{}{\overset{K_2}{\rightleftharpoons}} SL_2$$

on L_0: Concentració inicial de CSA

S_0: Concentració inicial de solut

La constant d'equilibri es defineix com:

$$K_1 = \frac{[SL]}{[L][S]} = \frac{[SL]}{(S_0 - [SL] - [SL_2])(S_0 - [SL] - [SL_2])} \qquad \textbf{Equació 1}$$

si $[SL_2] << 0$ llavors $[SL_2] \approx 0$ i l'equació 1 es simplifica segons:

$$K_1 = \frac{[SL]}{[L][S]} = \frac{[SL]}{(S_0 - [SL])(S_0 - [SL])} \qquad \textbf{Equació 2}$$

La diferència de desplaçament químic es defineix com:

$$\Delta\delta = \delta_{obs} - \delta_f = \frac{[SL]}{S_0}\delta_C \text{ ;} \delta_C \text{ = desplaçament del complex} \qquad \textbf{Equació 3}$$

llavors si considerem que $L_0 = S_0$ i substituïm [SL] dins l'equació 2 tenim que:

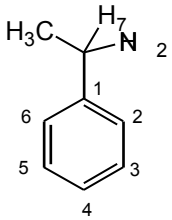
$$K_1 = \frac{[SL]}{(S_0 - [SL])^2} = \frac{S_0 \frac{\Delta\delta}{\delta_C}}{\left(S_0 - S_0 \frac{\Delta\delta}{\delta_C}\right)^2}$$

$$K_1^{1/2}\left(S_0 - S_0 \frac{\Delta\delta}{\delta_C}\right) = S_0^{1/2}\left(\frac{\Delta\delta}{\delta_C}\right)^{1/2}$$

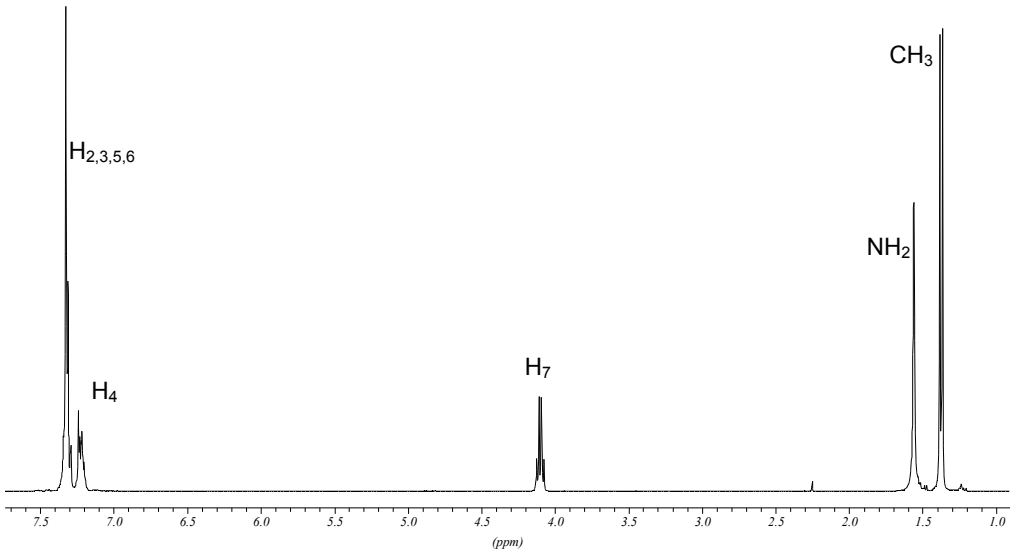
$$1 - \frac{\Delta\delta}{\delta_C} = \frac{\Delta\delta^{1/2}}{(S_0 K_1 \delta_C)^{1/2}}$$

$$\frac{\Delta\delta}{\delta_C} = 1 - \frac{\Delta\delta^{1/2}}{(S_0 K_1 \delta_C)^{1/2}} \quad \Longrightarrow \quad \boxed{\Delta\delta = \delta_C - \sqrt{\frac{\delta_C}{K_1}}\sqrt{\frac{\Delta\delta}{S_0}}}$$

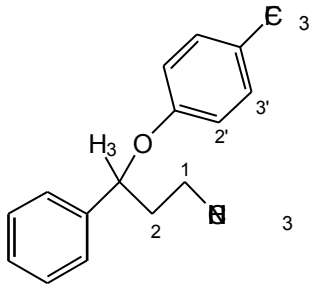
ESPECTRES DE ^{1}H RMN DELS SOLUTS EMPRATS EN ELS EXPERIMENTS DE SOLVATACIÓ



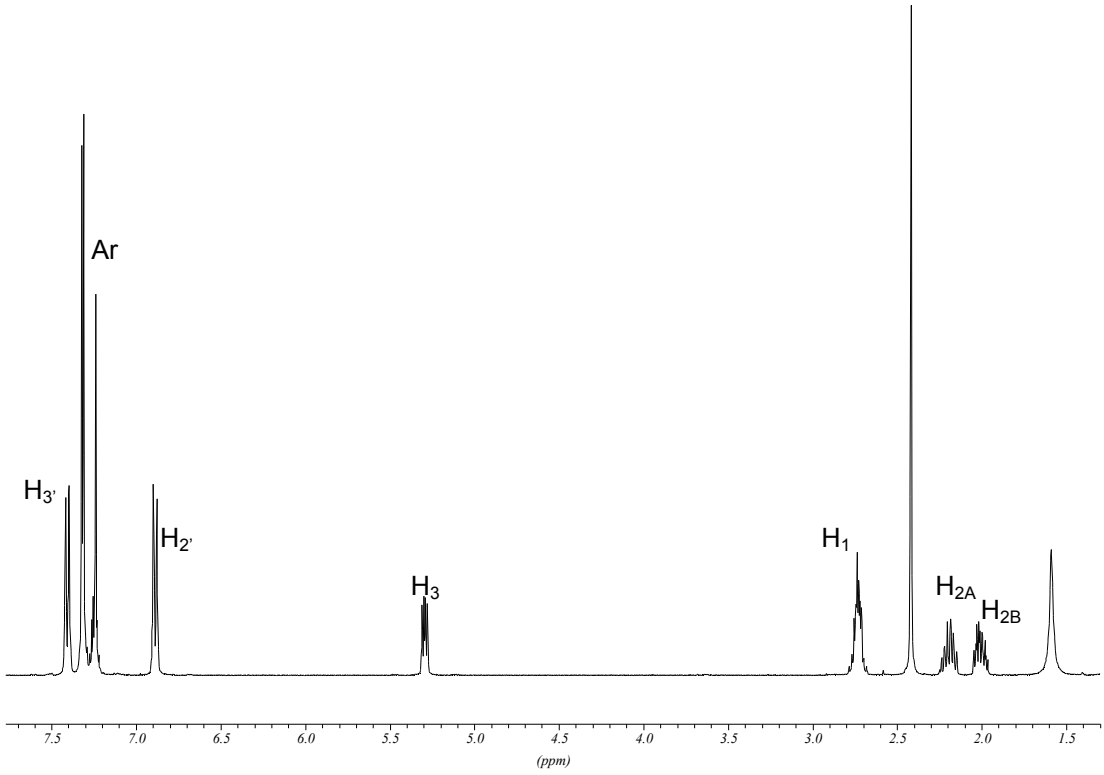
58



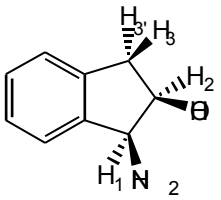
Espectre de ^{1}H RMN de **58** en $CDCl_3$ i 64 scans d'adquisició. Enregistrat en un aparell de 400 MHz.



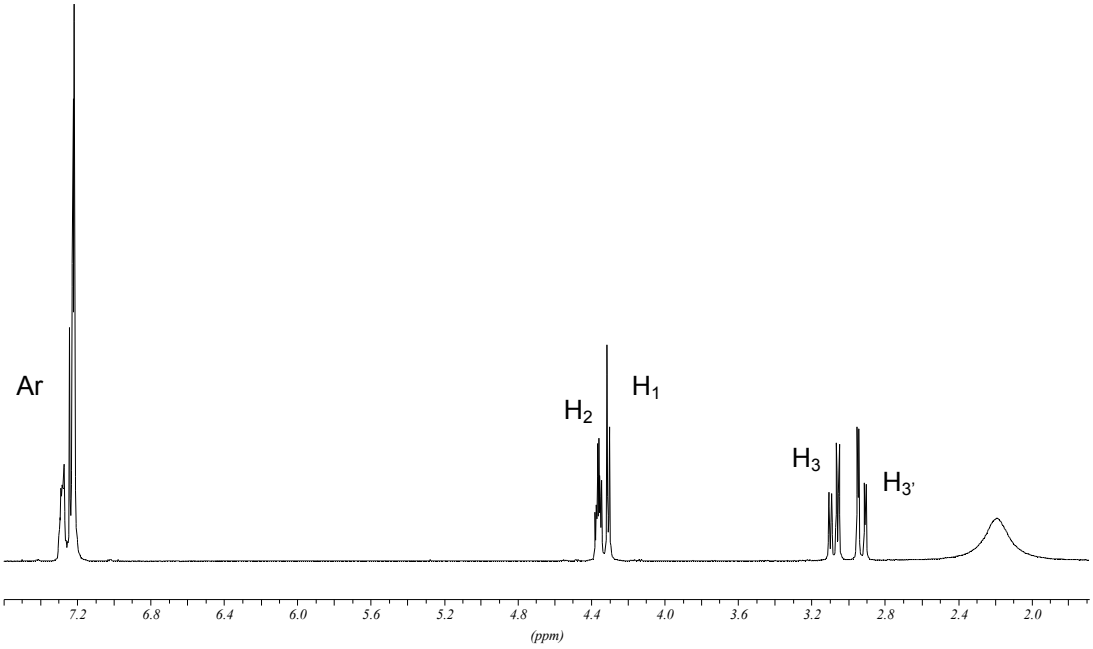
59



Espectre de ^{1}H RMN de **59** en $CDCl_3$ i 64 scans d'adquisició. Enregistrat en un aparell de 400 MHz.

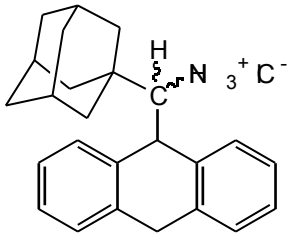


60

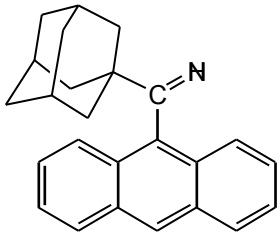


Espectre de ^{1}H RMN de **60** en $CDCl_3$ i 64 scans d'adquisició. Enregistrat en un aparell de 400 MHz.

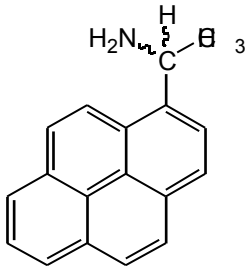
ESPECTRES EM I IR DELS COMPOSTOS SINTETITZATS



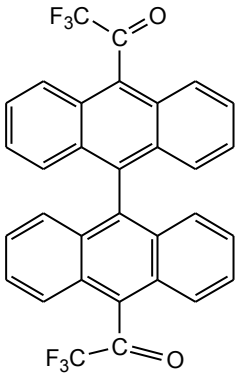
37



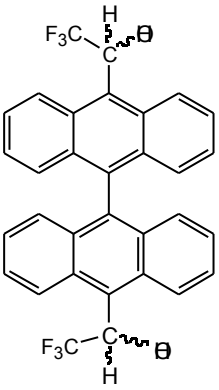
28



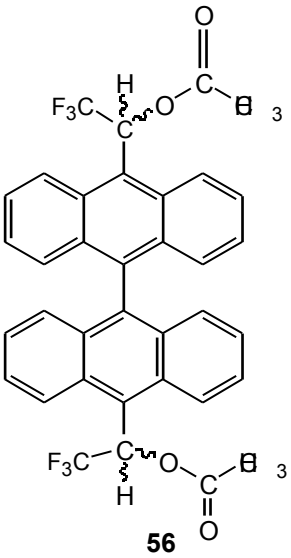
18



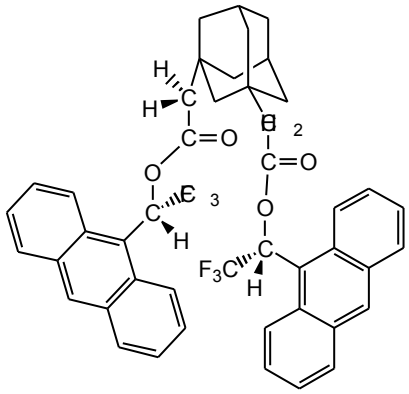
53



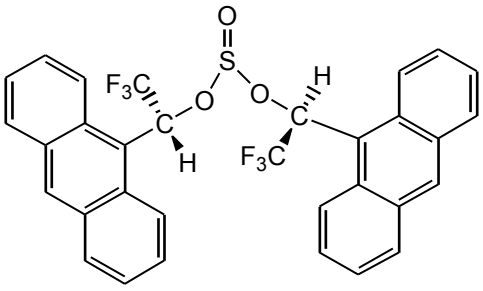
20



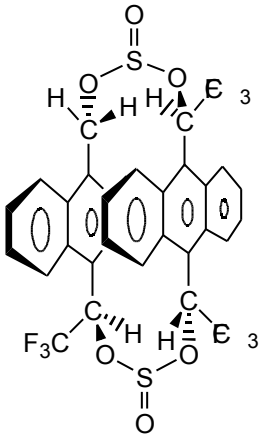
56



70



69



26