Supporting Information

A selective chromogenic molecular sensor for acetate anion in mixed acetonitrile/water media

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1. Titration of **1, 2, 3** with $[Me_4N]OH$ in MeCN solution.
2. Titration of **2** with anions in MeCN solution.
3. Titration of **1, 3** with anions in MeCN solution.
4. Titration of **2** with a mixture of F^-, AcO^- and $H_2PO_4^-$ in MeCN/H_2O solution.
5. Titration of **2** with anions in $CHCl_3$ solution.
6. Titration of **2** with AcO^- in $CHCl_3$/EtOH solution.
7. MS (ESI) spectra of **1, 2** and **3**.
8. ^1H NMR spectra of **1, 2** and **3.**
9. ^{13}C NMR spectra of **1** and **3.**
10. IR spectra of **2.**

1. Titration of 1,2,3 with $[Me_4N]OH$ in MeCN solution

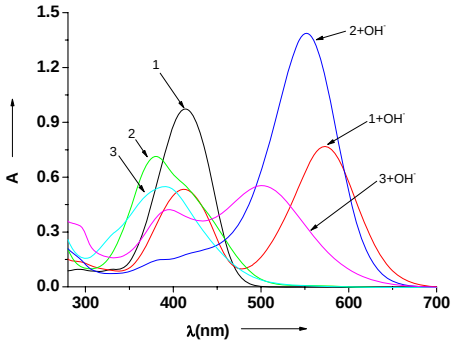


Fig. S1 Changes in the UV/vis absorption spectra of **1, 2, 3** (2.5×10^{-5} M) in MeCN solution upon addition of 20 equiv of $[Me_4N]OH$.

2. Titration of 2 with anions in MeCN solution

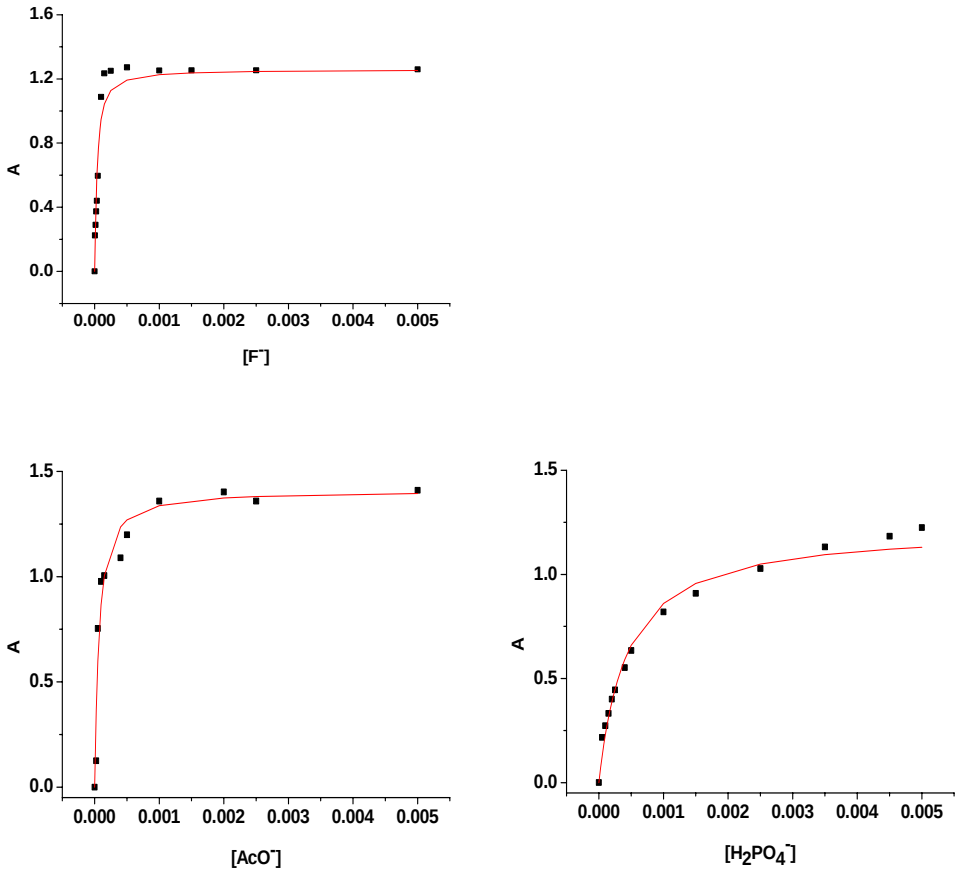
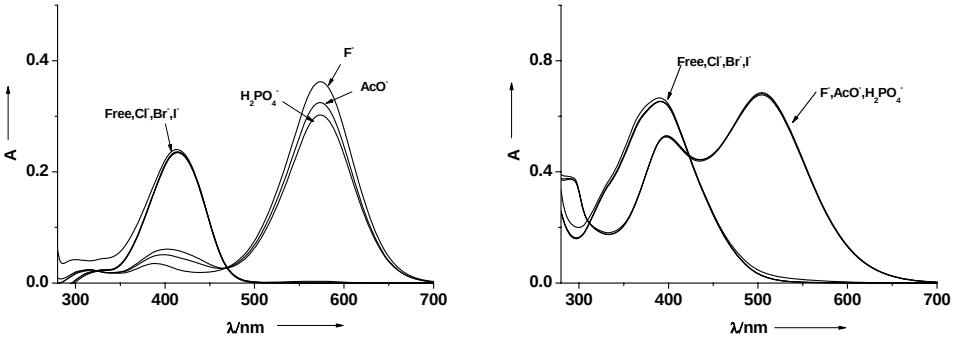


Fig. S2 The changes of absorption band centered at 552 nm as a function of $[F^-]$, $[AcO^-]$, $[H_2PO_4^-]$, red line represents calculated results. [**2**] was 2.5×10^{-5} M.

3. Titration of 1, 3 with anions in MeCN solution



a b

Fig. S3 a) Changes in the UV/vis absorption spectrum of **1** (2.5×10^{-6} M) in MeCN solution upon addition of 100 equiv of anions. b) Changes in the UV/vis absorption spectrum of **3** (5×10^{-5} M) in MeCN solution upon addition of 50 equiv of anions.

4. Titration of 2 with a mixture of F^-, AcO^- and $H_2PO_4^-$ in MeCN/H_2O solution

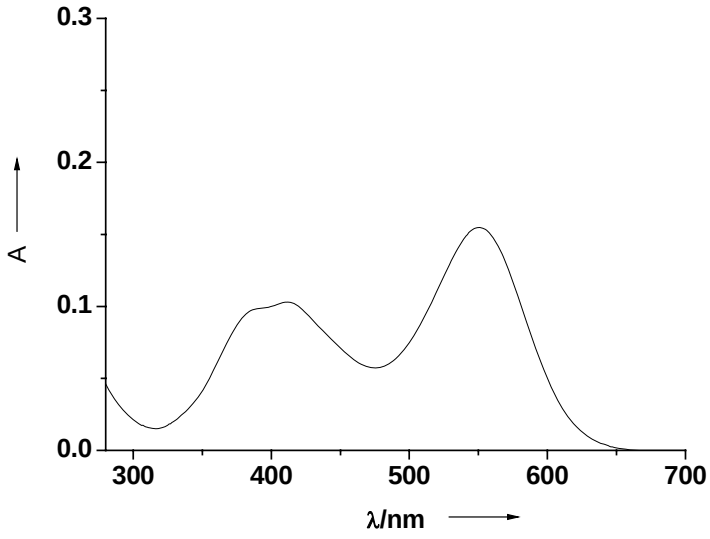


Fig. S4 Changes in the UV/vis absorption spectrum of **2** (6.25×10^{-6} M) in acetonitrile/water (90:10, v/v) solution upon addition of 200 equiv of F^-, AcO^- and $H_2PO_4^-$.

5. Titration of 2 with anions in $CHCl_3$ solution

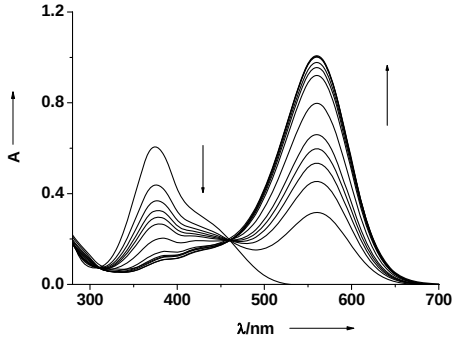


Fig. S5a UV/vis titration of **2** (2.5×10^{-5} M) in $CHCl_3$ solution upon addition of AcO^- (from 0 to 100 equiv).

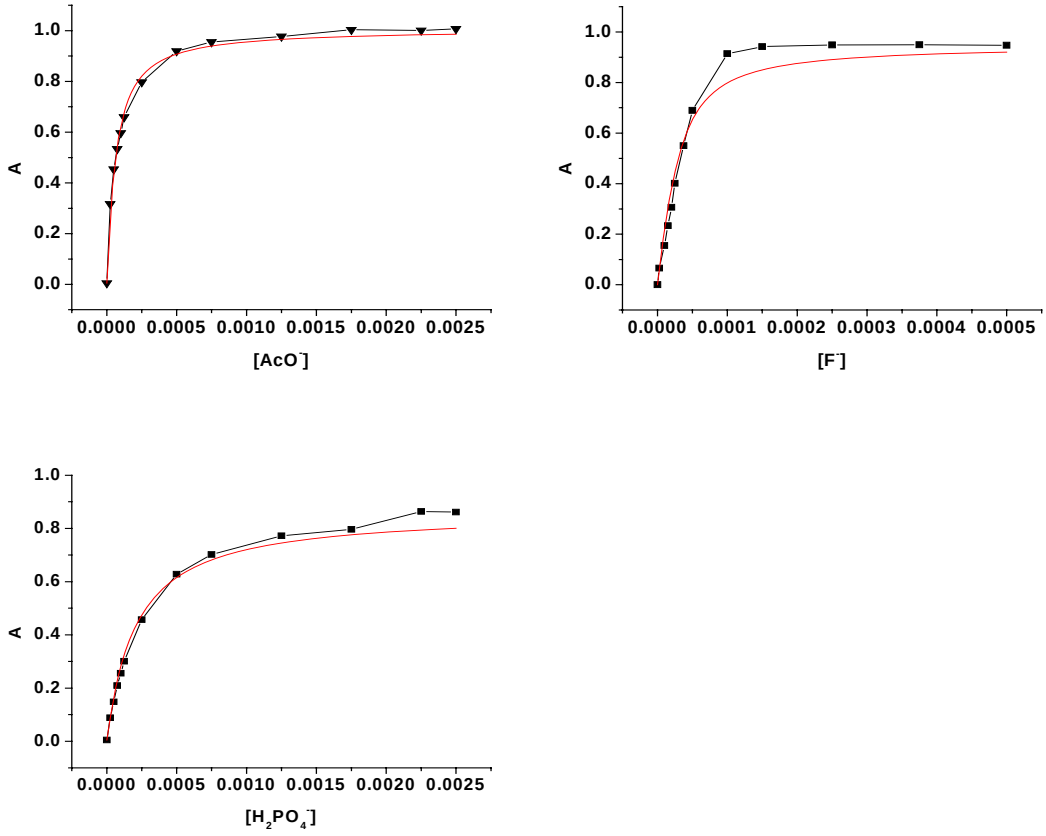
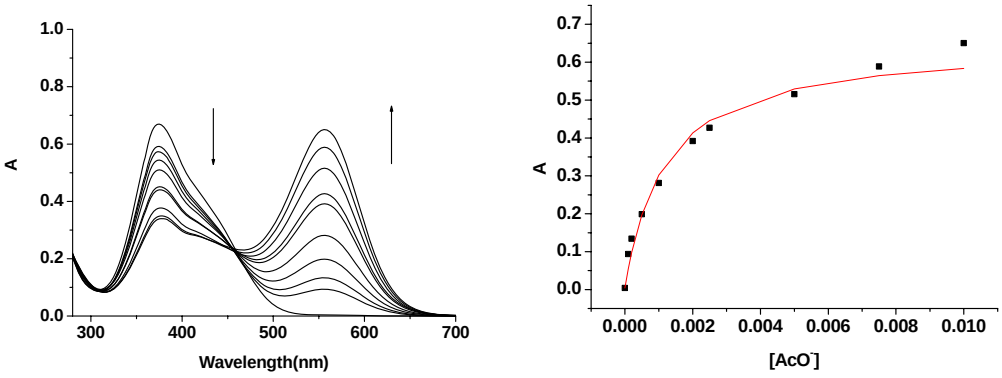


Fig. S5b The changes of absorption band centered at 560 nm as a function of [F^-], [AcO^-], [$H_2PO_4^-$], red line represents calculated results. [**2**] was 2.5×10^{-5} M. The equilibrium constant was calculated to be $(6.68\pm1)\times10^4$ M^{-1} for F^-, $1.90\times10^4\pm901$ M^{-1} for AcO^- and $5.10\times10^3\pm341$ M^{-1} for $H_2PO_4^-$.

6. Titration of 2 with AcO^- in $CHCl_3$/EtOH solution

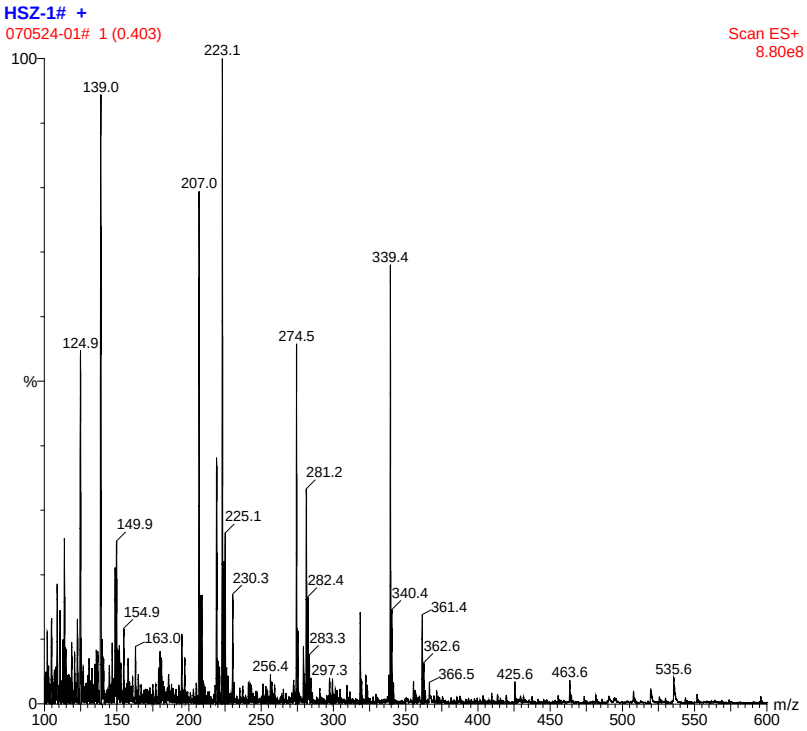


(a) (b)

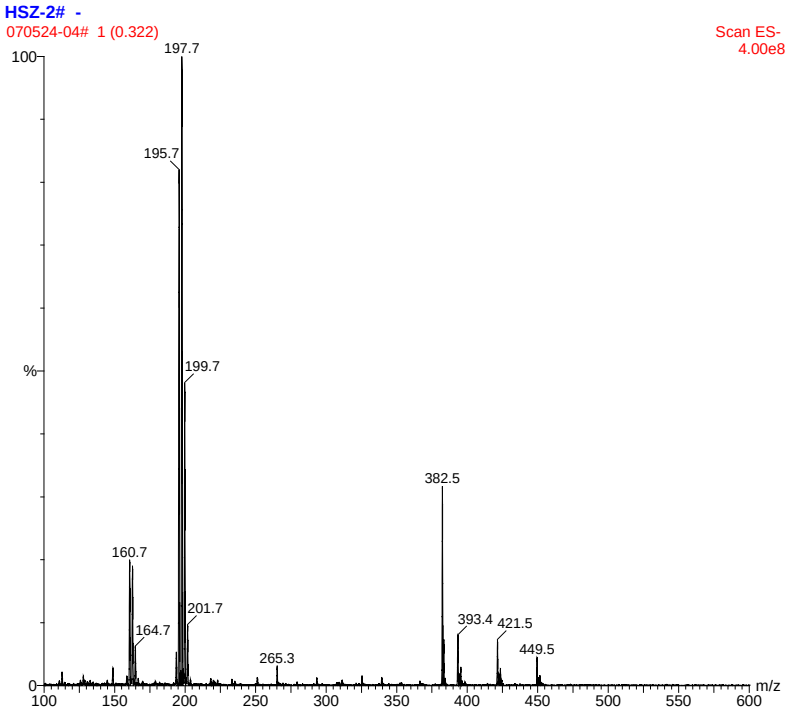
Fig. S6 (a) Changes in the UV-vis absorption spectrum of **2** in 1:1 $CHCl_3$/EtOH solution (2.5×10^{-5} M) upon addition of AcO^- (0-100 equiv); (b) the changes of absorption band centered at 560 nm as a function of [AcO^-], red line represents calculated results.

7. MS (ESI) spectra of 1, 2 and 3

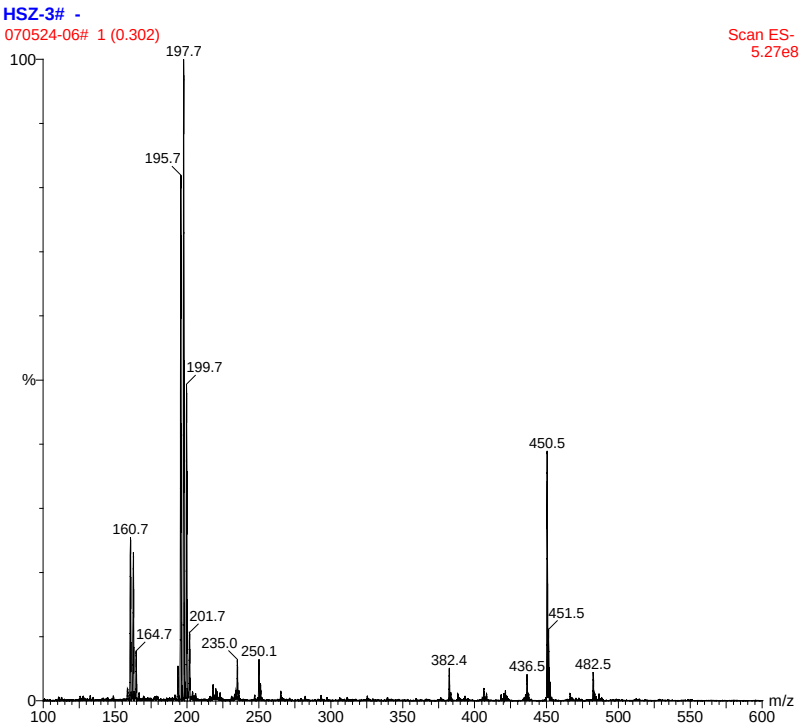
MS (ESI) spectra of 1



MS (ESI) spectra of 2

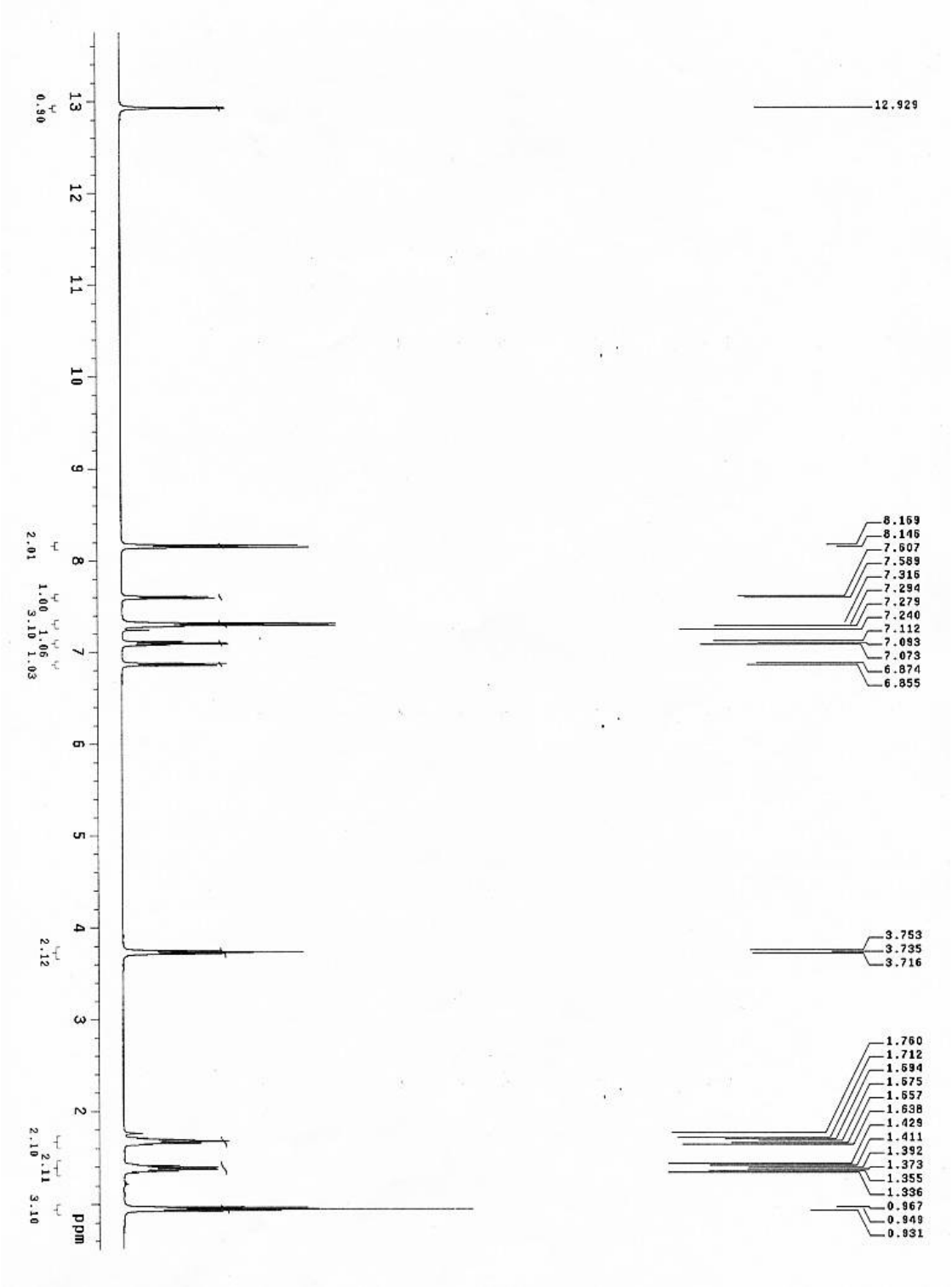


MS (ESI) spectra of 3

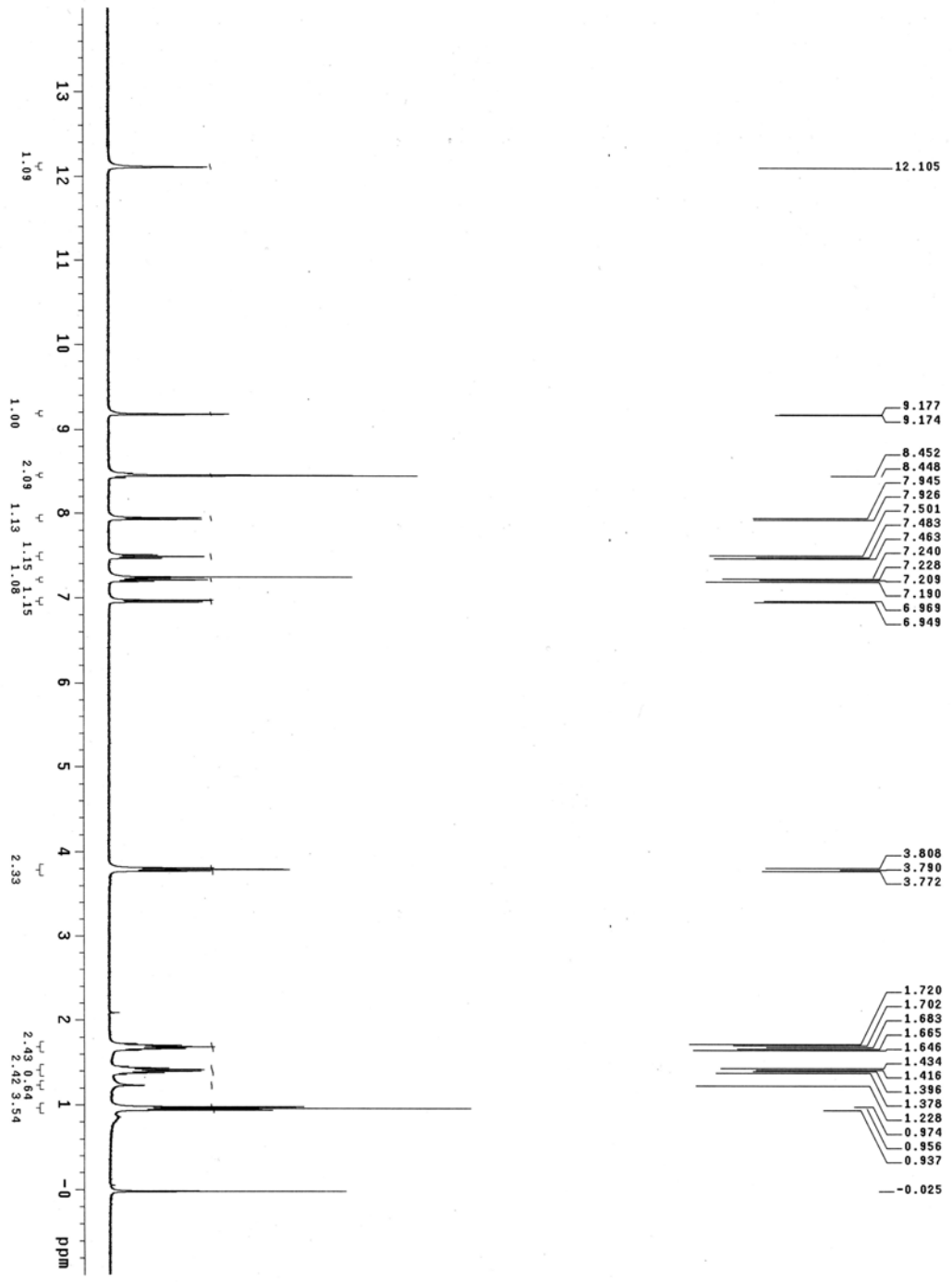


8. ^{1}H NMR spectra of 1, 2 and 3

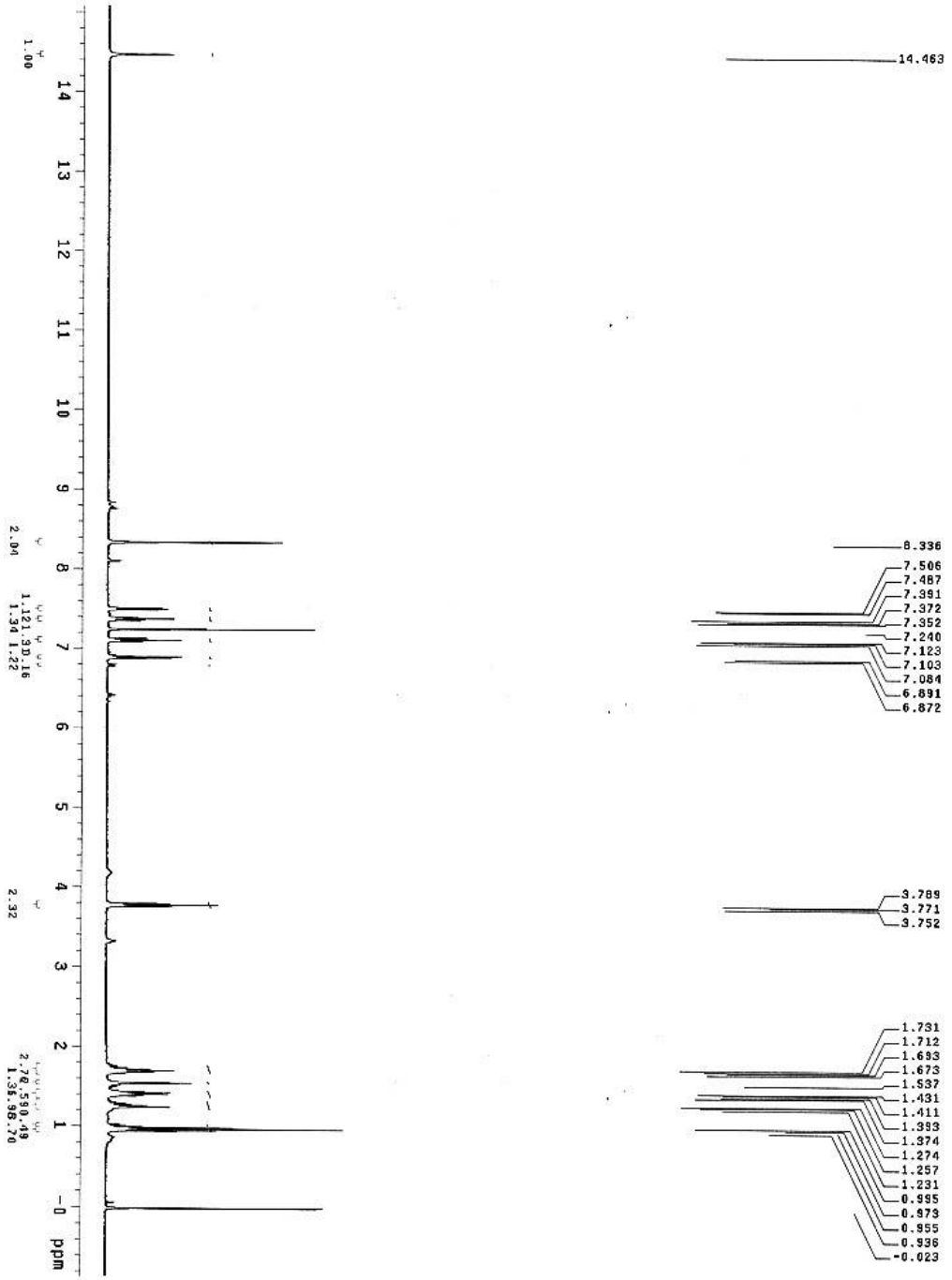
^{1}H NMR spectra of 1 ($CDCl_3$, 400 MHz)



^{1}H NMR spectra of 2 ($CDCl_3$, 400 MHz)

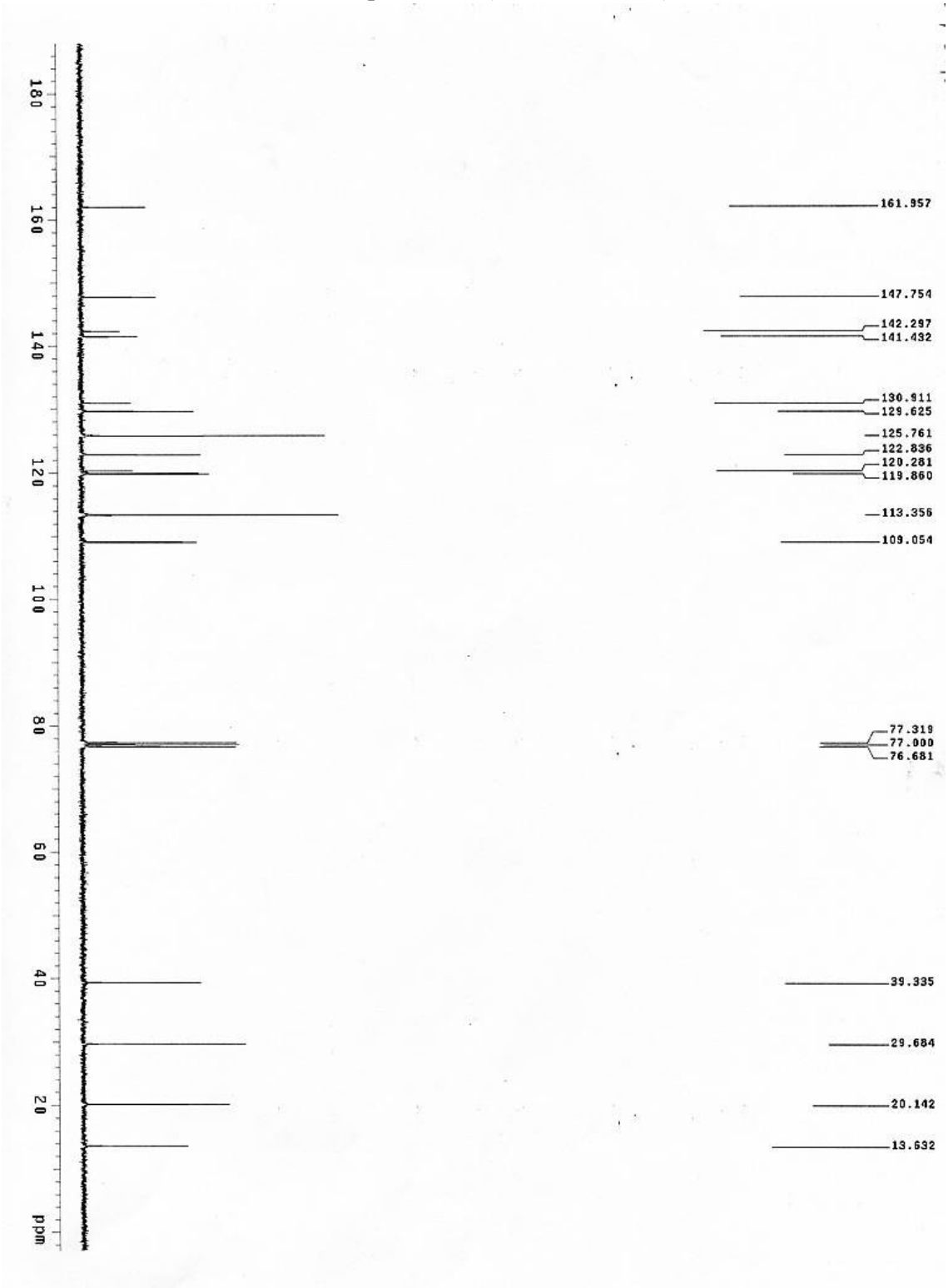


^{1}H NMR spectra of 3 ($CDCl_3$, 400 MHz)

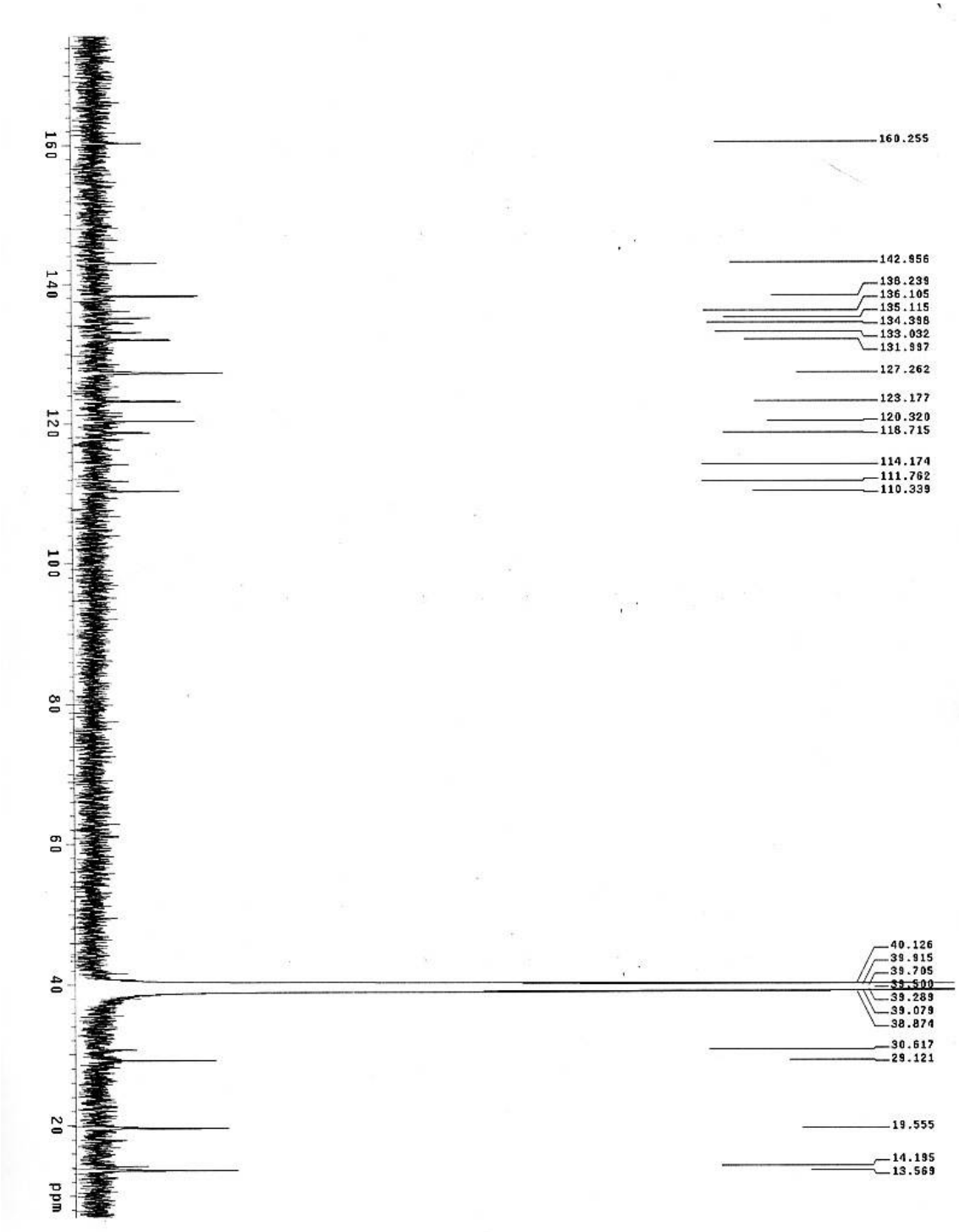


9. ^{13}C NMR spectra of 1 and 3

^{13}C NMR spectra of 1 ($CDCl_3$, 400 MHz)



^{13}C NMR spectra of 3 (DMSO-d_6, 400 MHz)



10. IR spectra of 2