

## *Electronic Supplementary Information*

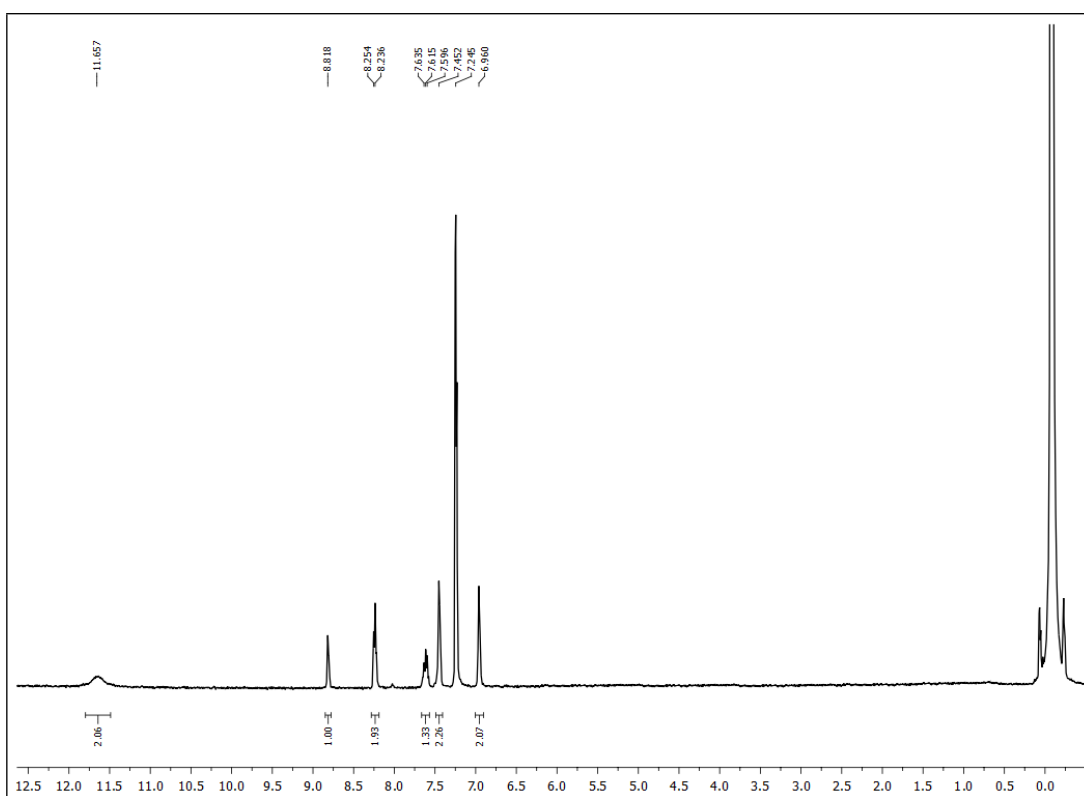
### **A Series of Ditopic Receptors for Succinic Acid Binding**

Swapan Dey,<sup>\*a</sup> Dibyendu Sain,<sup>a</sup> Ashish Kumar<sup>a</sup> and Chanda Kumari.<sup>a</sup>

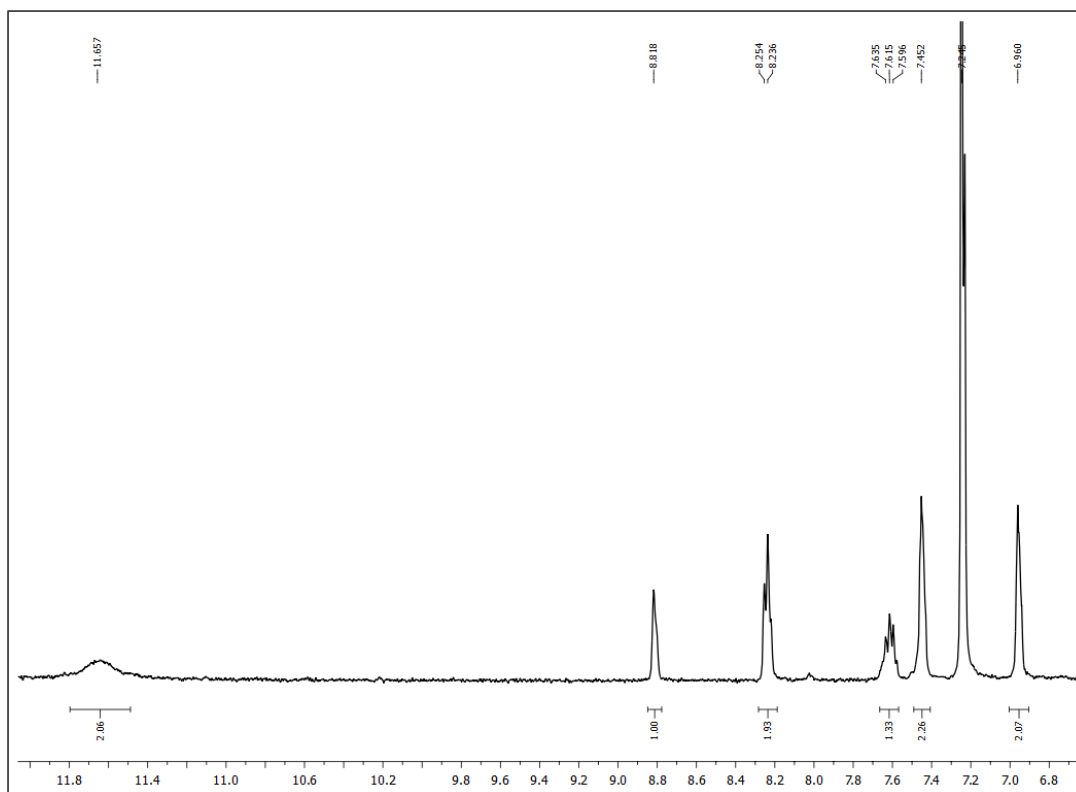
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*Ph: +913262235607, Fax: +913262296563, E-mail: [dey.s.ac@ismdhanbad.ac.in](mailto:dey.s.ac@ismdhanbad.ac.in)*

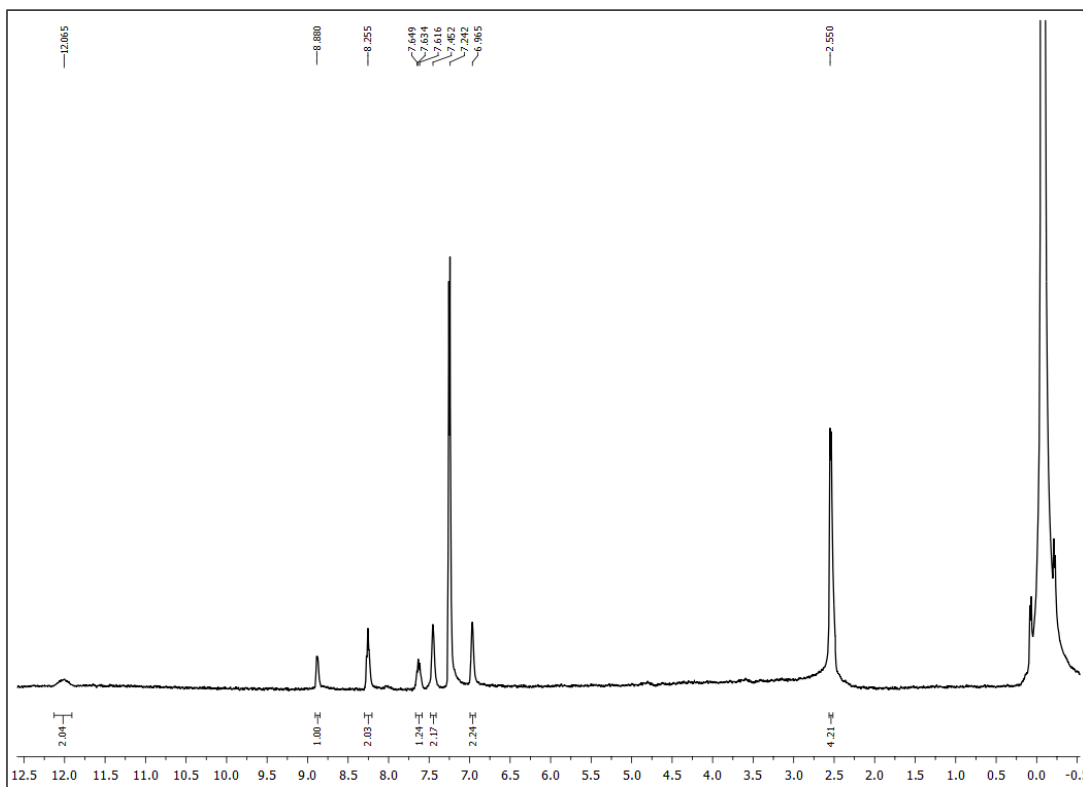
#### **<sup>1</sup>H NMR spectra of R1:**



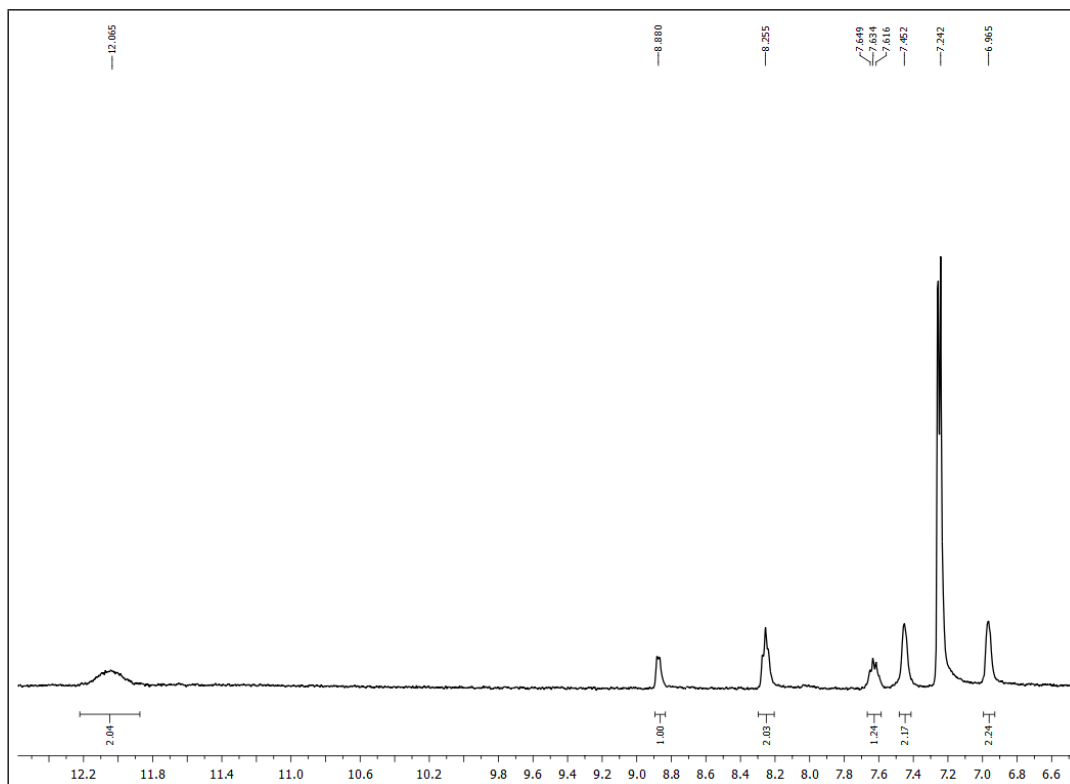
**$^1\text{H}$  NMR spectra of R1 (expanded form):**



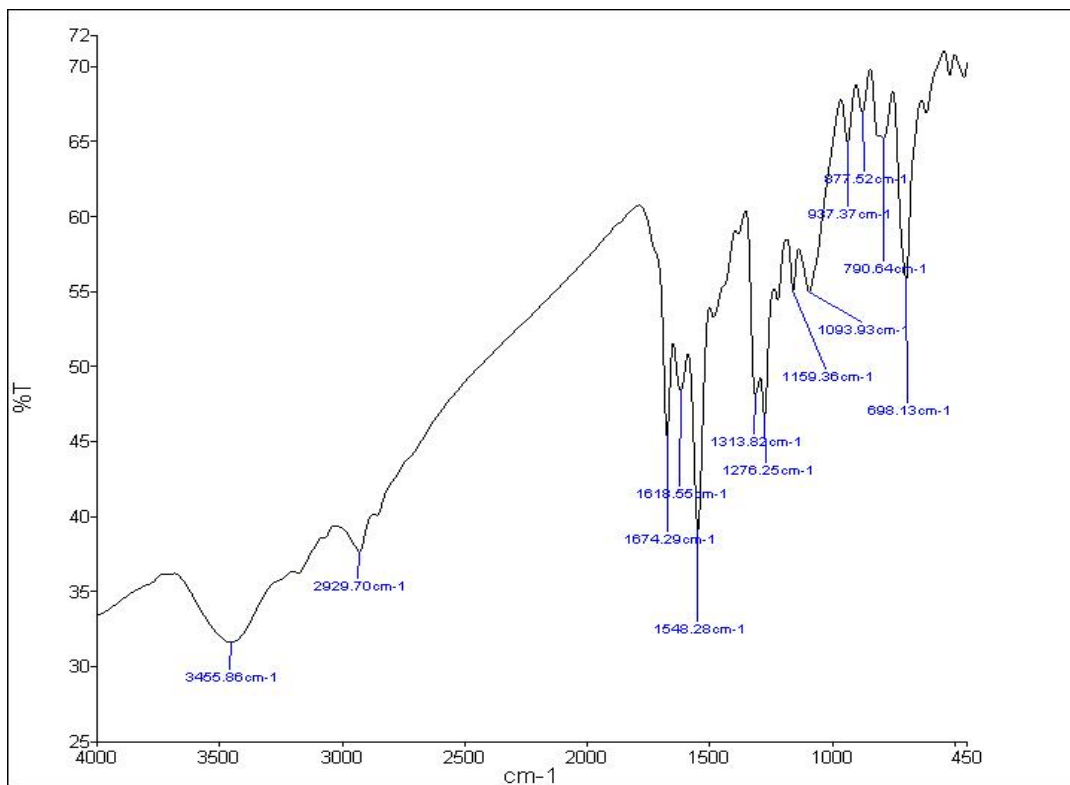
**$^1\text{H}$  NMR spectra of R1-succinic acid complex (1:1):**



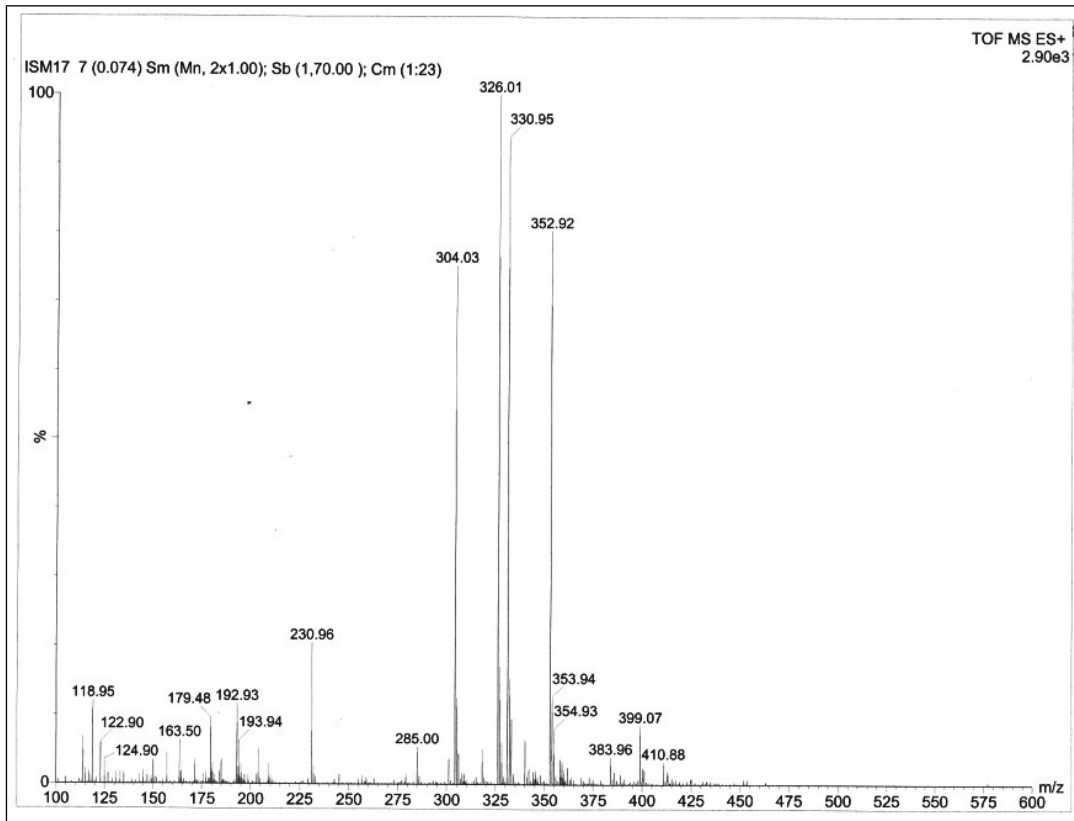
**<sup>1</sup>H NMR spectra of R1-succinic acid complex (1:1) (expanded form):**



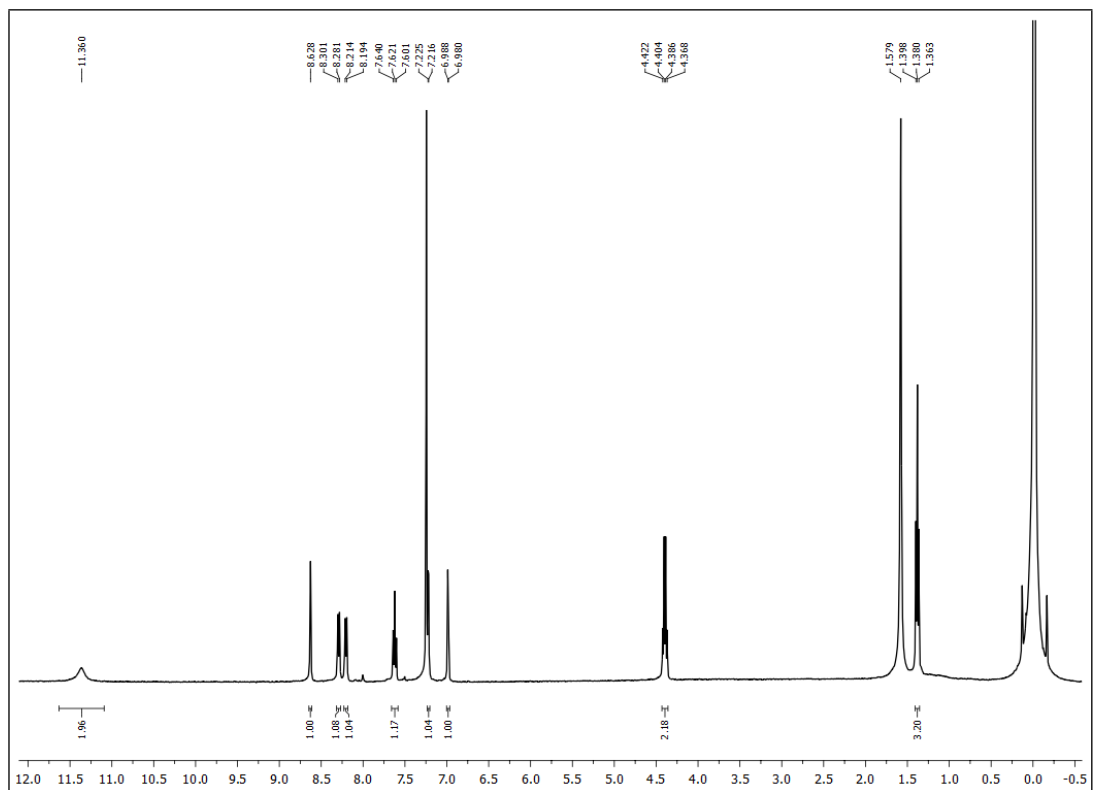
**IR spectra of R1:**



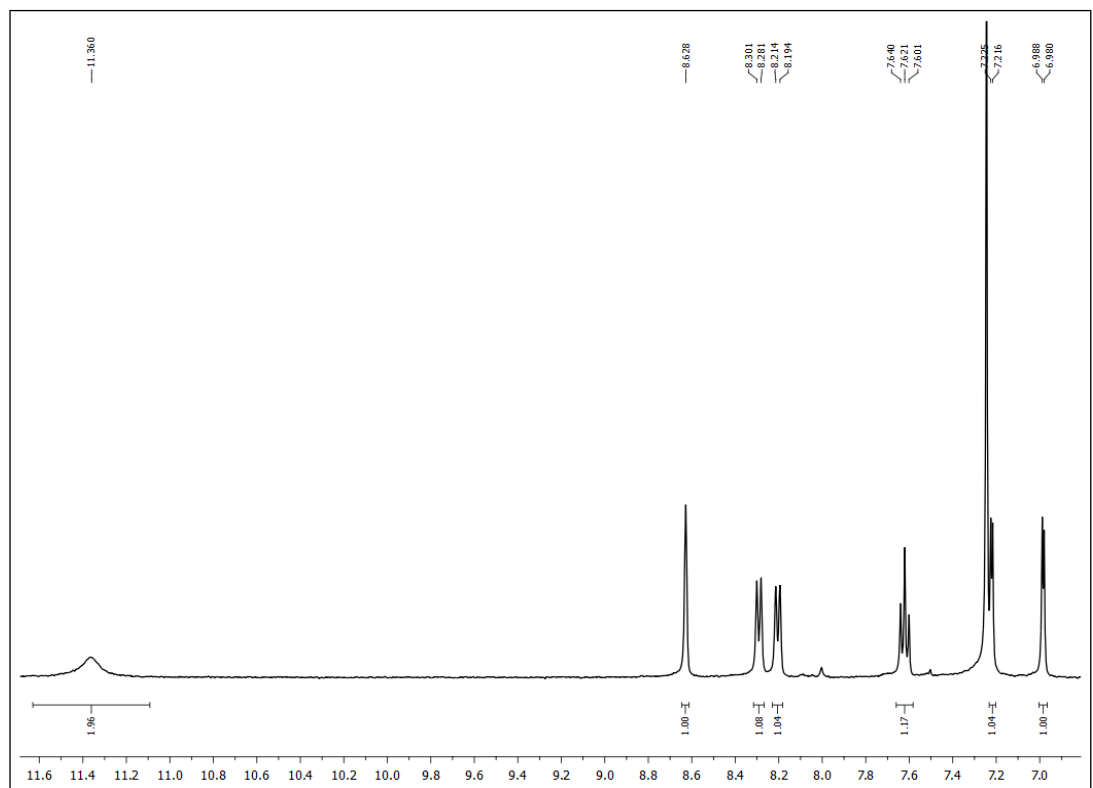
# Mass spectra of R1:



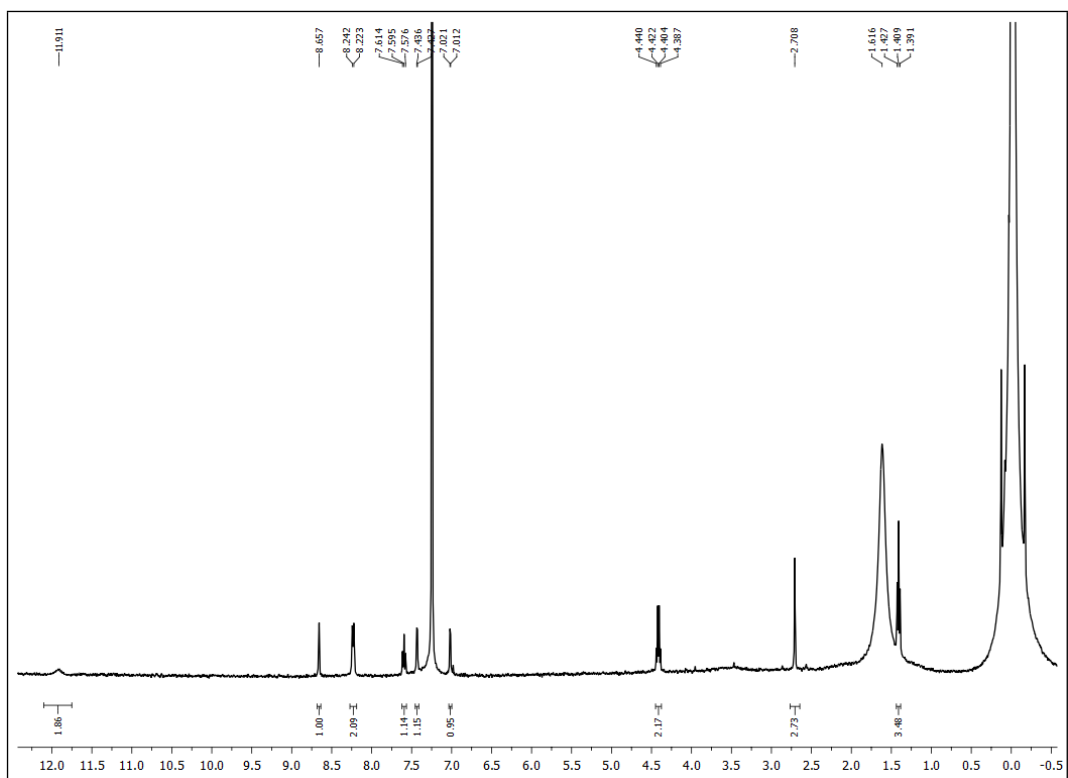
### <sup>1</sup>H NMR spectra of R2:



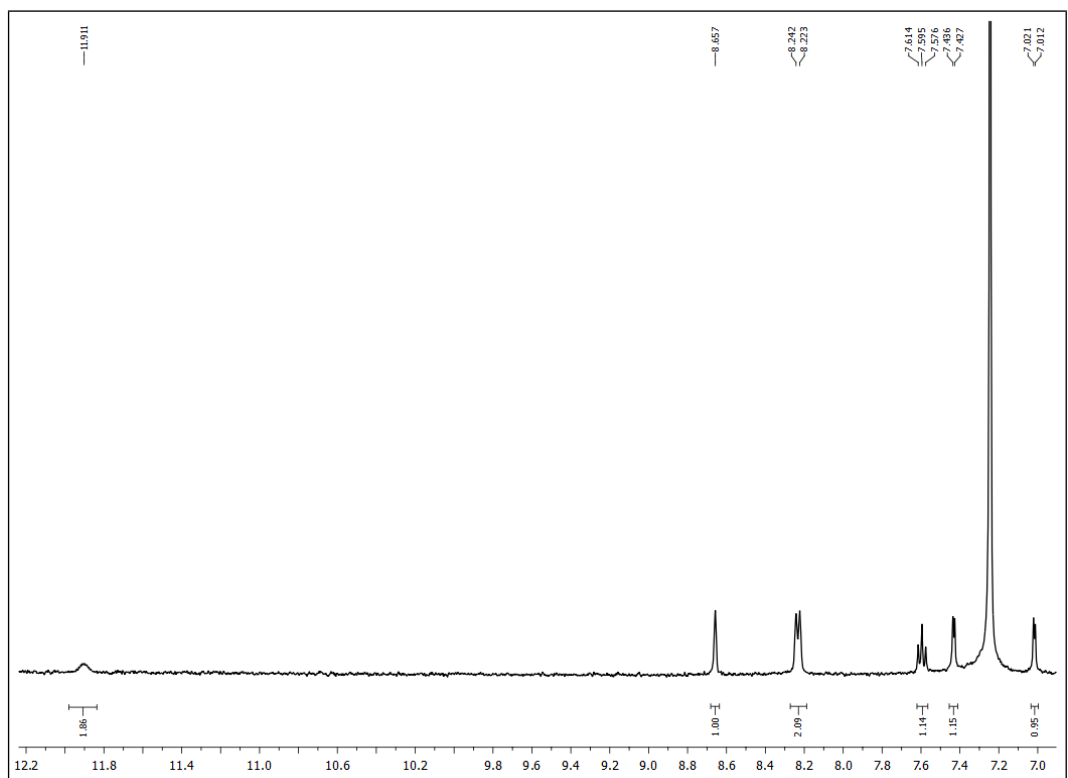
### <sup>1</sup>H NMR spectra of R2 (expanded form):



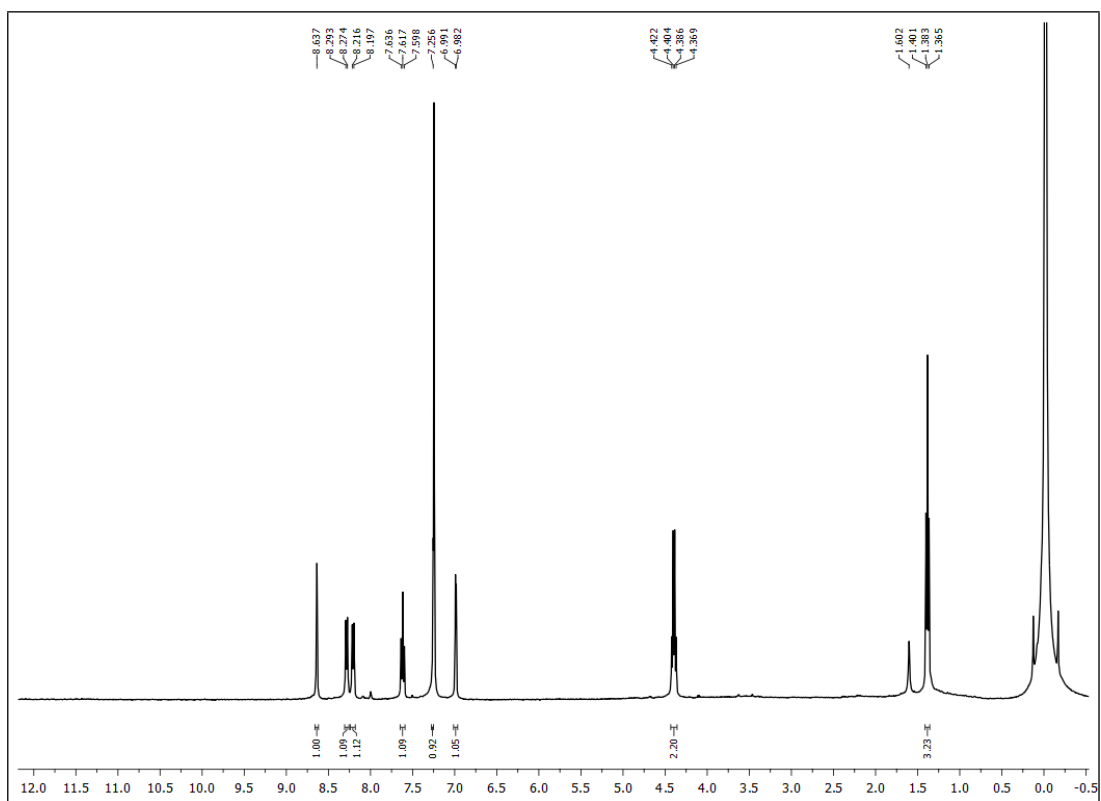
### $^1\text{H}$ NMR spectra of R2-succinic acid complex (1:1):



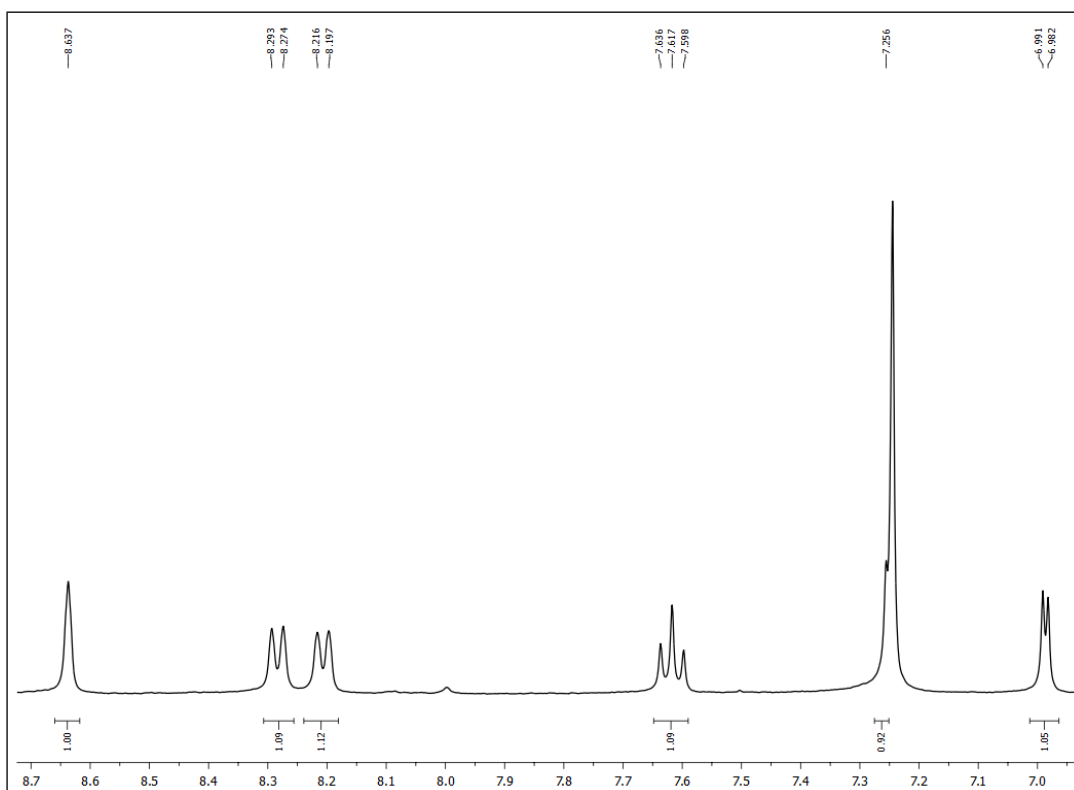
### $^1\text{H}$ NMR spectra of R2-succinic acid complex (1:1) (expanded form):



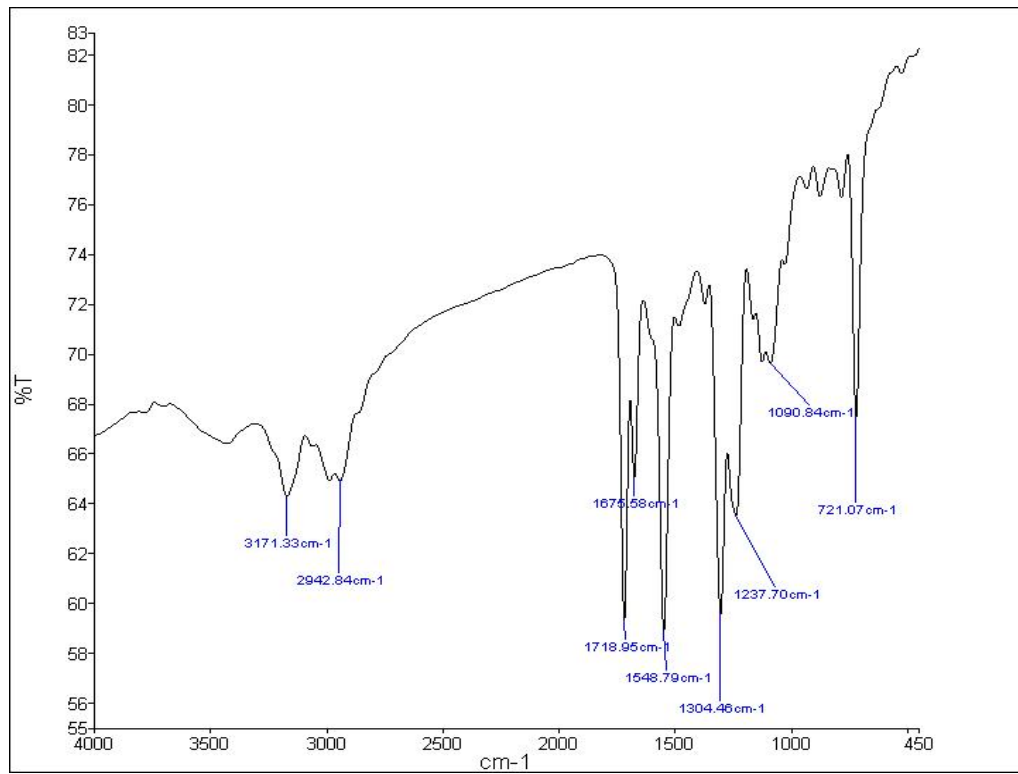
**$^1\text{H}$  NMR spectra of R2 after  $\text{D}_2\text{O}$  exchange:**



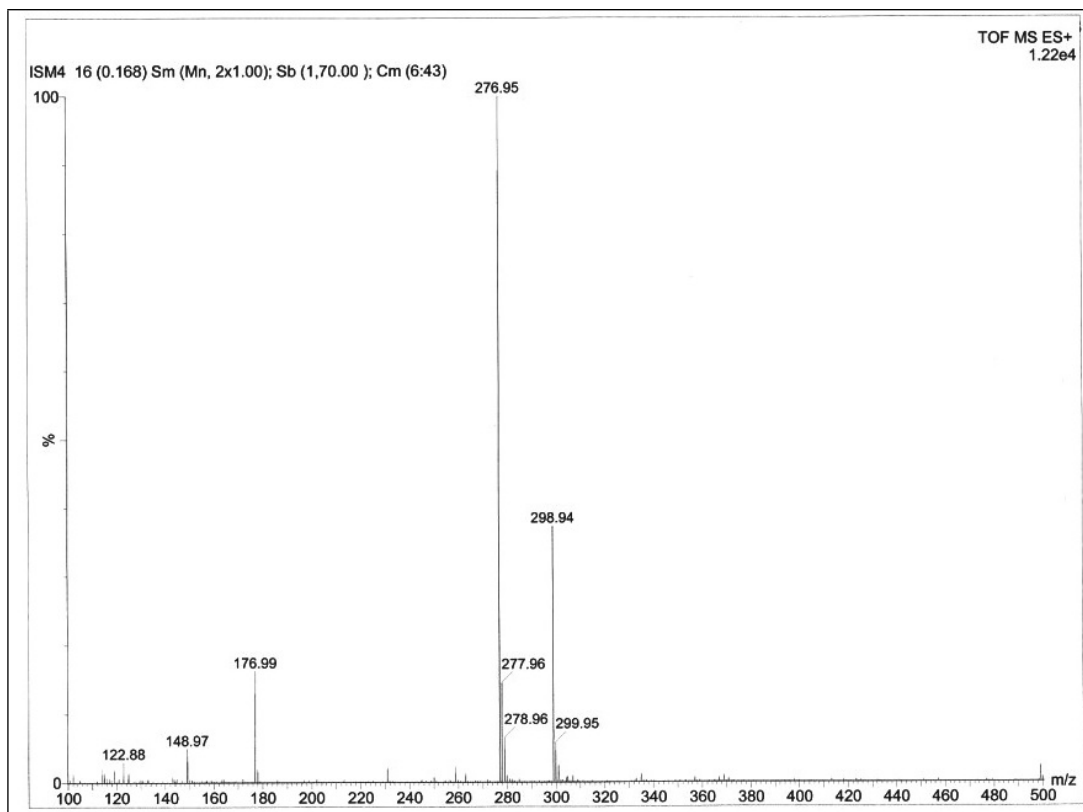
**$^1\text{H}$  NMR spectra of R2 after  $\text{D}_2\text{O}$  exchange (expanded form):**



## IR spectra of R2:

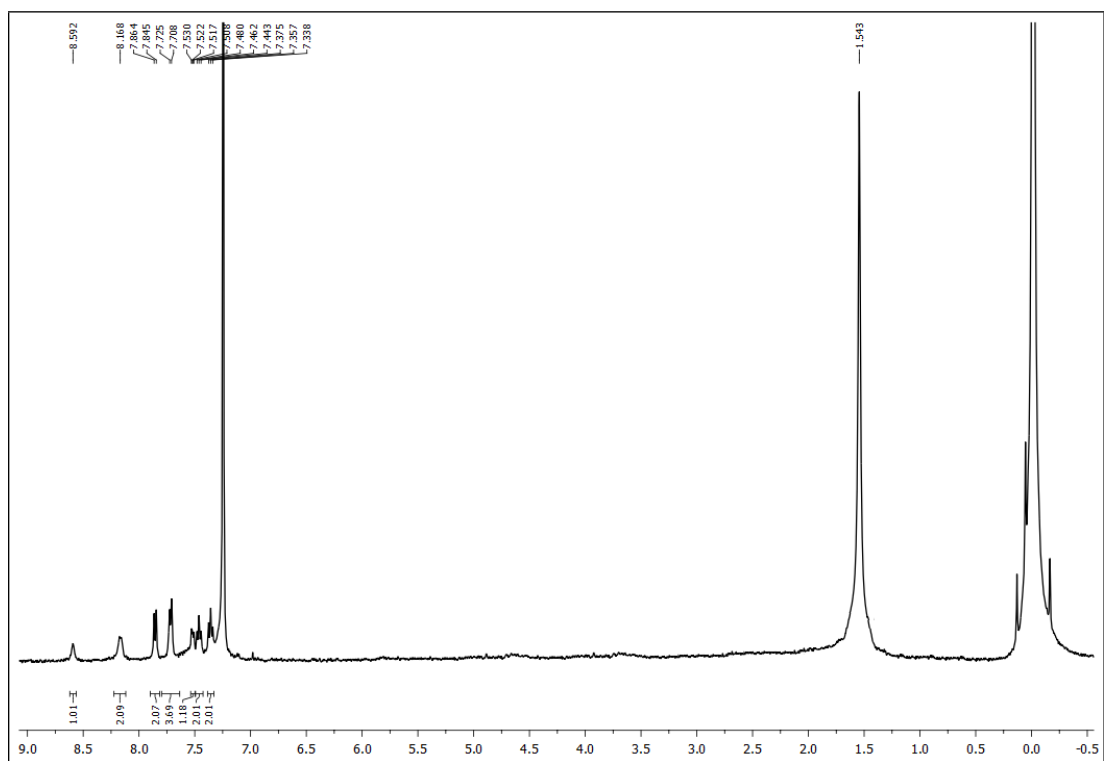


## Mass spectra of R2:

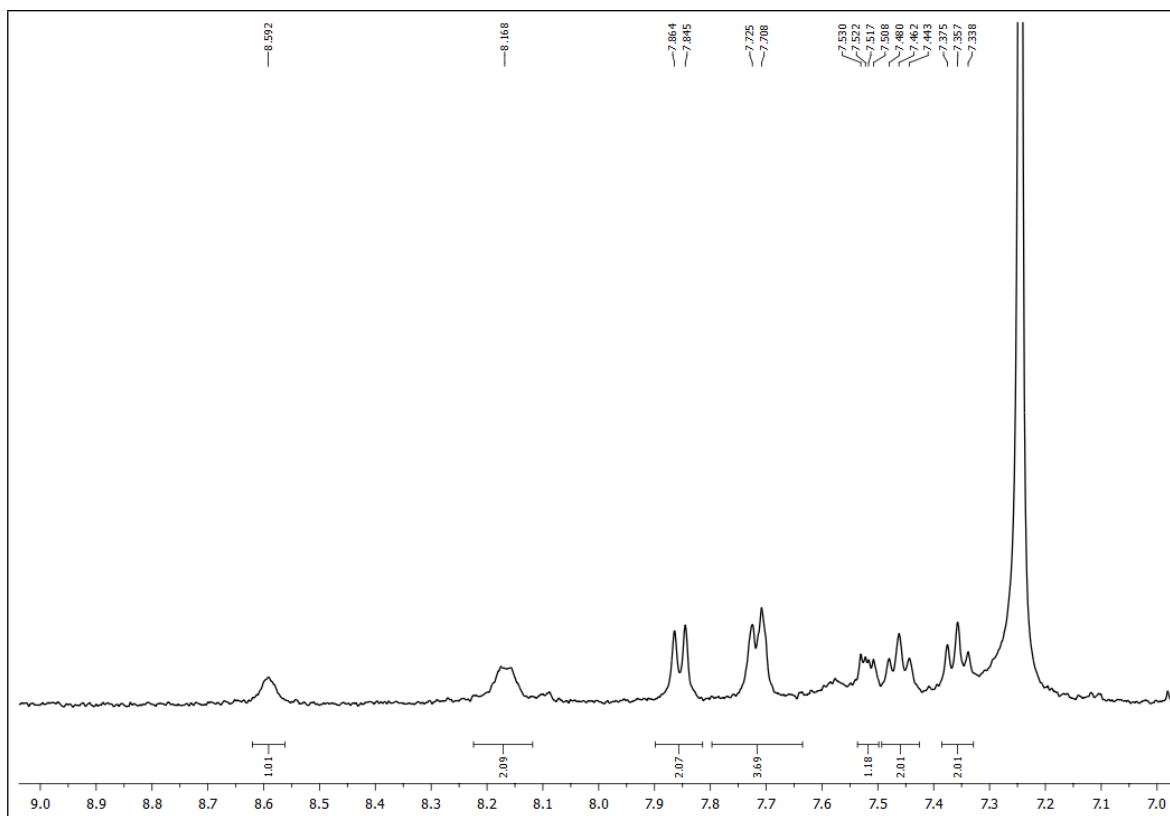




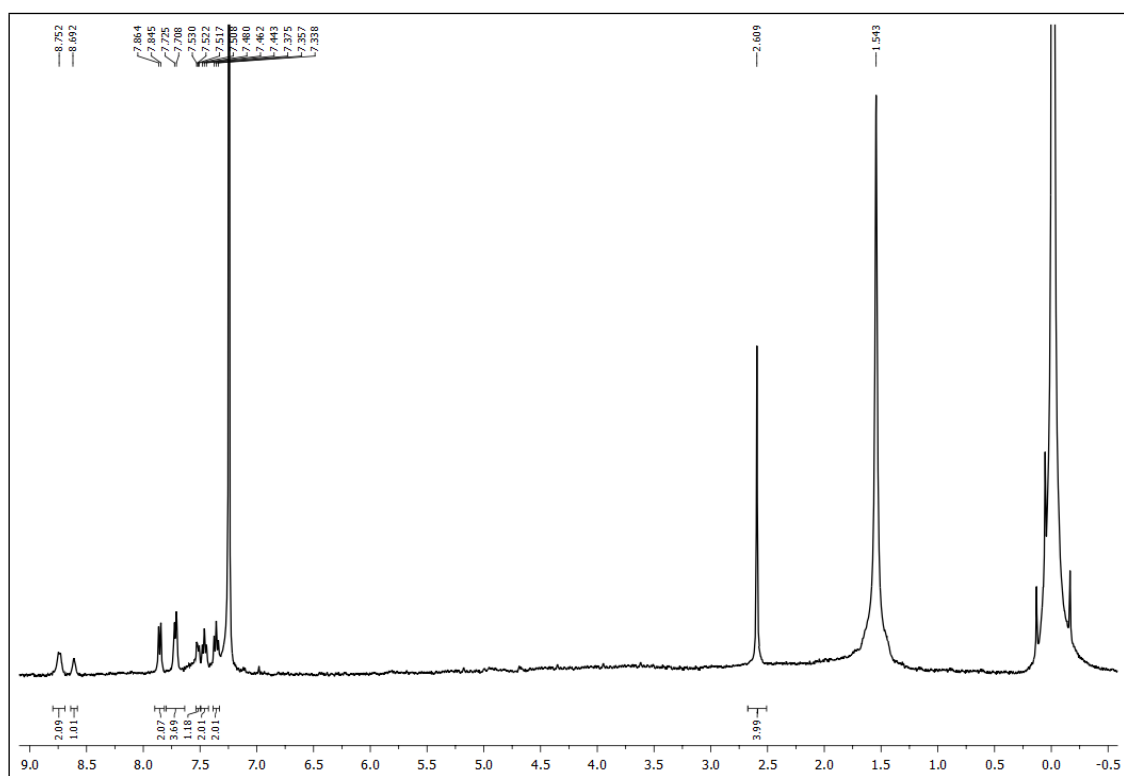
### <sup>1</sup>H NMR spectra of R3:



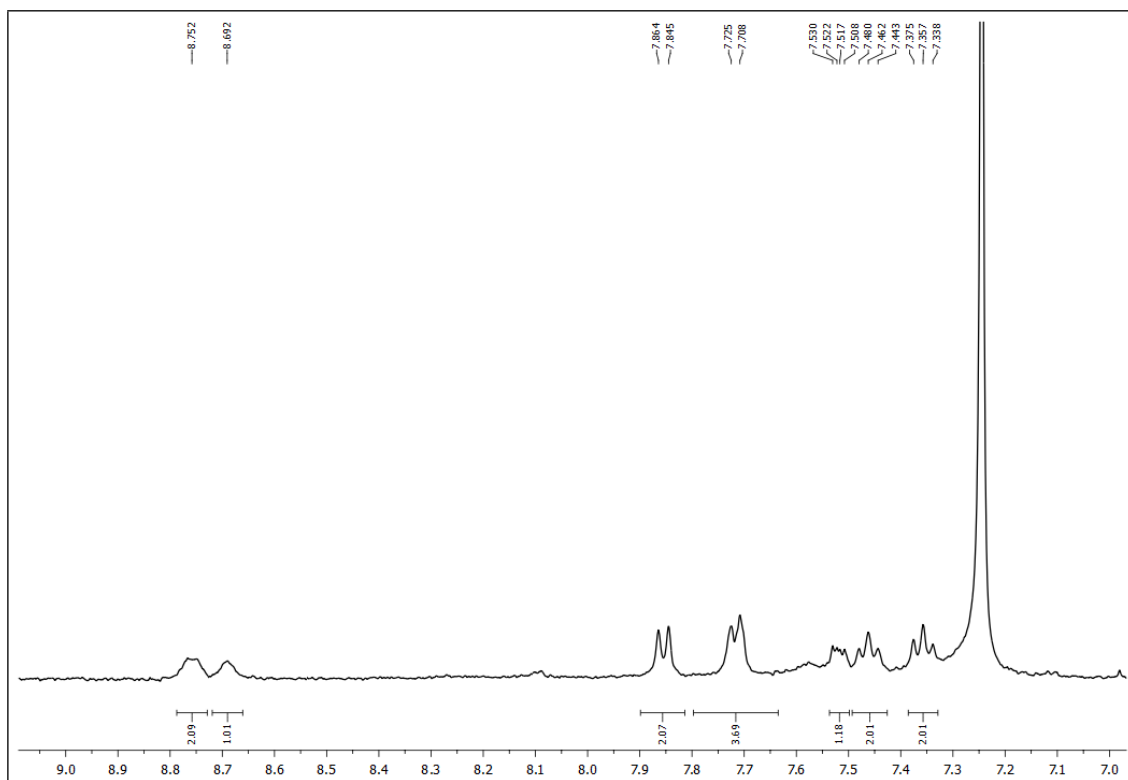
### <sup>1</sup>H NMR spectra of R3 (expanded form):



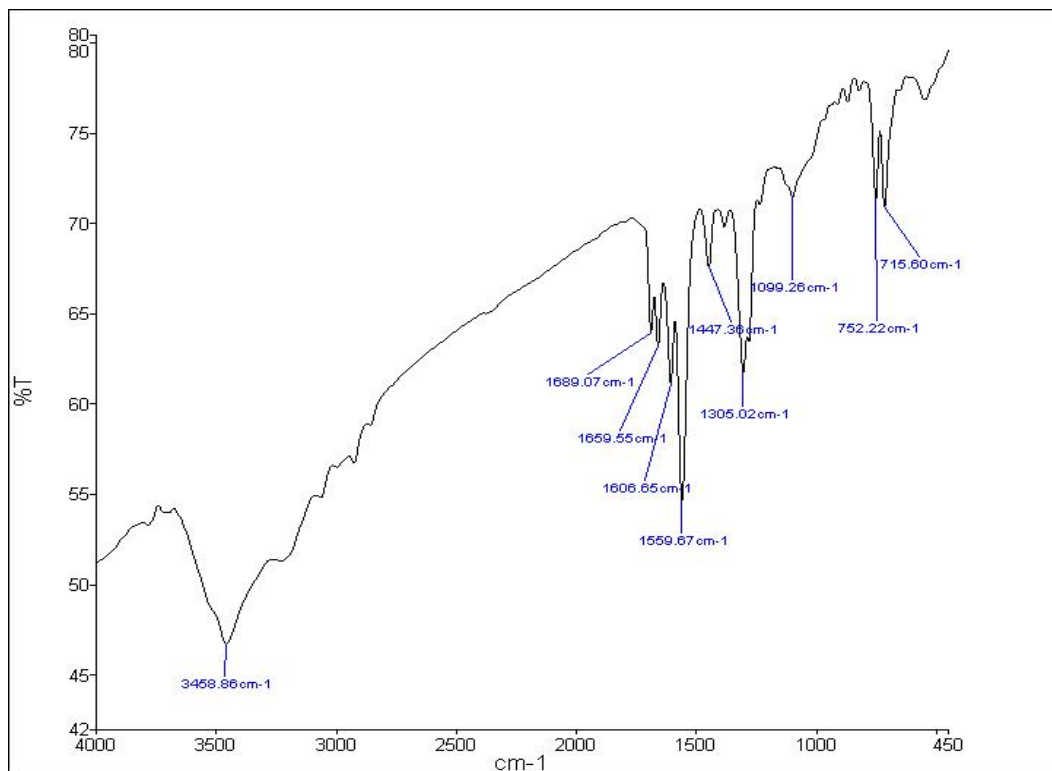
**$^1\text{H}$  NMR spectra of R3-succinic acid complex (1:1):**



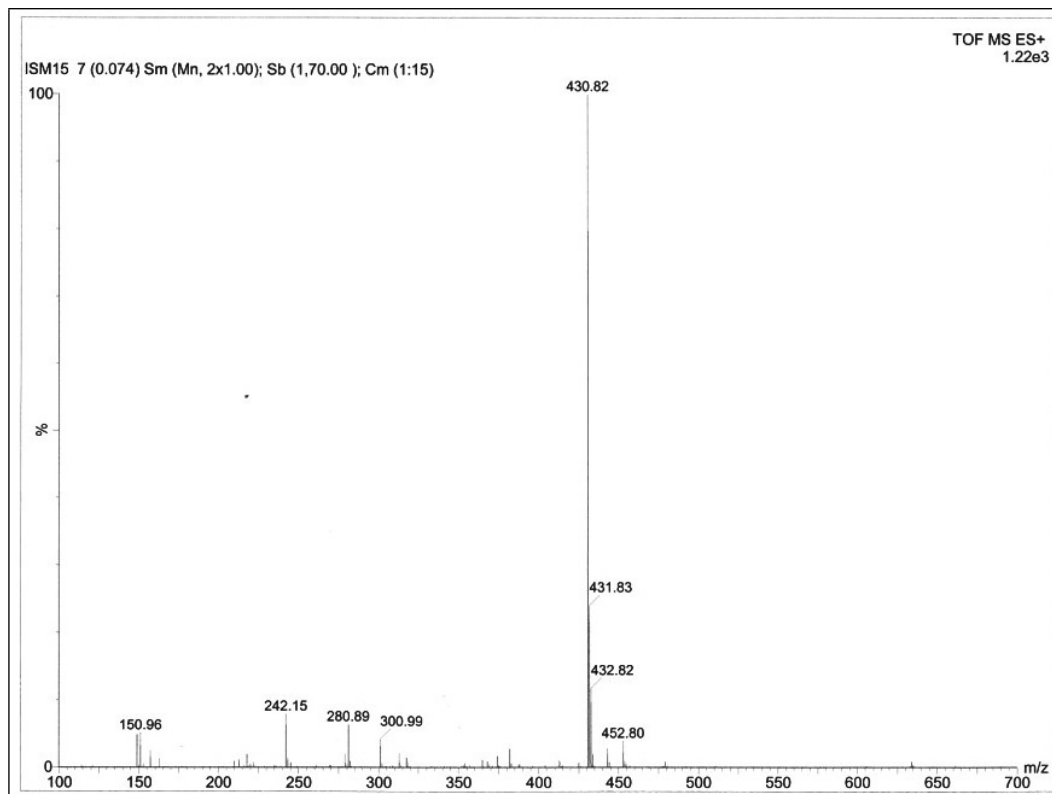
**$^1\text{H}$  NMR spectra of R3-succinic acid complex (1:1) (expanded form):**



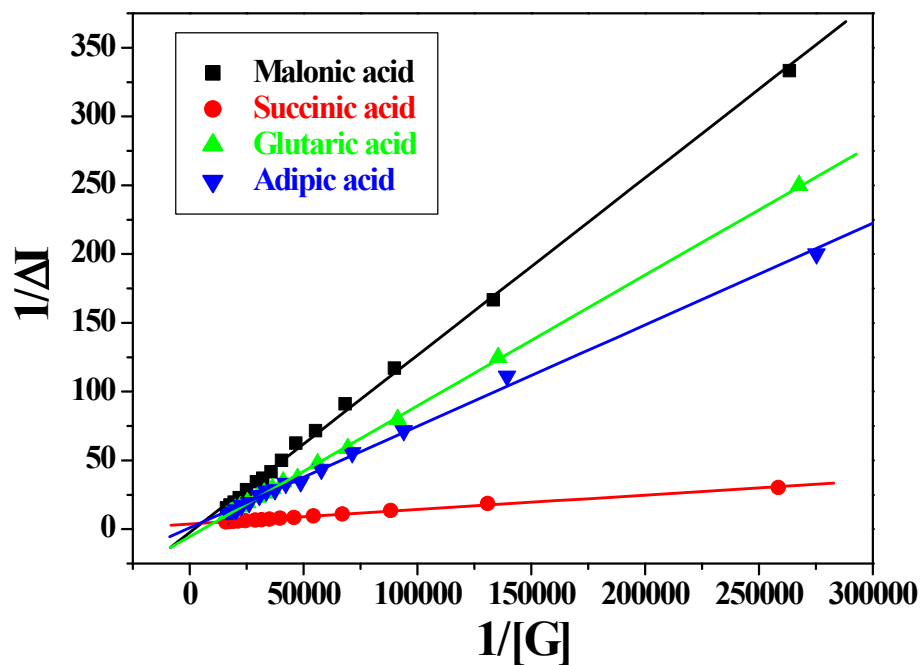
### IR spectra of R3:



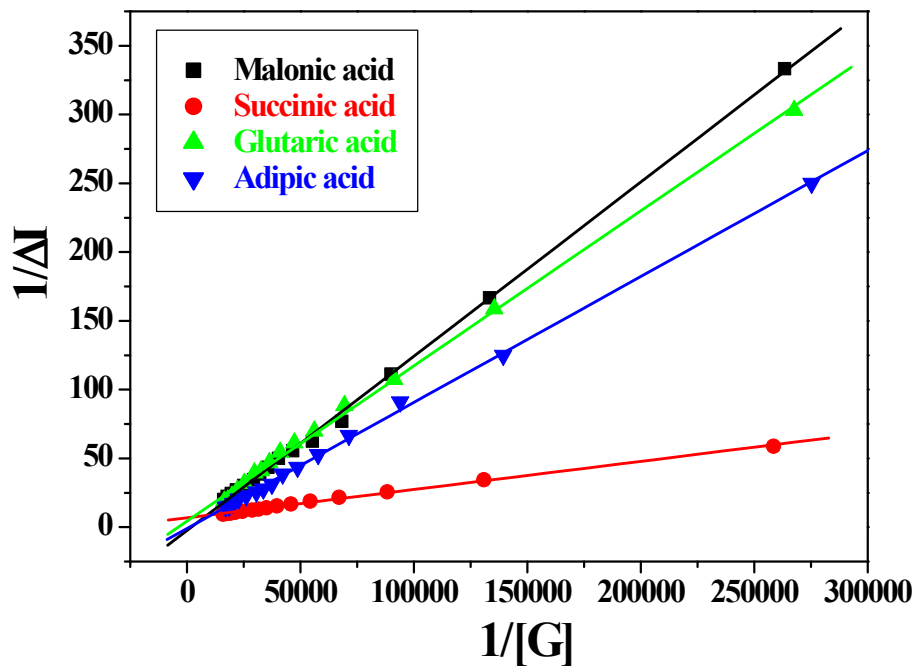
### Mass spectra of R3:



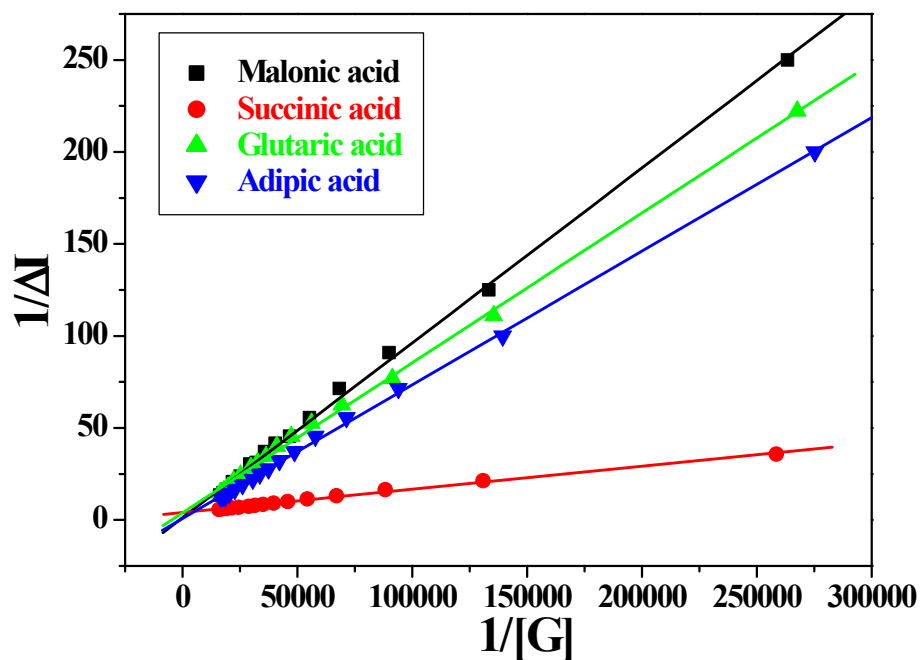
Binding constant calculation by UV titration method of R1 with malonic, succinic, glutaric and adipic acid respectively using linear regression analysis.



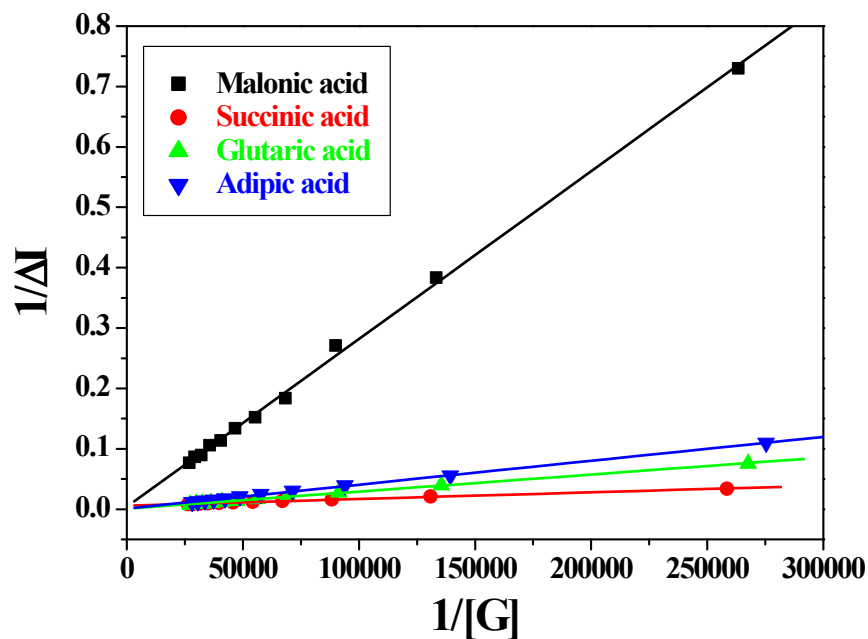
Binding constant calculation by UV titration method of R2 with malonic, succinic, glutaric and adipic acid respectively using linear regression analysis.



Binding constant calculation by UV titration method of R3 with malonic, succinic, glutaric and adipic acid respectively using linear regression analysis.



Binding constant calculation by Fluorescence titration method of R3 with malonic, succinic, glutaric and adipic acid respectively using linear regression analysis.



### Calculation of limit of detection (LOD):

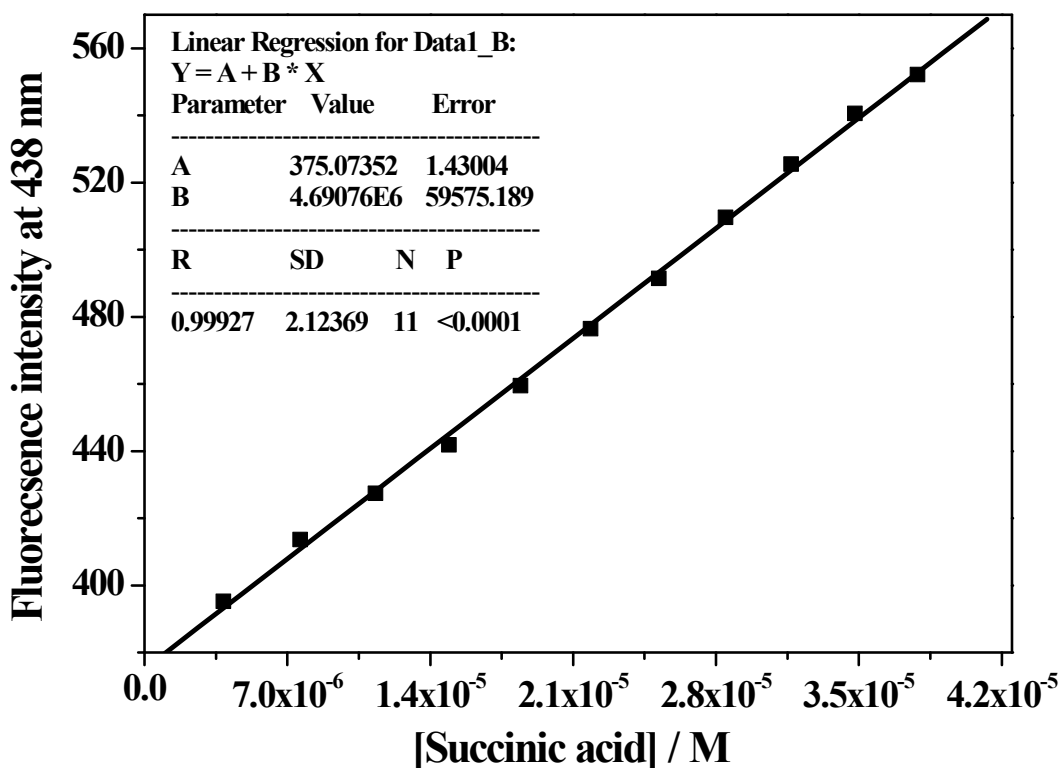
The detection limit of **R3** for succinic acid was calculated on the basis of fluorescence titration. To determine the standard deviation for the fluorescence intensity, the emission intensity of **R3** without any guest was measured by 10 times and the standard deviation of blank measurements was calculated.

The limit of detection (LOD) of **R3** for sensing succinic acid was determined from the following equation:

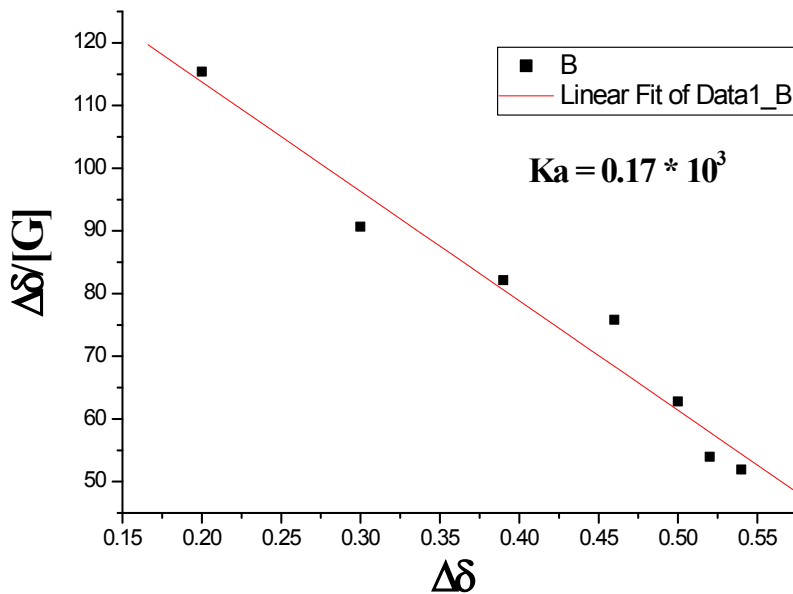
$$\text{LOD} = K \times \text{SD}/S$$

Where  $K = 2$  or  $3$  (we take  $3$  in this case);  $\text{SD}$  is the standard deviation of the blank receptor (**R3**);  $S$  is the slope of the calibration curve.

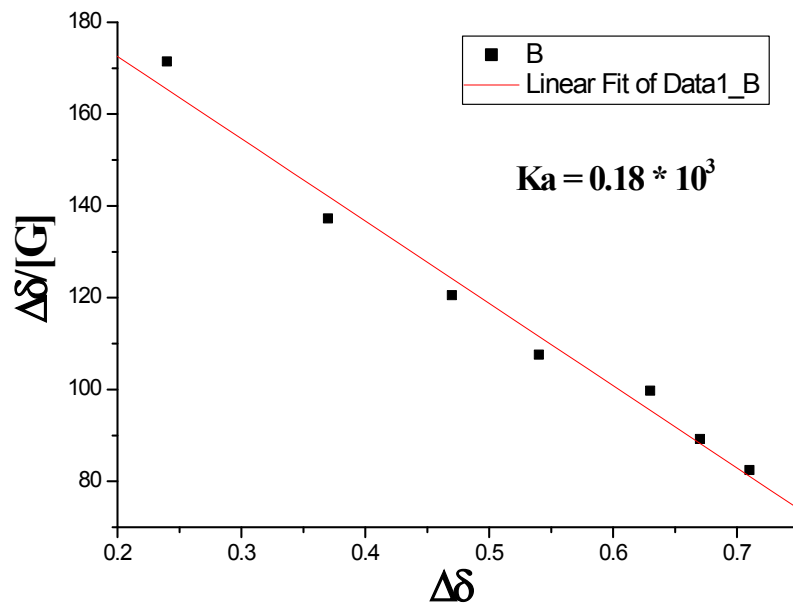
From the linear fit graph we get slope =  $4.69 \times 10^6$ , and  $\text{SD}$  value is  $0.50148$ . Thus using the above formula we get the Limit of Detection =  $3.21 \times 10^{-7}$  M i.e. **R3** can detect succinic acid up to this very lower concentration by fluorescence techniques.



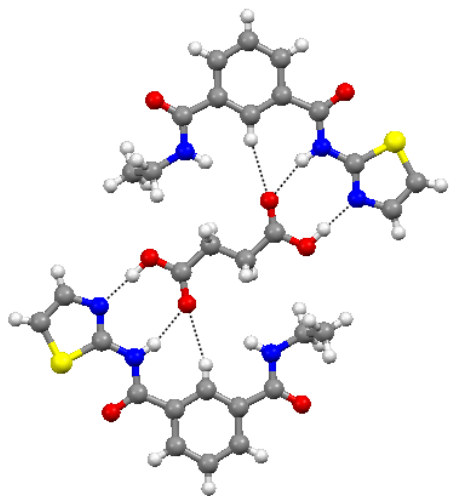
Binding constant calculation by  $^1\text{H-NMR}$  method of R1 with succinic acid using linear method:



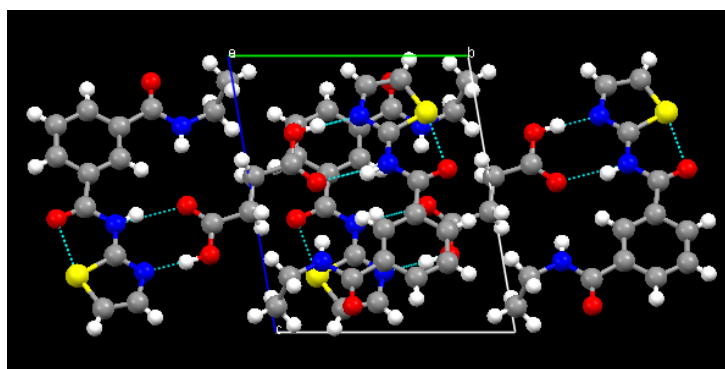
Binding constant calculation by  $^1\text{H-NMR}$  method of R3 with succinic acid using linear method:



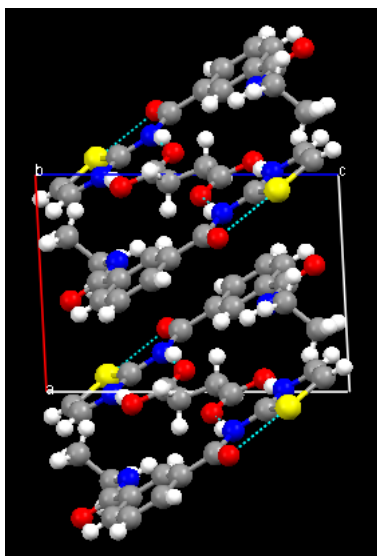
Different crystal structure of R2-Succinic acid complex (CCDC No. 1012219):



View through Crystallographic *a*-axis:



View through Crystallographic *b*-axis:





View through Crystallographic *c*-axis:

