

Supporting Information

Hydroxychalcone dyes that serve as color indicators for pH and fluoride ions

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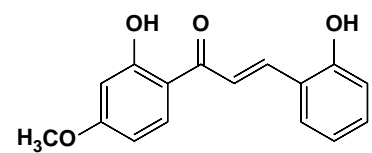
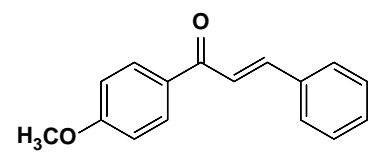
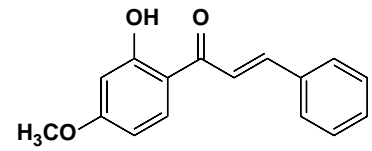
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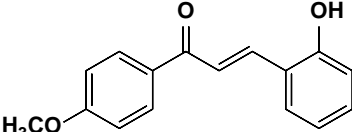
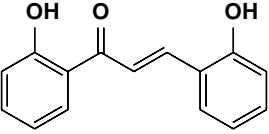
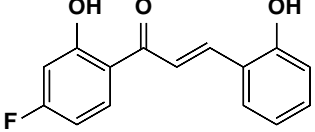
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1. Checklist of characterization data of all compounds

Compound	Know/Unknown	¹ H NMR	¹³ C NMR	HRMS	UV-Vis
 CLN1	Unknown	√	√	√	√
 CLN2	Unknown	√	√	√	√
 CLN3	Unknown	√	√	√	√

Compound	Know/Unknown	¹ H NMR	¹³ C NMR	HRMS	UV-Vis
 <p>CLN4</p>	Unknown	√	√	√	√
 <p>CLN5</p>	Unknown	√	√	√	√
 <p>CLN6</p>	Unknown	√	√	√	√

2. UV-vis absorption spectral titrations and Job plots of CLN5 and CLN6 with TBAF

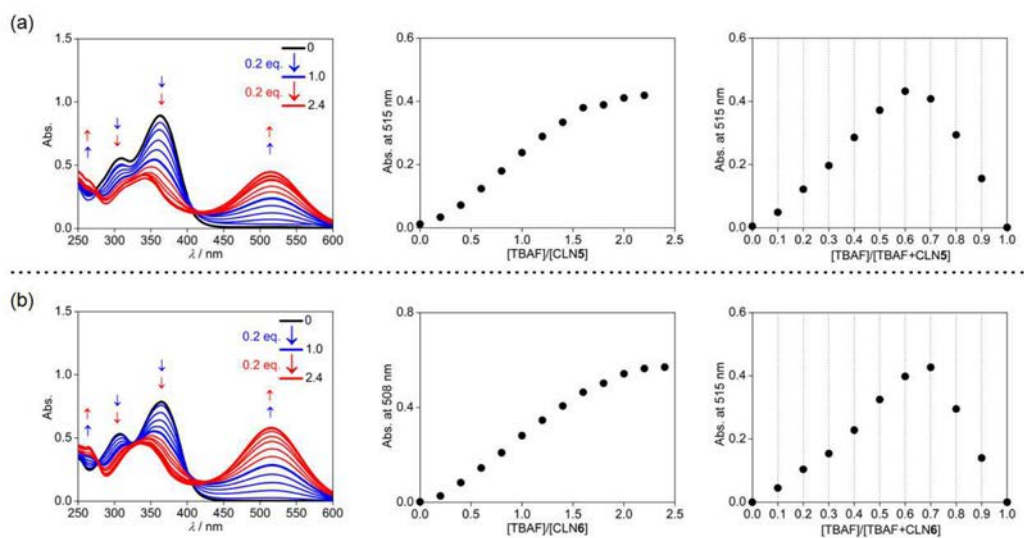


Fig. 1 UV-vis absorption spectral titrations of (a) CLN5 ($4.0 \times 10^{-5} \text{ mol}\cdot\text{L}^{-1}$) and (b) CLN6 ($4.0 \times 10^{-5} \text{ mol}\cdot\text{L}^{-1}$) with TBAF in CH_3CN at 298 K (left), plots of the absorbance changes at λ_{max} with respect to $[\text{TBAF}]/[\text{CLN}]$ (centre), and Job plots for the absorbance changes with respect to $[\text{TBAF}]/[\text{TBAF} + \text{CLN}]$ (right).

3. Changes in the ^1H NMR spectra of CLN2 upon mixing with TBAF

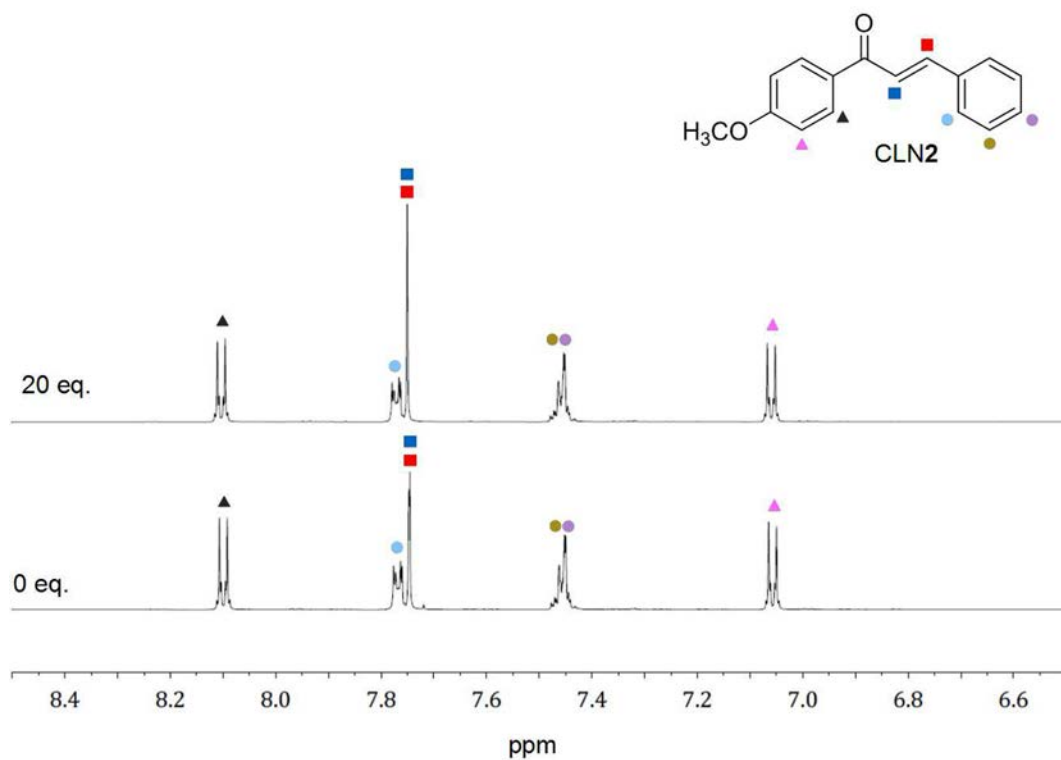


Fig.2 Changes in the ^1H NMR spectra (600 MHz) of CLN2 ($1.4 \times 10^{-2} \text{ mol} \cdot \text{L}^{-1}$) upon mixing with TBAF in CD_3CN at 293 K.

4. UV-vis absorption spectra of CLN1 and CLN1 + TBAF in CH₂Cl₂

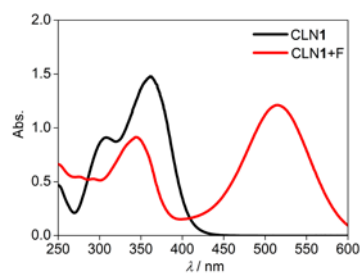
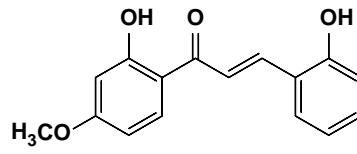
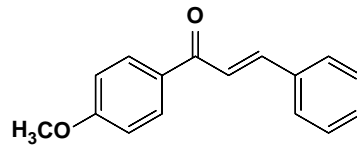
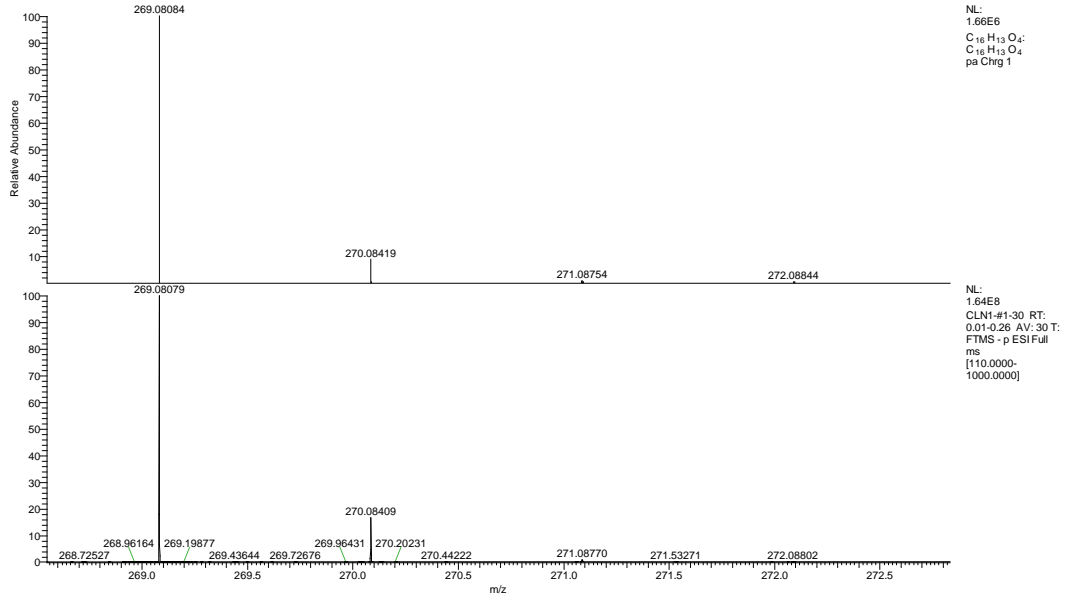


Fig. 3 UV-vis absorption spectra of CLN1 and a mixture of CLN1 and 5 equiv. amounts of TBAF in CH₂Cl₂ ($4.0 \times 10^{-5} \text{ mol} \cdot \text{L}^{-1}$) at 298 K.

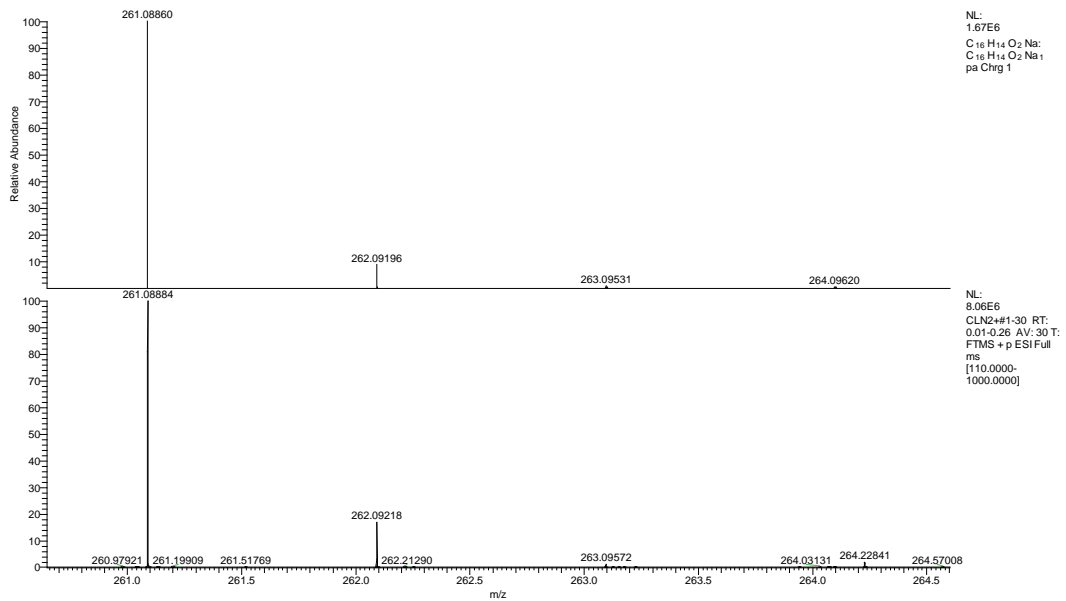
5. Mass spectra

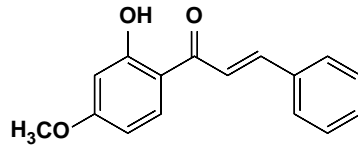


CLN1

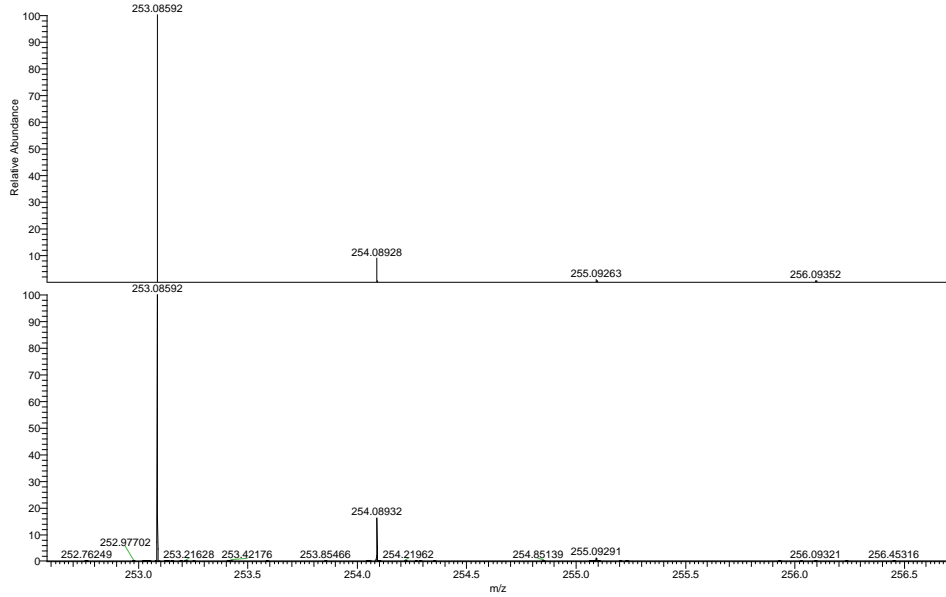


CLN2



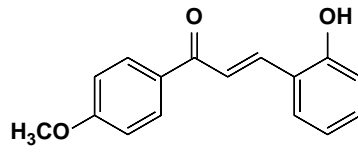


CLN3

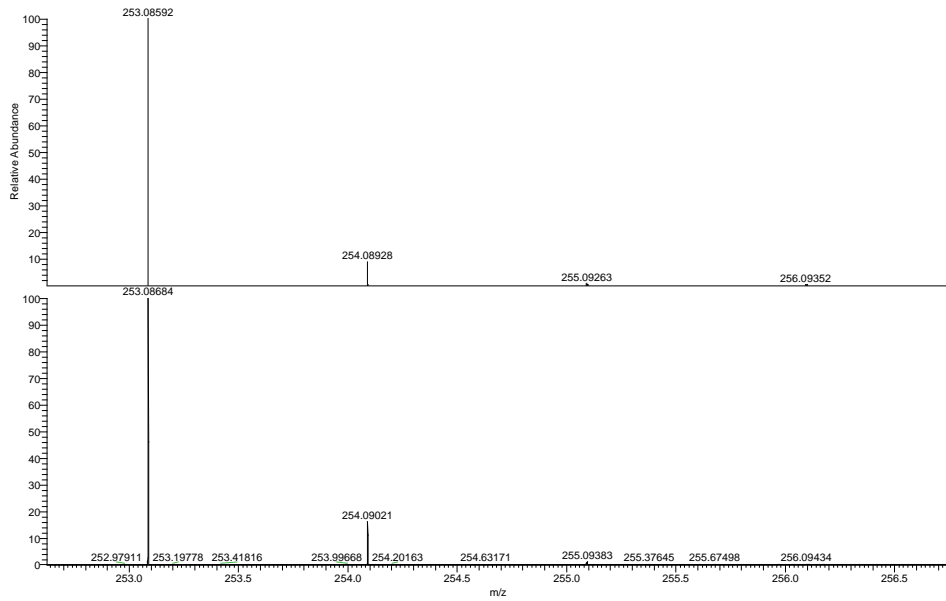


NL:
1.67E6
C₁₆H₁₃O₃⁺
C₁₆H₁₃O₃
pa Chrg 1

NL:
9.25E6
CLN3-#1-30 RT:
0.01-0.26 AV: 30 T:
FTMS - p ESI Full
ms
[110.0000-
1000.0000]

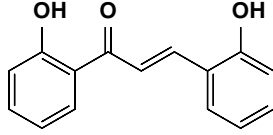


CLN4

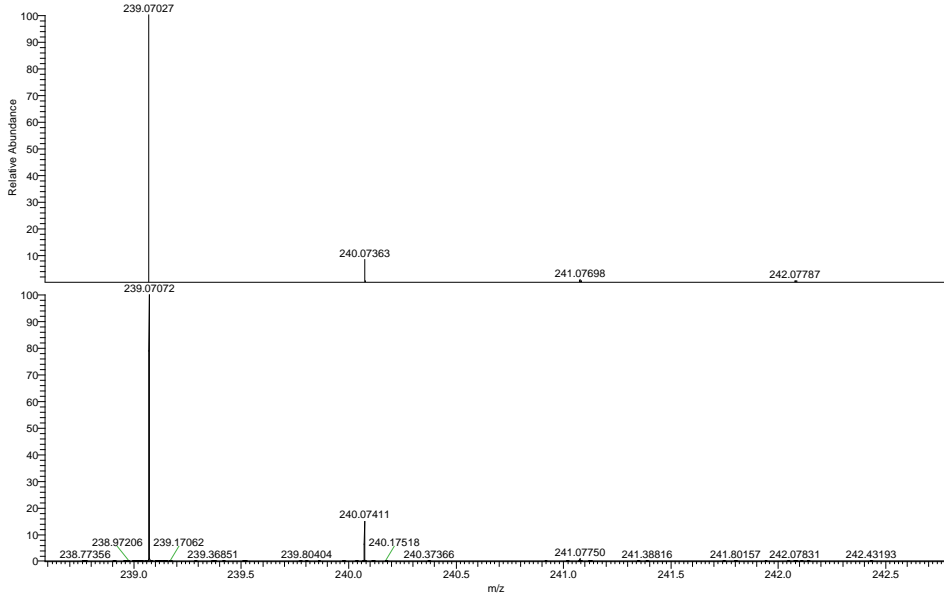


NL:
1.67E6
C₁₆H₁₃O₃⁺
C₁₆H₁₃O₃
pa Chrg 1

NL:
3.65E6
CLN4-#1-30 RT:
0.01-0.26 AV: 30 T:
FTMS - p ESI Full
ms
[110.0000-
1000.0000]

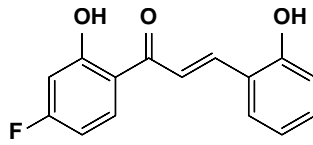


CLN5

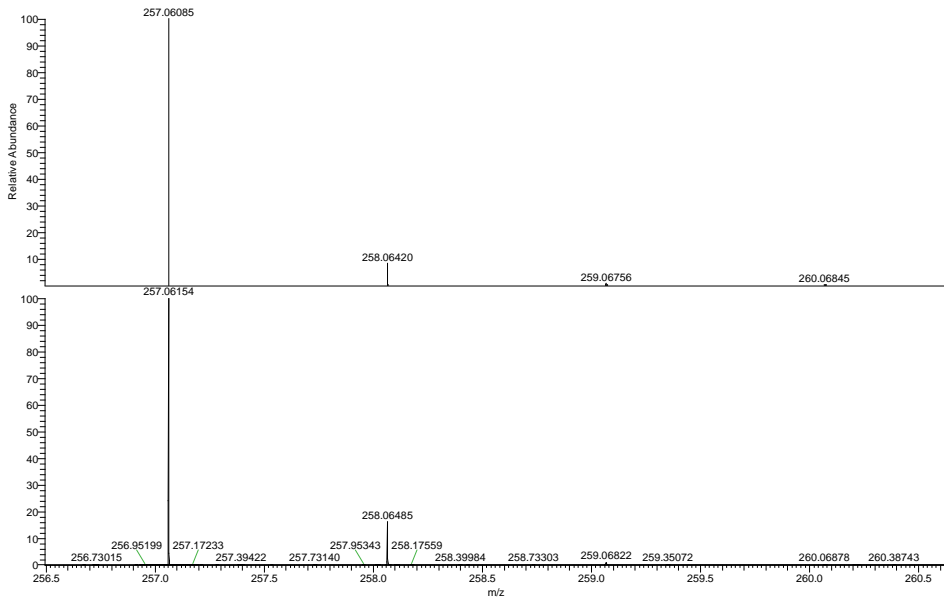


NL:
1.69E6
C₁₅H₁₁O₂
C₁₅H₁₁O₃
pa Chrg 1

NL:
4.74E7
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0.01-0.26 AV: 30 T:
FTMS - p ESI Full
ms
[110.0000-
1000.0000]



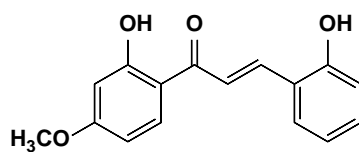
CLN6



NL:
1.69E6
C₁₅H₁₀O₃F
C₁₅H₁₀O₃F₁
pa Chrg 1

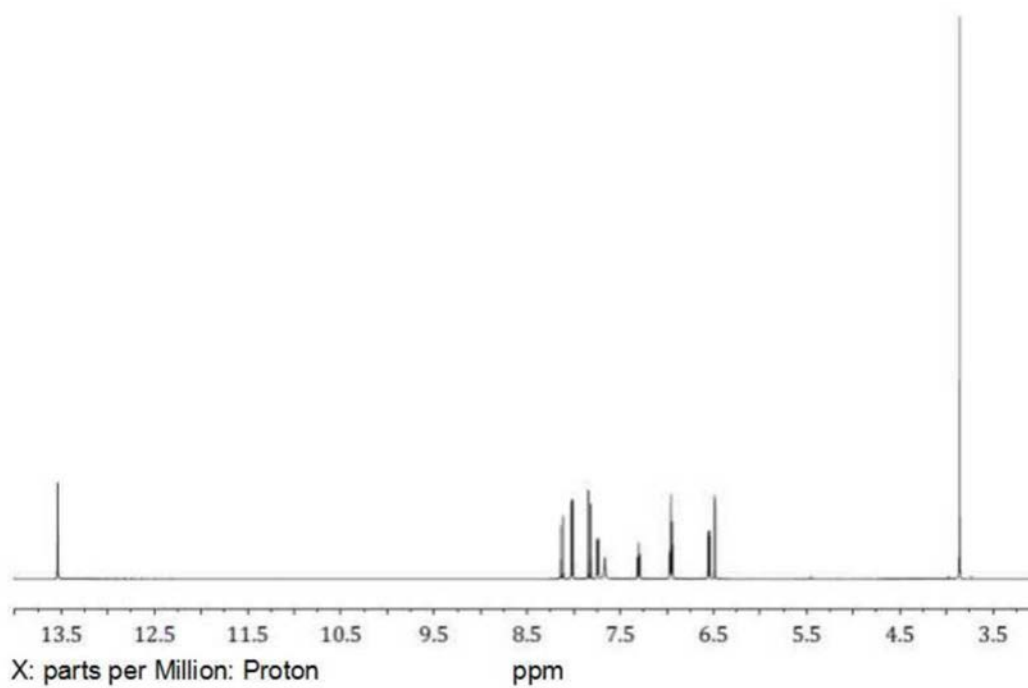
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CLN6-#1-30 RT:
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FTMS - p ESI Full
ms
[110.0000-
1000.0000]

6. ^1H and ^{13}C NMR spectra

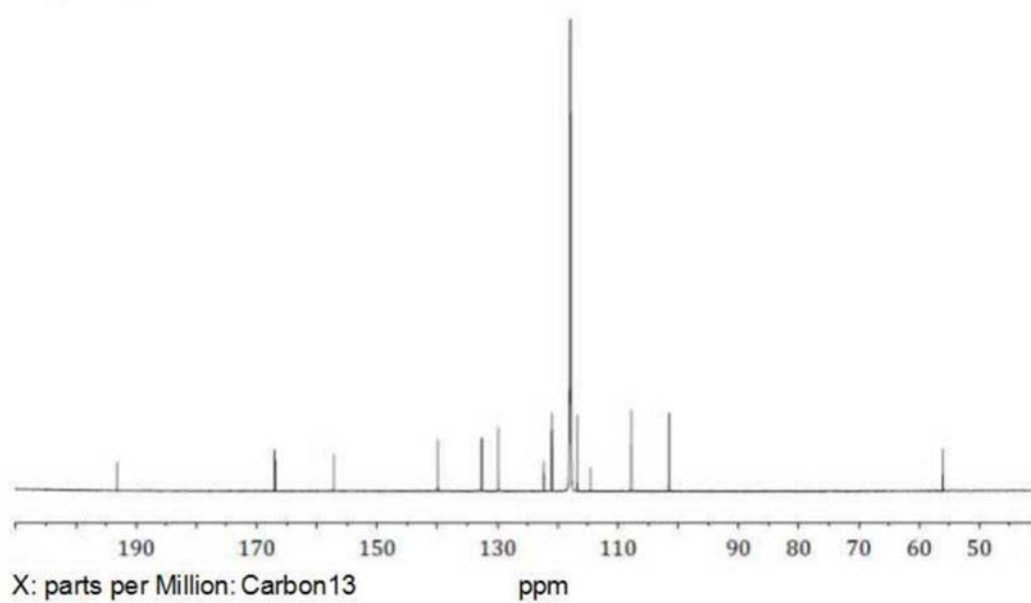


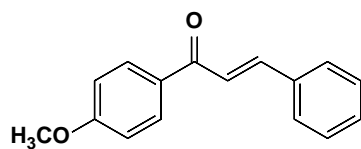
CLN1

^1H NMR (600 MHz, CD_3CN , 293 K)



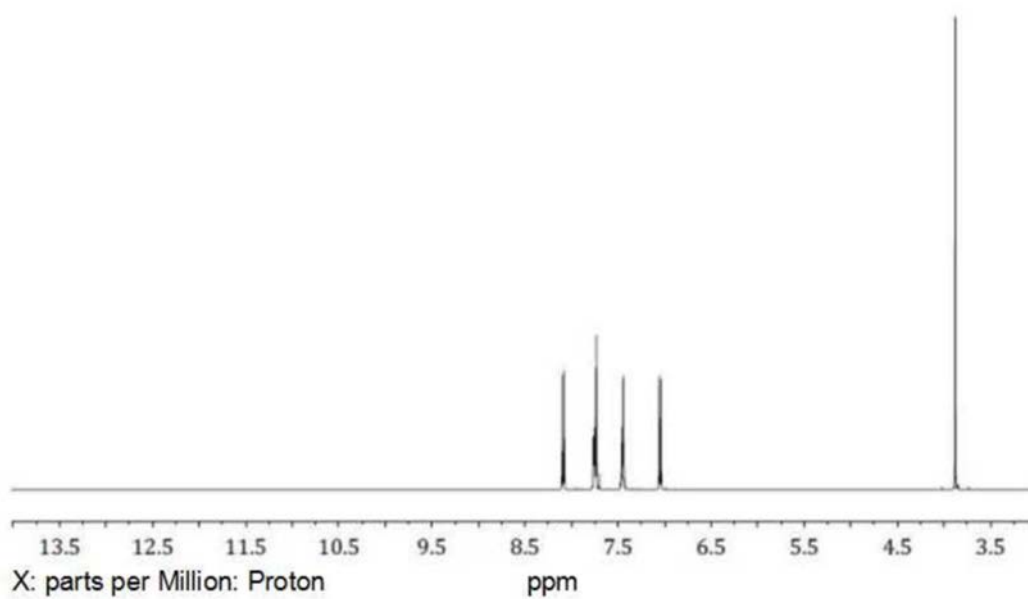
^{13}C NMR (150 MHz, CD_3CN , 293 K)



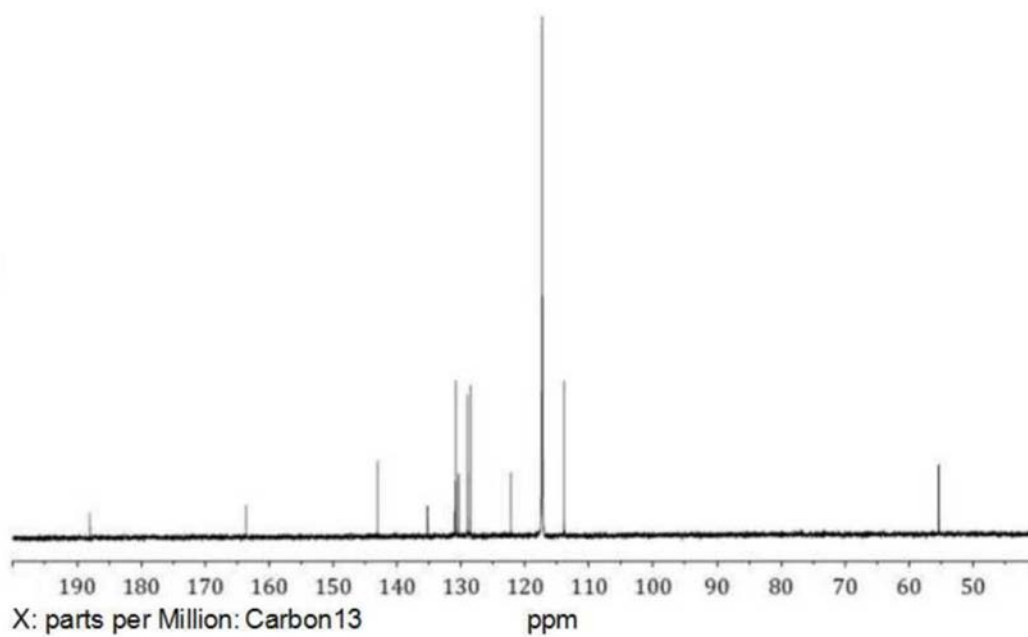


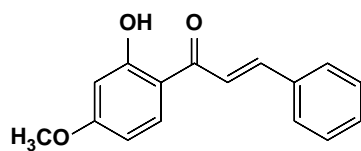
CLN2

^1H NMR (500 MHz, CD_3CN , 293 K)



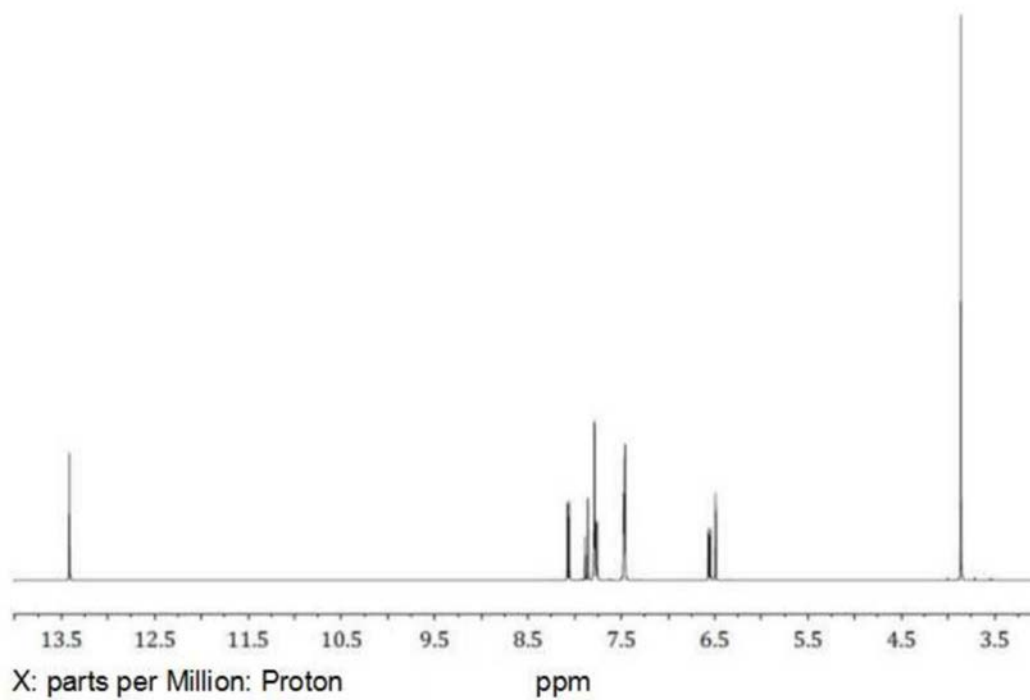
^{13}C NMR (125 MHz, CD_3CN , 293 K)



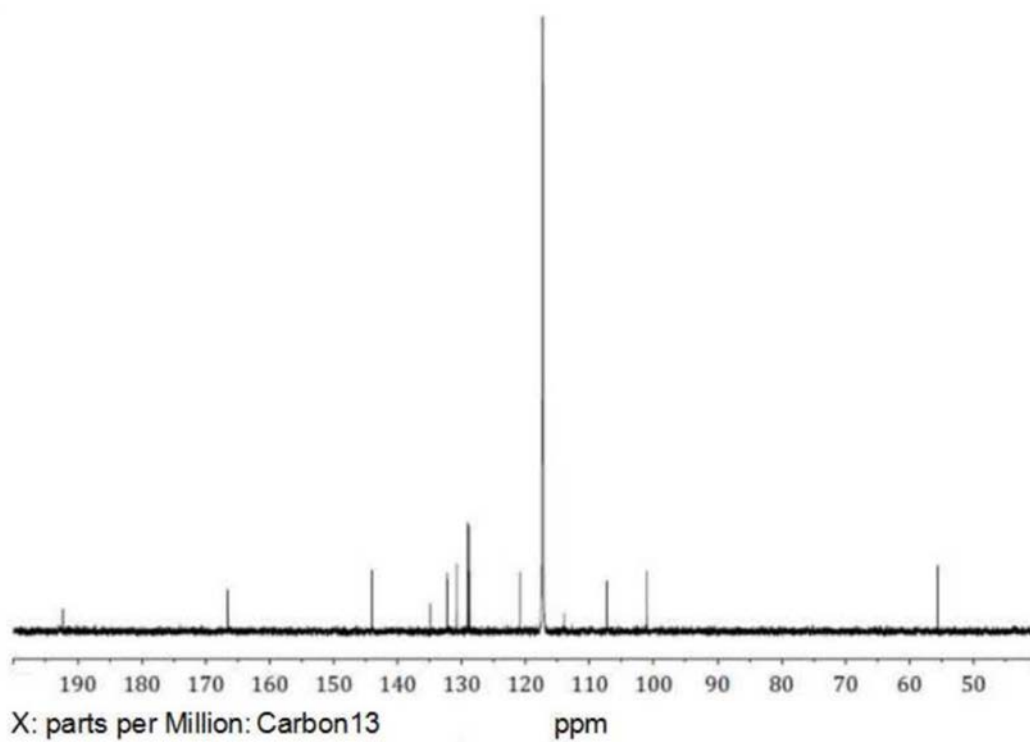


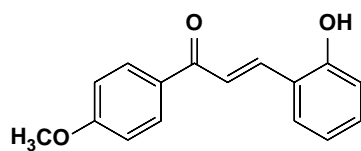
CLN3

^1H NMR (500 MHz, CD_3CN , 293 K)



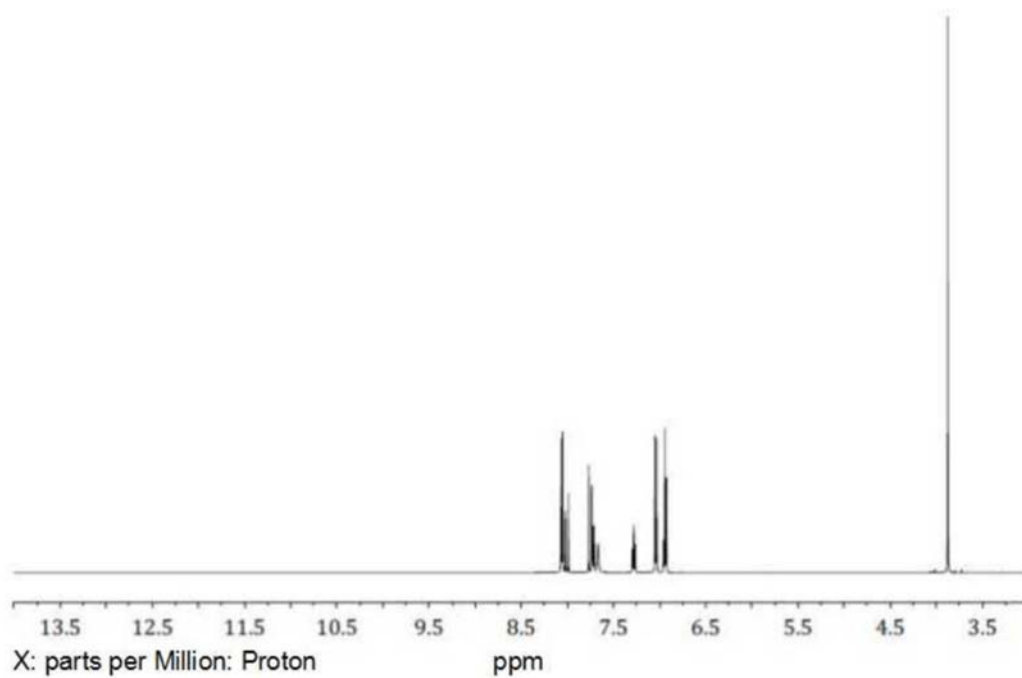
^{13}C NMR (125 MHz, CD_3CN , 293 K)



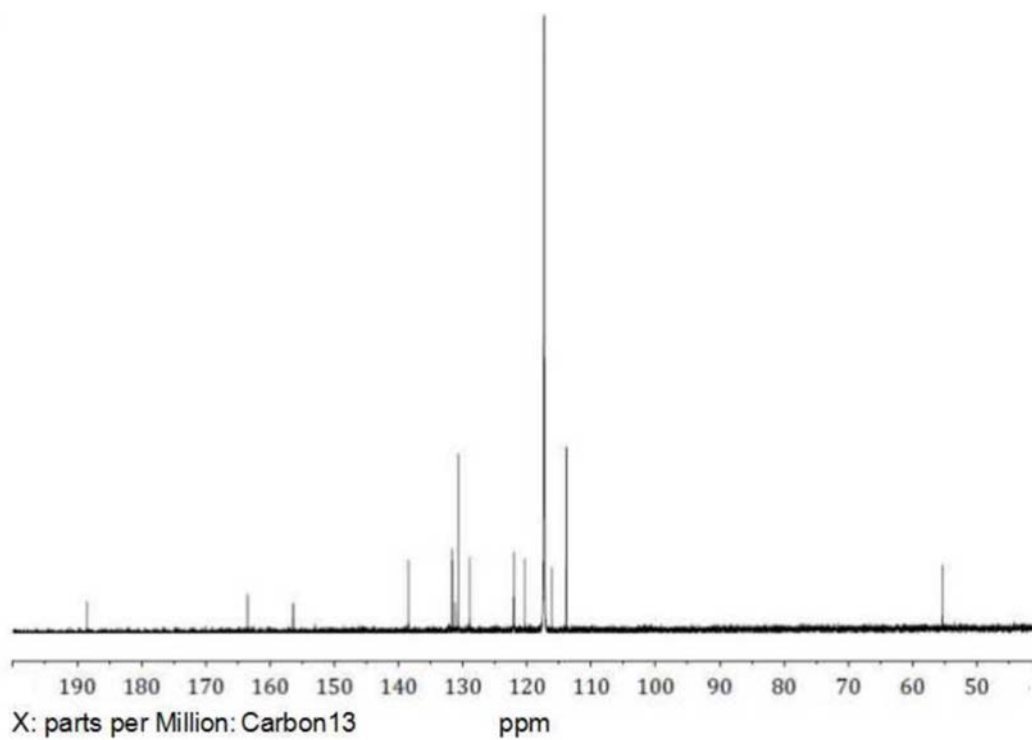


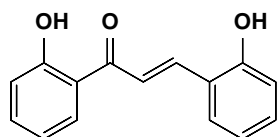
CLN4

^1H NMR (600 MHz, CD_3CN , 293 K)



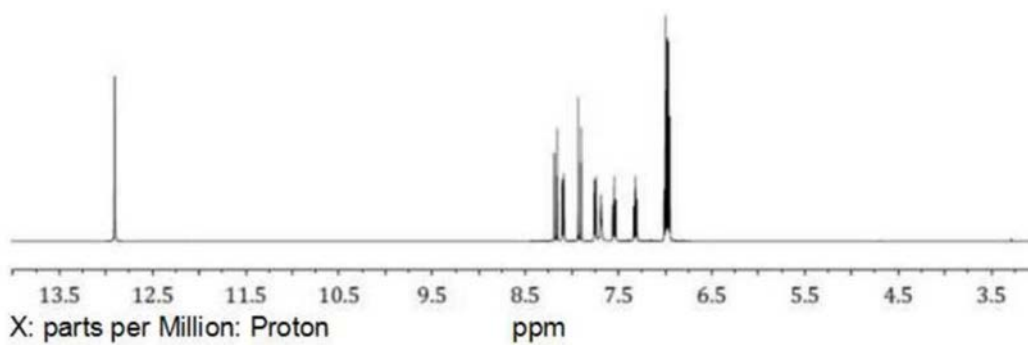
^{13}C NMR (150 MHz, CD_3CN , 293 K)



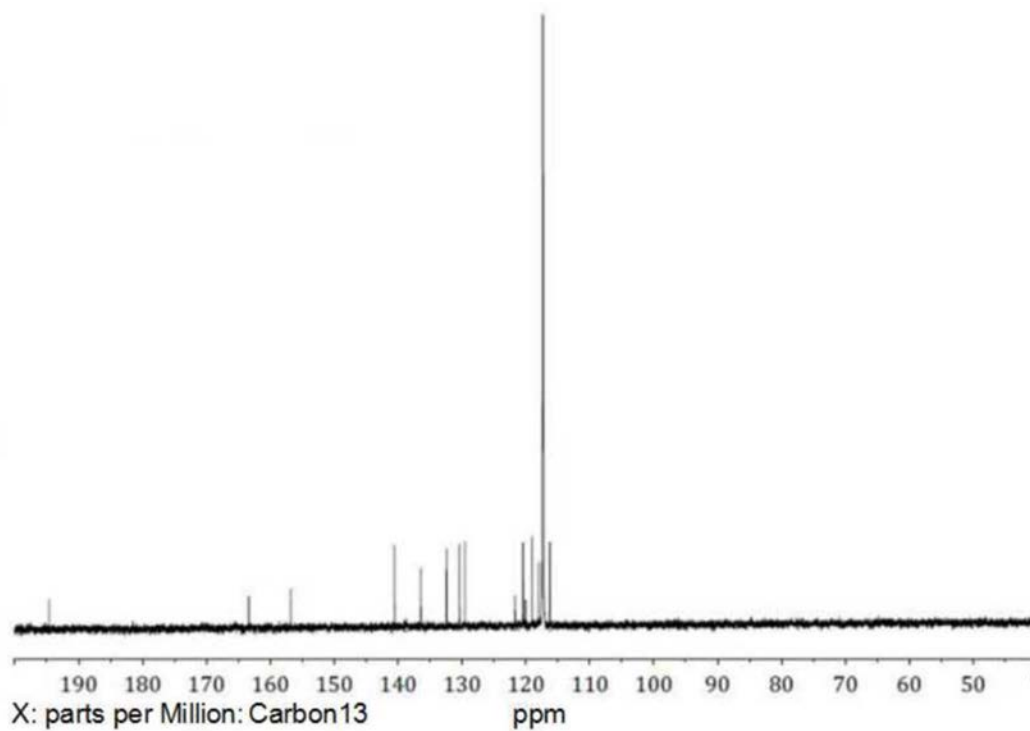


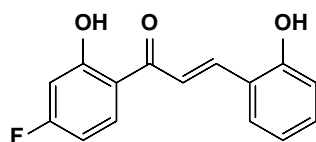
CLN5

^1H NMR (500 MHz, CD_3CN , 293 K)



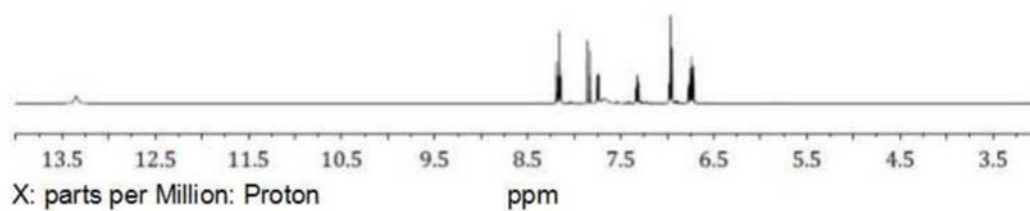
^{13}C NMR (125 MHz, CD_3CN , 293 K)





CLN6

^1H NMR (500 MHz, CD_3CN , 293 K)



^{13}C NMR (125 MHz, CD_3CN , 293 K)

