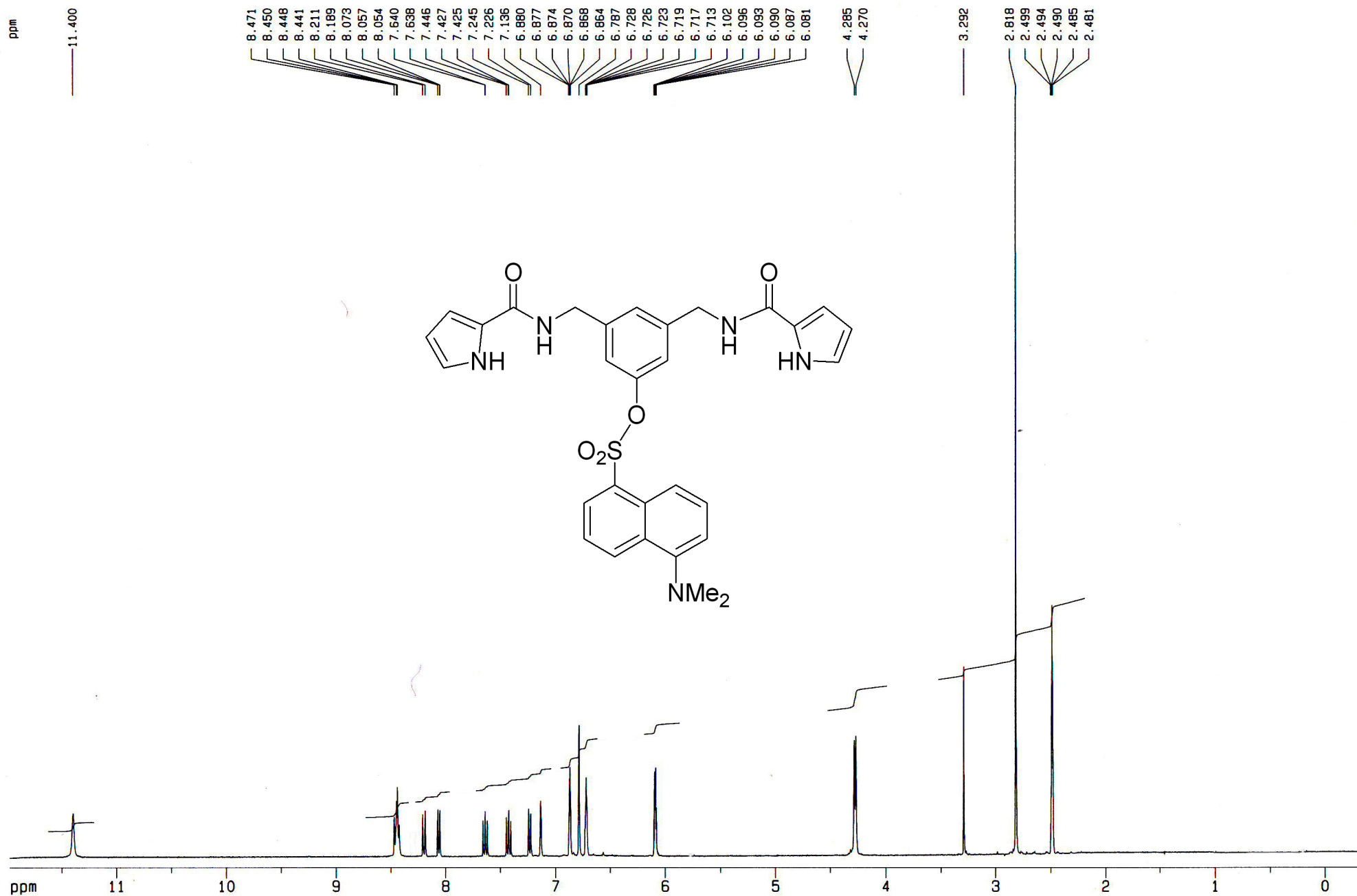


### **Supplementary material:**

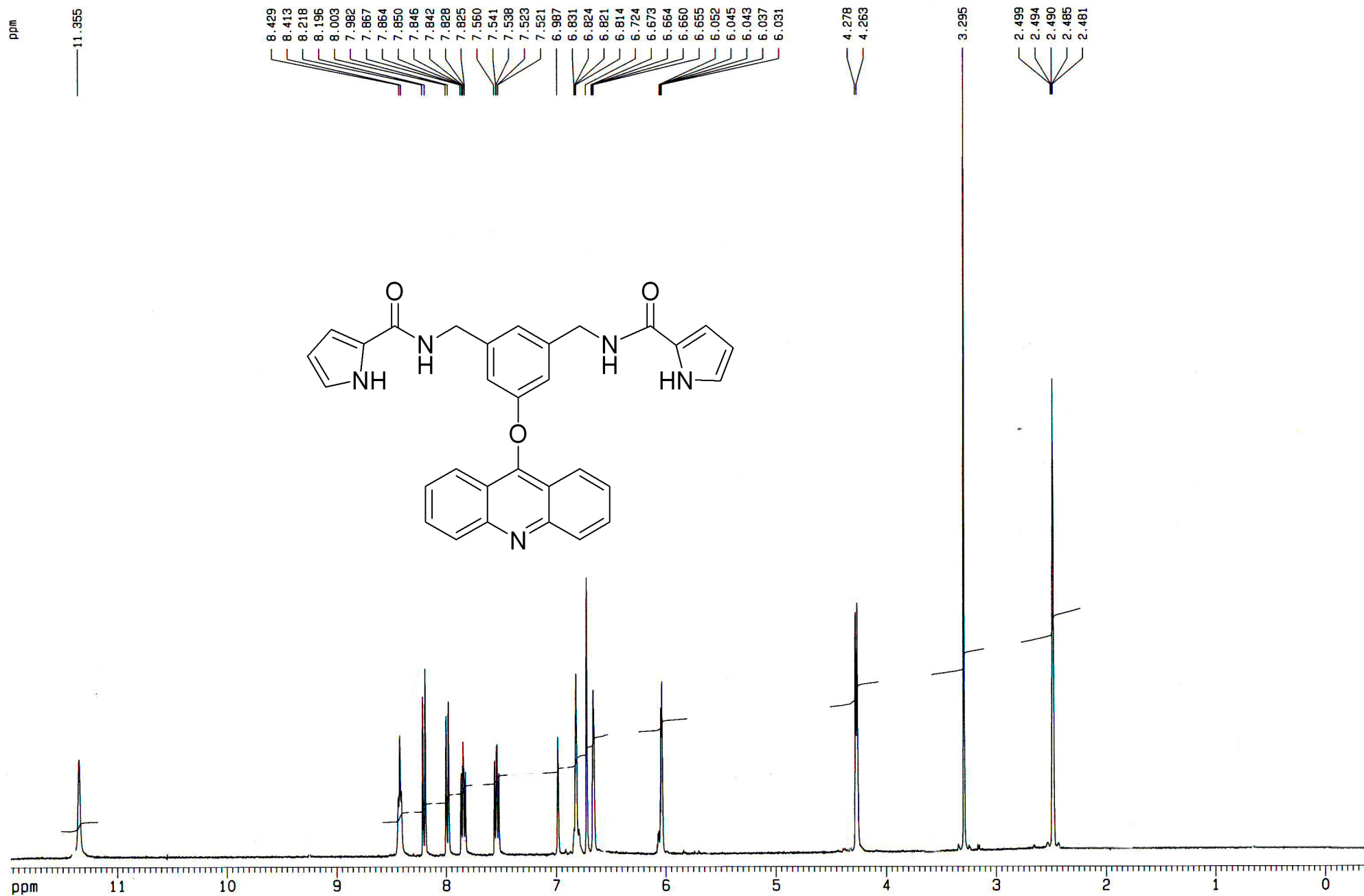
|                                                                                  |       |
|----------------------------------------------------------------------------------|-------|
| 1.- $^1\text{H}$ and $^{13}\text{C}$ -NMR spectra of <b>1</b> and <b>2</b> ..... | p. 2  |
| 2.- HRMS of <b>1</b> and <b>2</b> .....                                          | p. 7  |
| 3a.- Titration spectra of <b>1</b> with dicarboxylates .....                     | p. 11 |
| 3b.- Titration spectra of <b>2</b> with dicarboxylates .....                     | p. 17 |
| 4a.- Titration curves of <b>1</b> .....                                          | p. 23 |
| 4b.- Titration curves of <b>2</b> .....                                          | p. 31 |
| 5.- Fluorescence experiments of <b>1</b> with glutarate TBA-salt .....           | p. 39 |

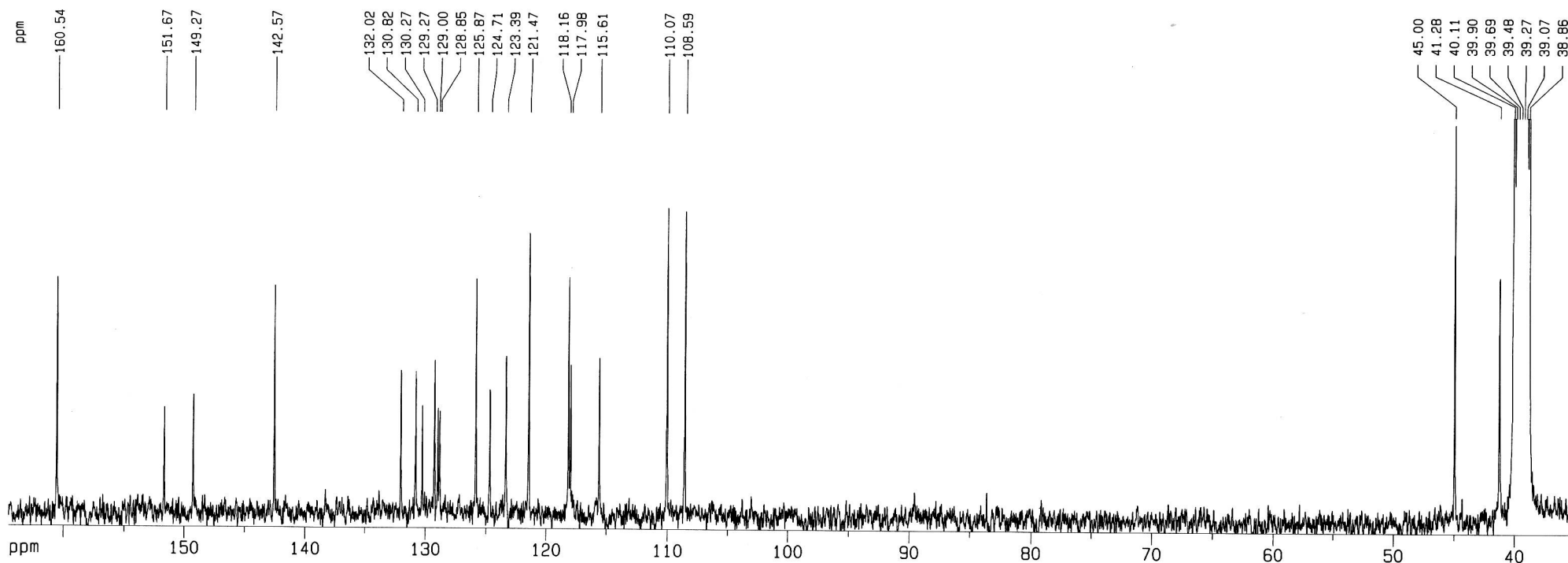
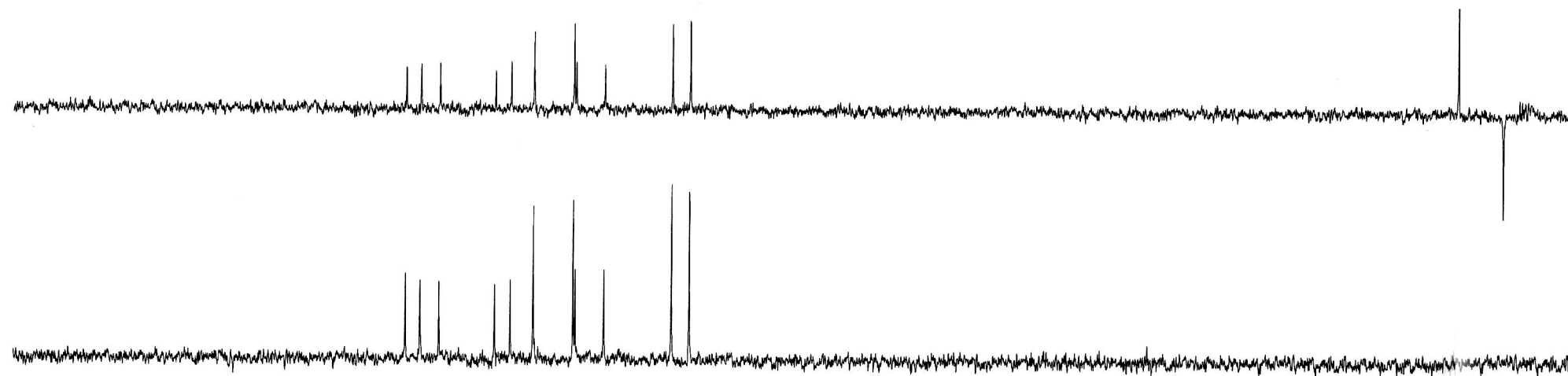
1.-  $^1\text{H}$  and  $^{13}\text{C}$ -NMR spectra of **1** and **2**

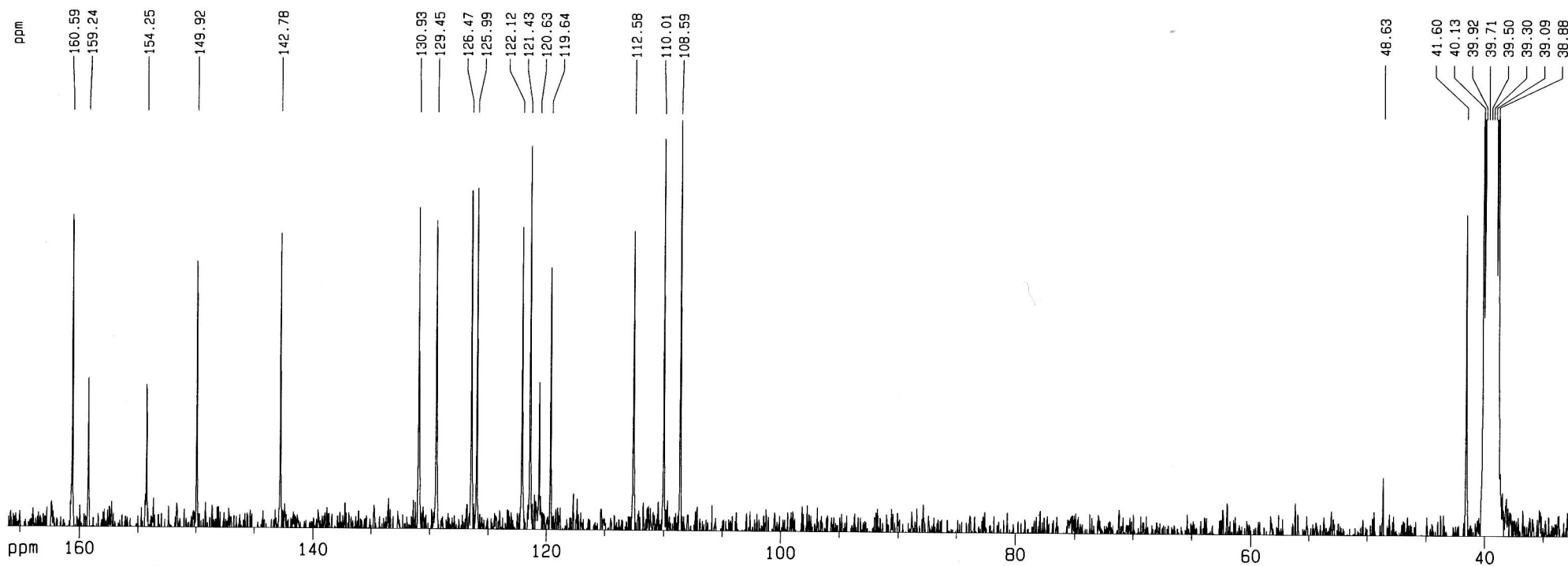
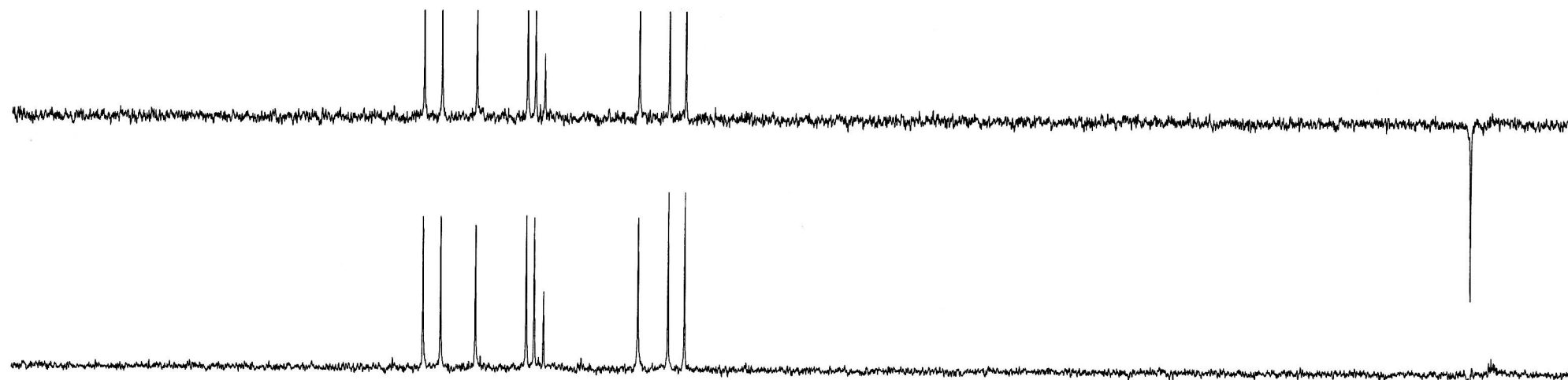
belen-20 receptor 4  
1H DMSO-d6



belen-19 receptor 3  
1H DMSO-d6



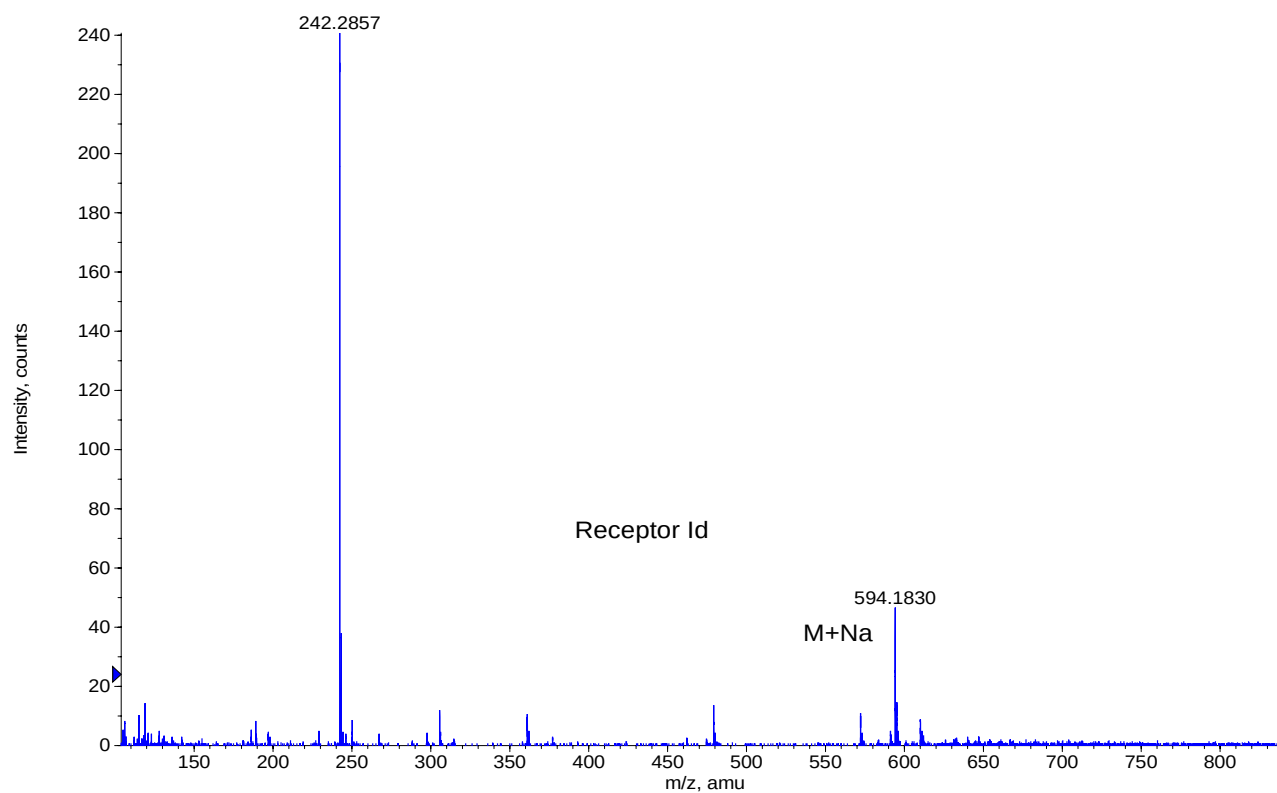




2.- HRMS of **1** and **2**

+TOF MS: 0.183 to 0.217 min from Sample 5 (receptor Id) of nov080612.wiff  
a=3.56022533717758410e-004, t0=-1.04130907076505540e+001 R;, subtracted (0.033 to 0...

Max. 240.7 counts.

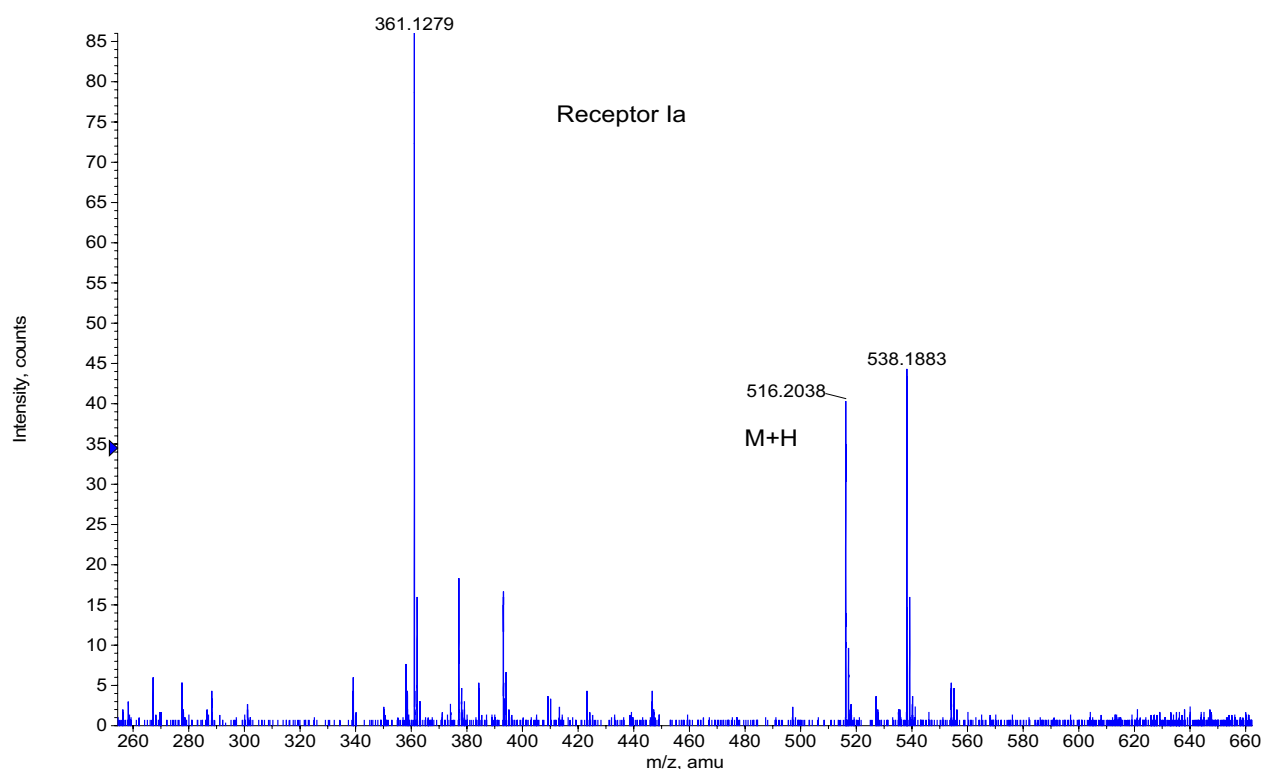


| Formula             | CalculatedMass | mDaError | ppmError  | RDB  |
|---------------------|----------------|----------|-----------|------|
| C23 H33 N5 O10 Na S | 594.184036     | -1.03568 | -1.74303  | 9.5  |
| C32 H28 N5 O5 S     | 594.180568     | 2.43242  | 4.093718  | 21.5 |
| C25 H32 N5 O10 S    | 594.186441     | -3.44094 | -5.791039 | 12.5 |
| C30 H29 N5 O5 Na S  | 594.178162     | 4.83768  | 8.141727  | 18.5 |



+TOF MS: 0.167 to 0.200 min from Sample 4 (receptor Ia) of nov080612.wiff  
a=3.56022533717758410e-004, t0=-1.04130907076505540e+001 R;, subtracted (0.034 to ...

Max. 1757.7 counts.



| Formula              | CalculatedMass | mDaError  | ppmError  | RDB  |
|----------------------|----------------|-----------|-----------|------|
| C18 H27 N11 O6 Na    | 516.203799     | 0.000872  | 0.001689  | 10.5 |
| C25 H31 N5 O4 Na Si  | 516.203754     | 0.04564   | 0.088415  | 13.5 |
| C10 H34 N9 O13 Si    | 516.203988     | -0.187572 | -0.363368 | -0.5 |
| C18 H34 N3 O14       | 516.20353      | 0.270236  | 0.523506  | 3.5  |
| C23 H26 N11 O2 Si    | 516.203474     | 0.325772  | 0.631091  | 17.5 |
| C31 H26 N5 O3        | 516.203016     | 0.78358   | 1.517965  | 21.5 |
| C34 H27 N3 O Na      | 516.204634     | -0.833864 | -1.615376 | 22.5 |
| C9 H31 N13 O9 Na Si  | 516.20292      | 0.880376  | 1.70548   | 1.5  |
| C26 H34 N O8 Si      | 516.204822     | -1.022308 | -1.980433 | 11.5 |
| C19 H30 N7 O10       | 516.204867     | -1.067076 | -2.067158 | 8.5  |
| C26 H27 N9 Na Si     | 516.205092     | -1.291672 | -2.502249 | 18.5 |
| C19 H23 N15 O2 Na    | 516.205136     | -1.33644  | -2.588975 | 15.5 |
| C17 H31 N7 O10 Na    | 516.202462     | 1.338184  | 2.592353  | 5.5  |
| C21 H35 N O12 Na     | 516.205147     | -1.347208 | -2.609835 | 4.5  |
| C24 H35 N O8 Na Si   | 516.202417     | 1.382952  | 2.679079  | 8.5  |
| C11 H30 N13 O9 Si    | 516.205325     | -1.524884 | -2.954032 | 4.5  |
| C15 H26 N13 O8       | 516.202182     | 1.618316  | 3.13503   | 9.5  |
| C22 H30 N7 O6 Si     | 516.202137     | 1.663084  | 3.221755  | 12.5 |
| C13 H35 N7 O11 Na Si | 516.205605     | -1.805016 | -3.496708 | 0.5  |
| C30 H30 N O7         | 516.201679     | 2.120892  | 4.108629  | 16.5 |
| C27 H30 N5 O4 Si     | 516.20616      | -2.35962  | -4.571097 | 16.5 |
| C20 H26 N11 O6       | 516.206204     | -2.404388 | -4.657822 | 13.5 |
| C6 H30 N15 O11 Si    | 516.201302     | 2.49782   | 4.83882   | 0.5  |

|                      |            |          |           |      |
|----------------------|------------|----------|-----------|------|
| C16 H35 N3 O14 Na    | 516.201125 | 2.675496 | 5.183017  | 0.5  |
| C22 H31 N5 O8 Na     | 516.206485 | -2.68452 | -5.200499 | 9.5  |
| C21 H27 N11 O2 Na Si | 516.201069 | 2.731032 | 5.290602  | 14.5 |
| C14 H30 N9 O12       | 516.200844 | 2.955628 | 5.725694  | 4.5  |

### 3 a.- Titration spectra of **1** with dicarboxylates

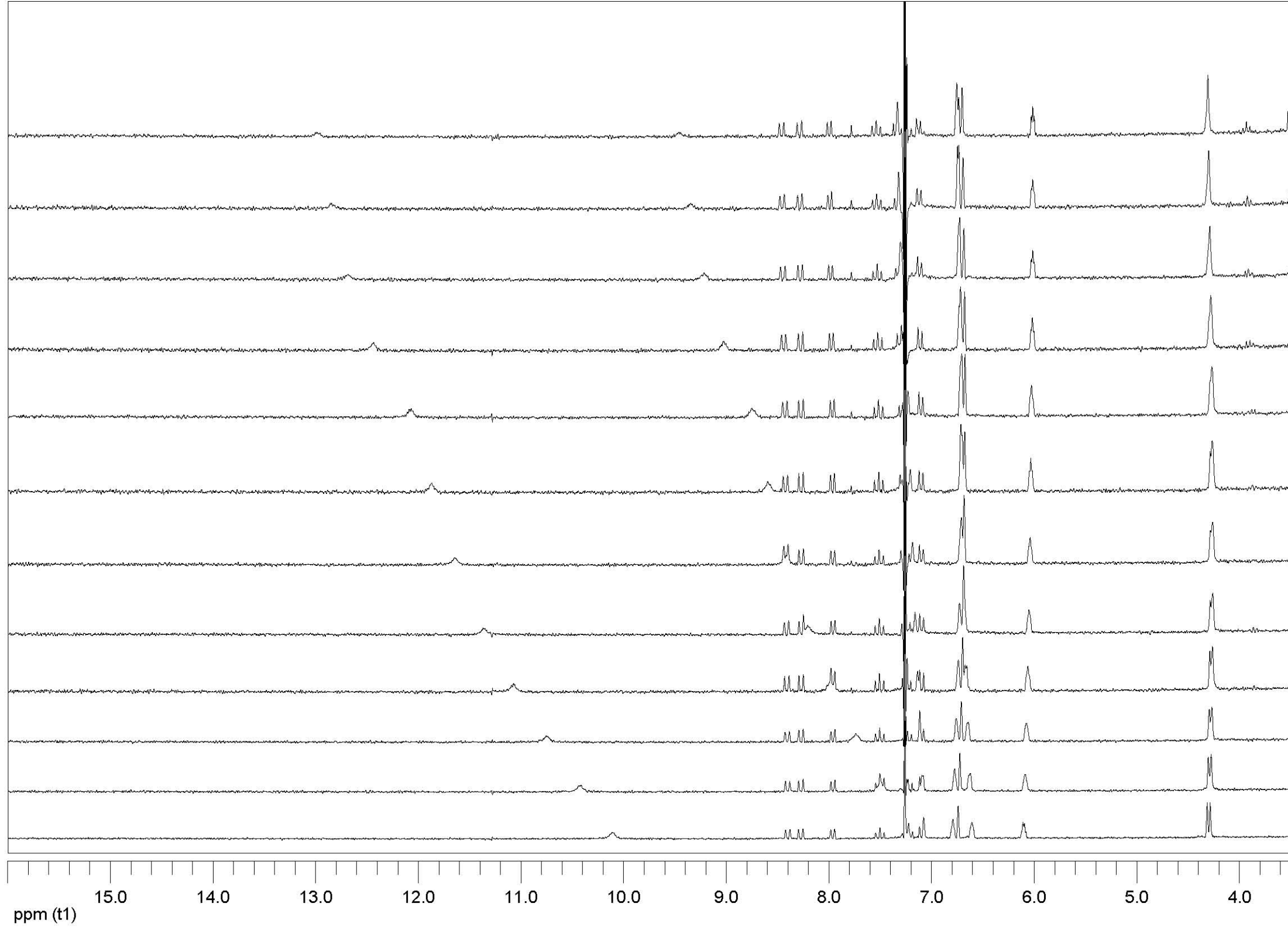
3.1. Succinate

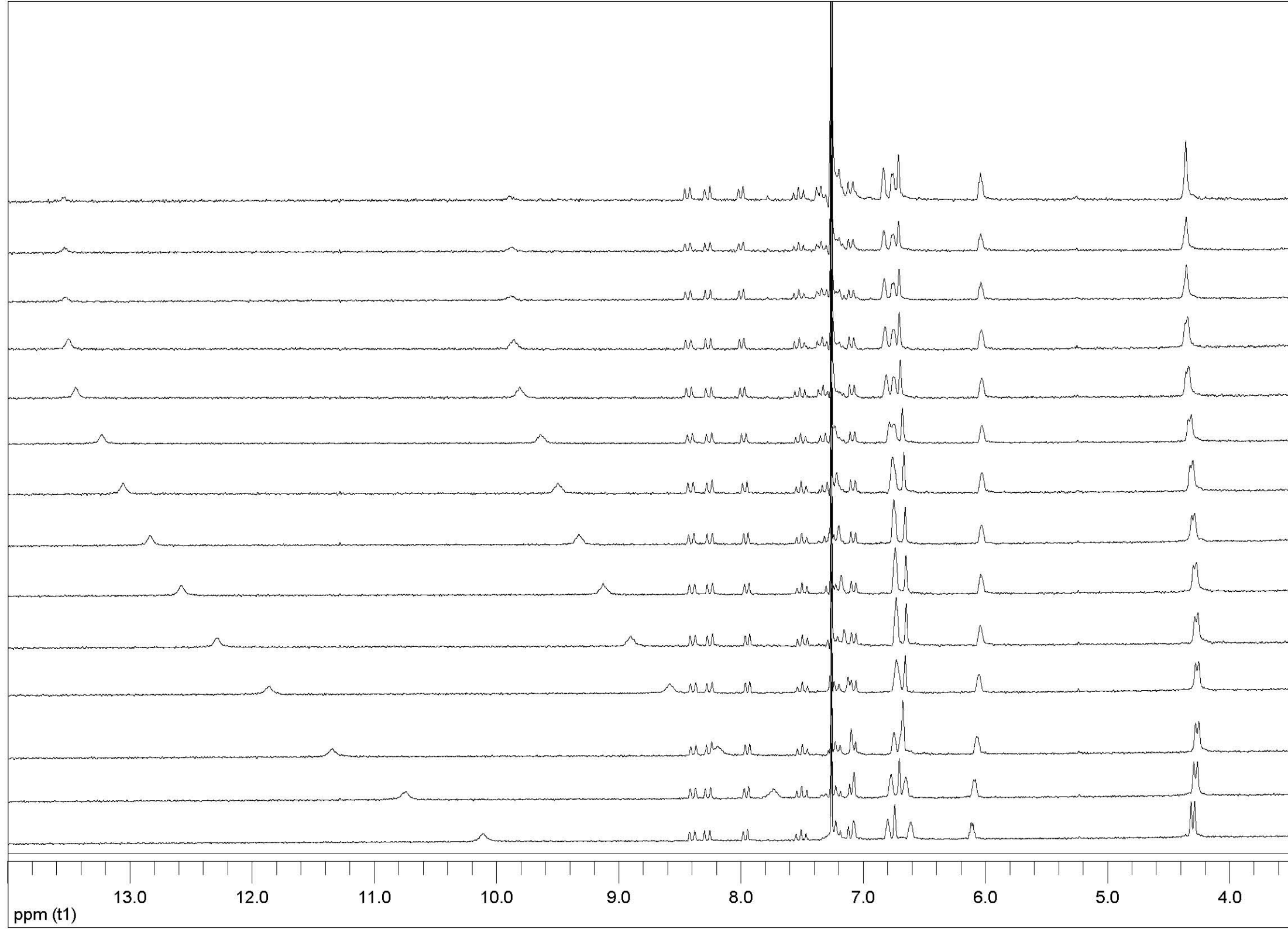
3.2. Adipate

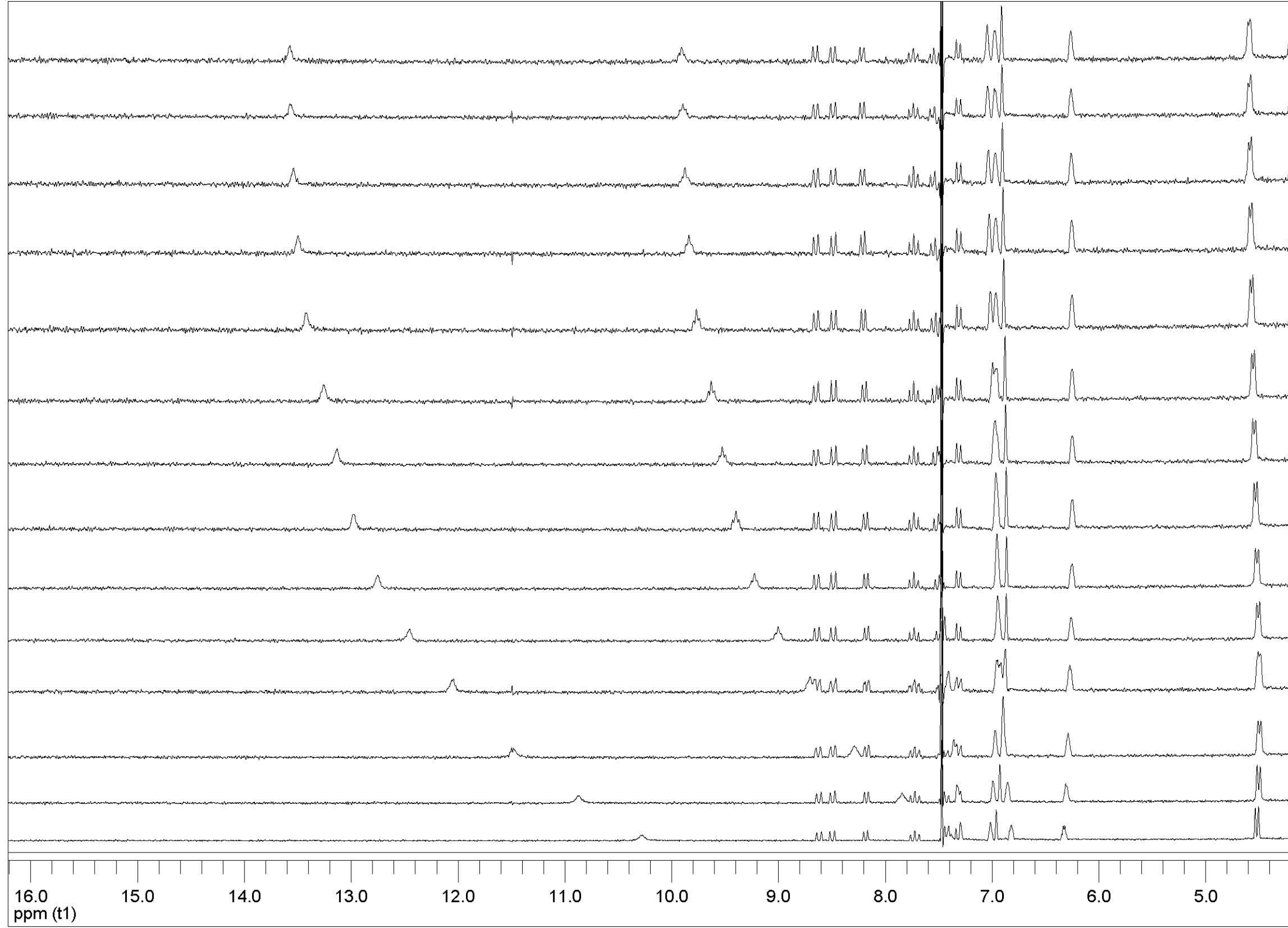
3.3. Pimelate

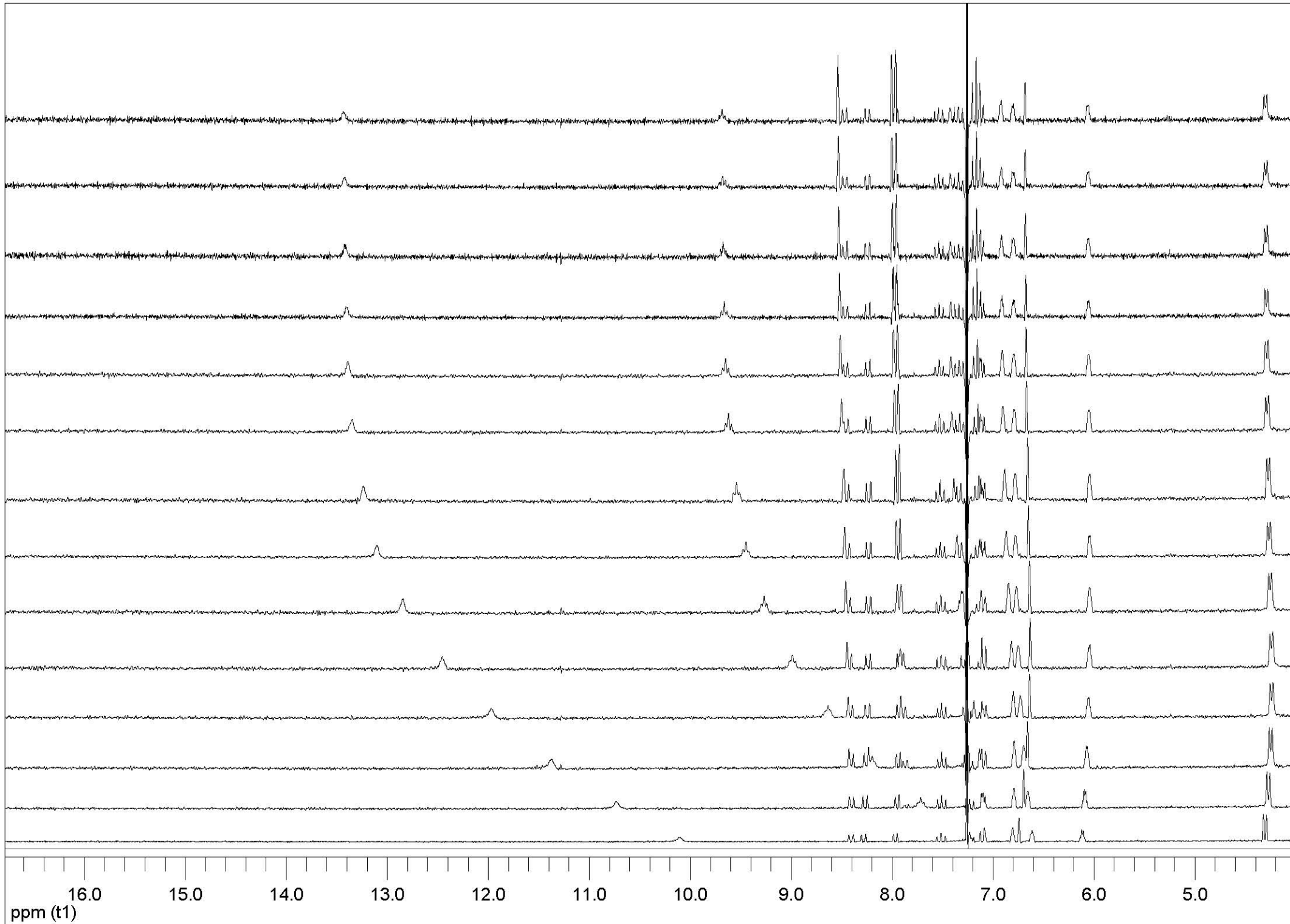
3.4. Isophthalate

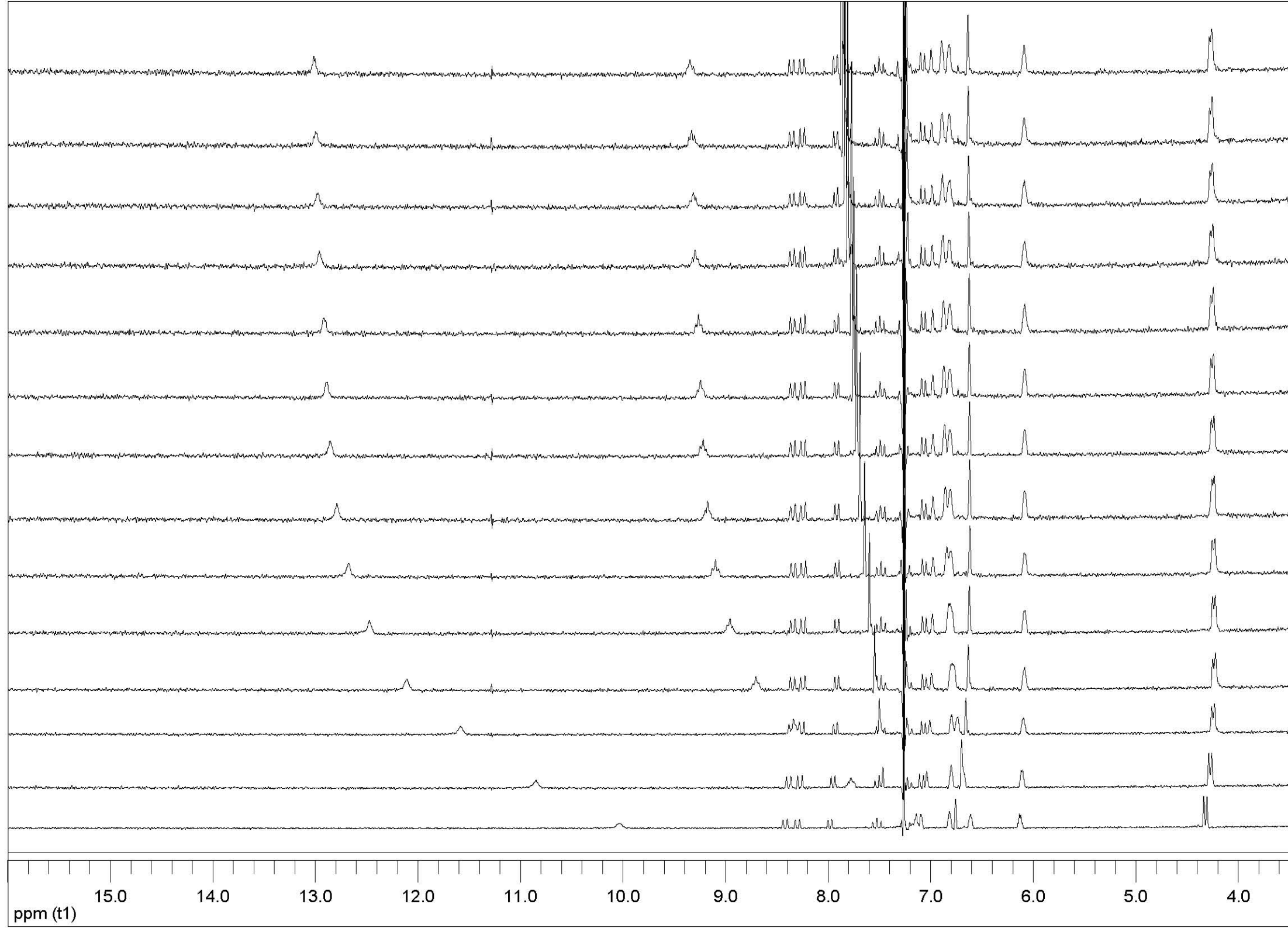
3.5. Terphthalate













### 3 b.- Titration spectra of **2** with dicarboxylates

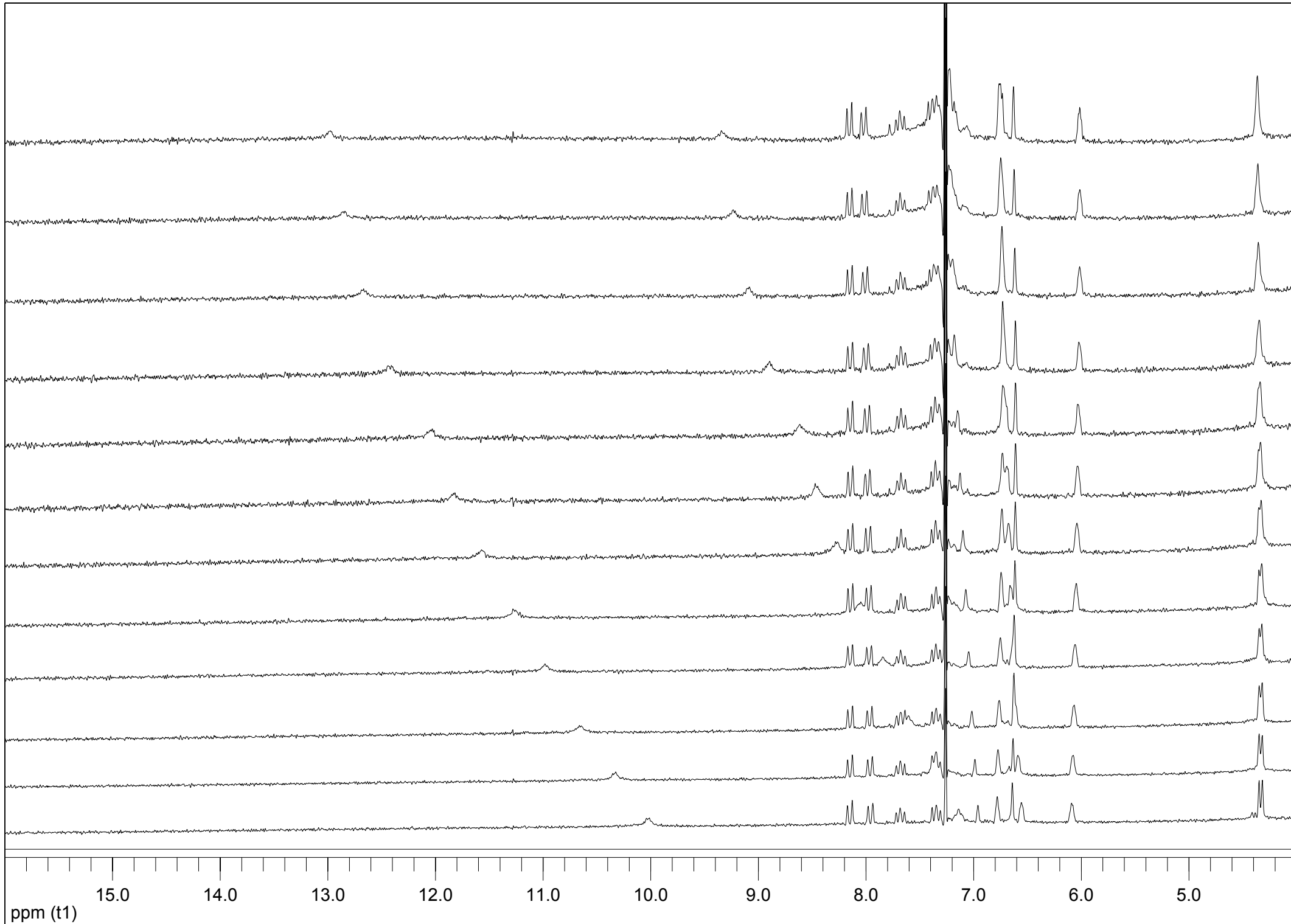
3.1. Succinate

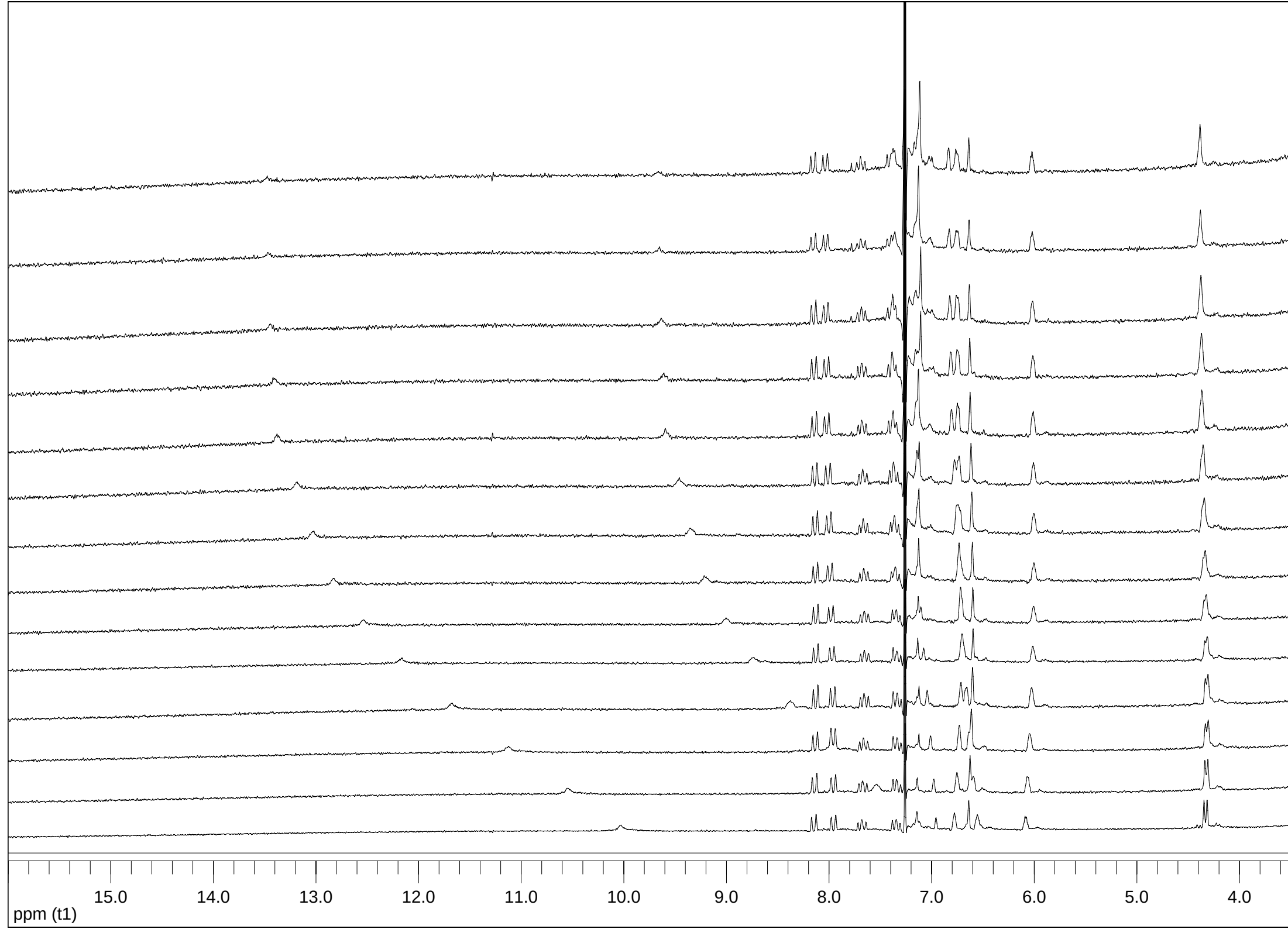
3.2. Glutarate

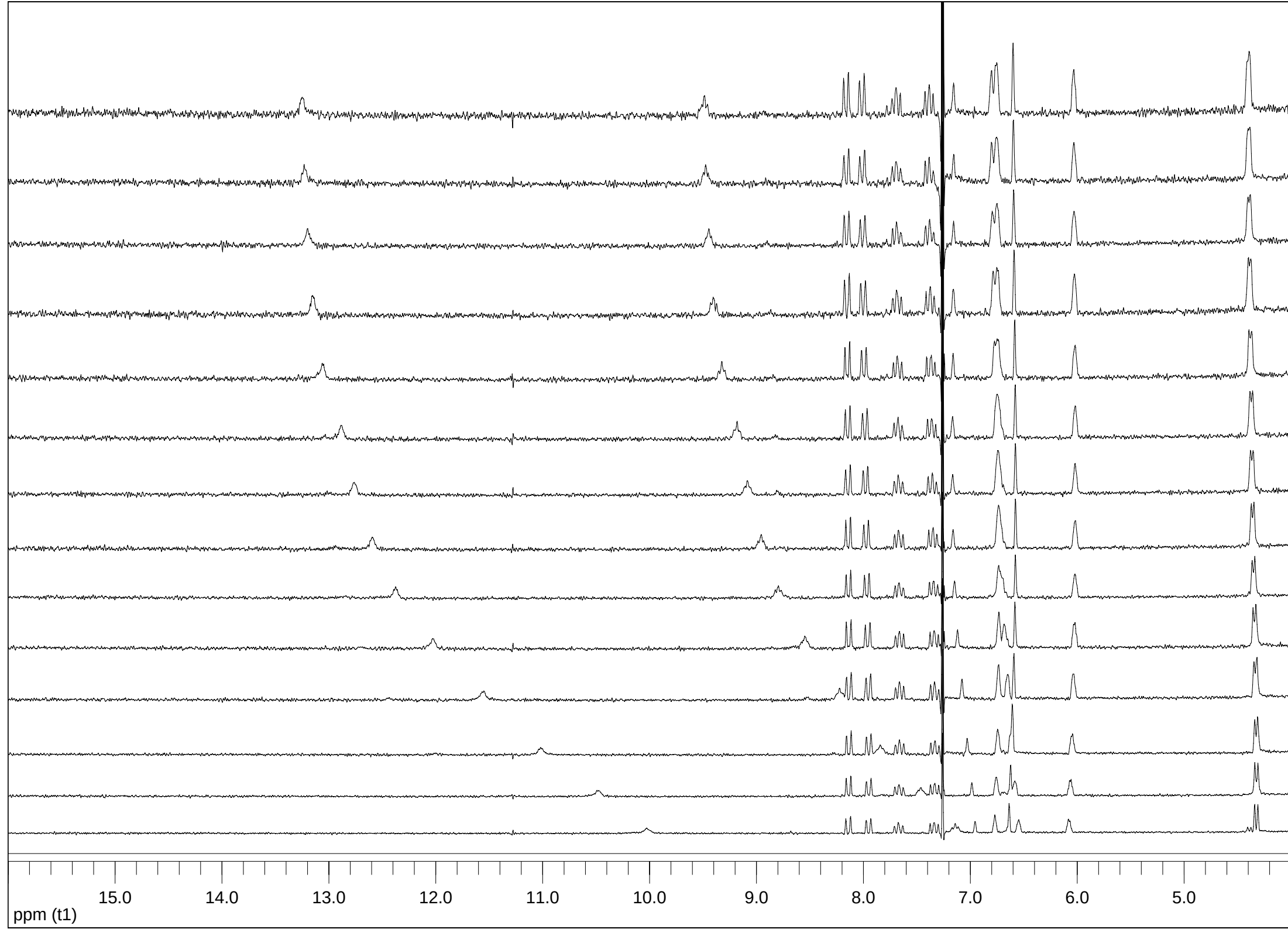
3.3. Pimelate

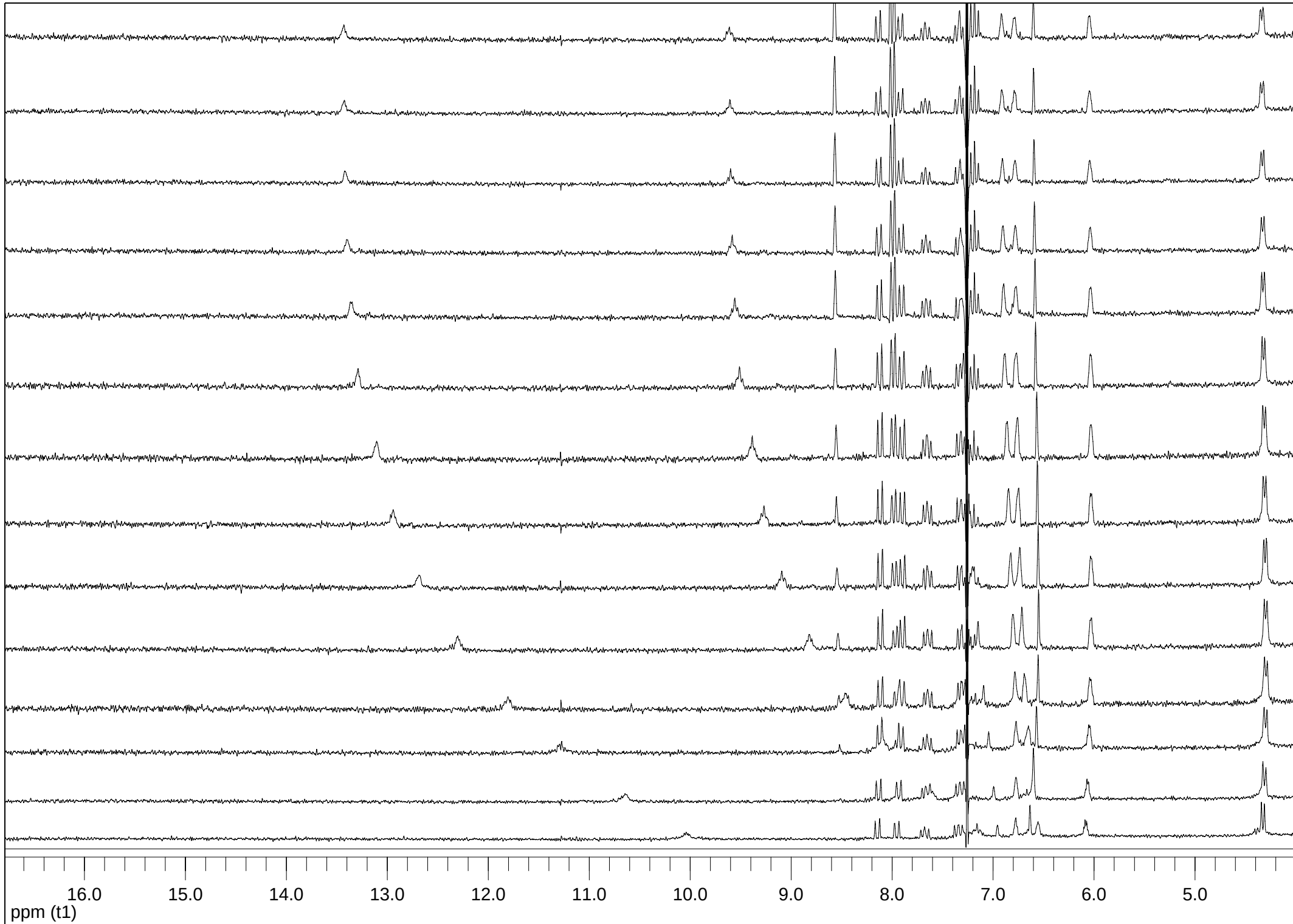
3.4. Isophthalate

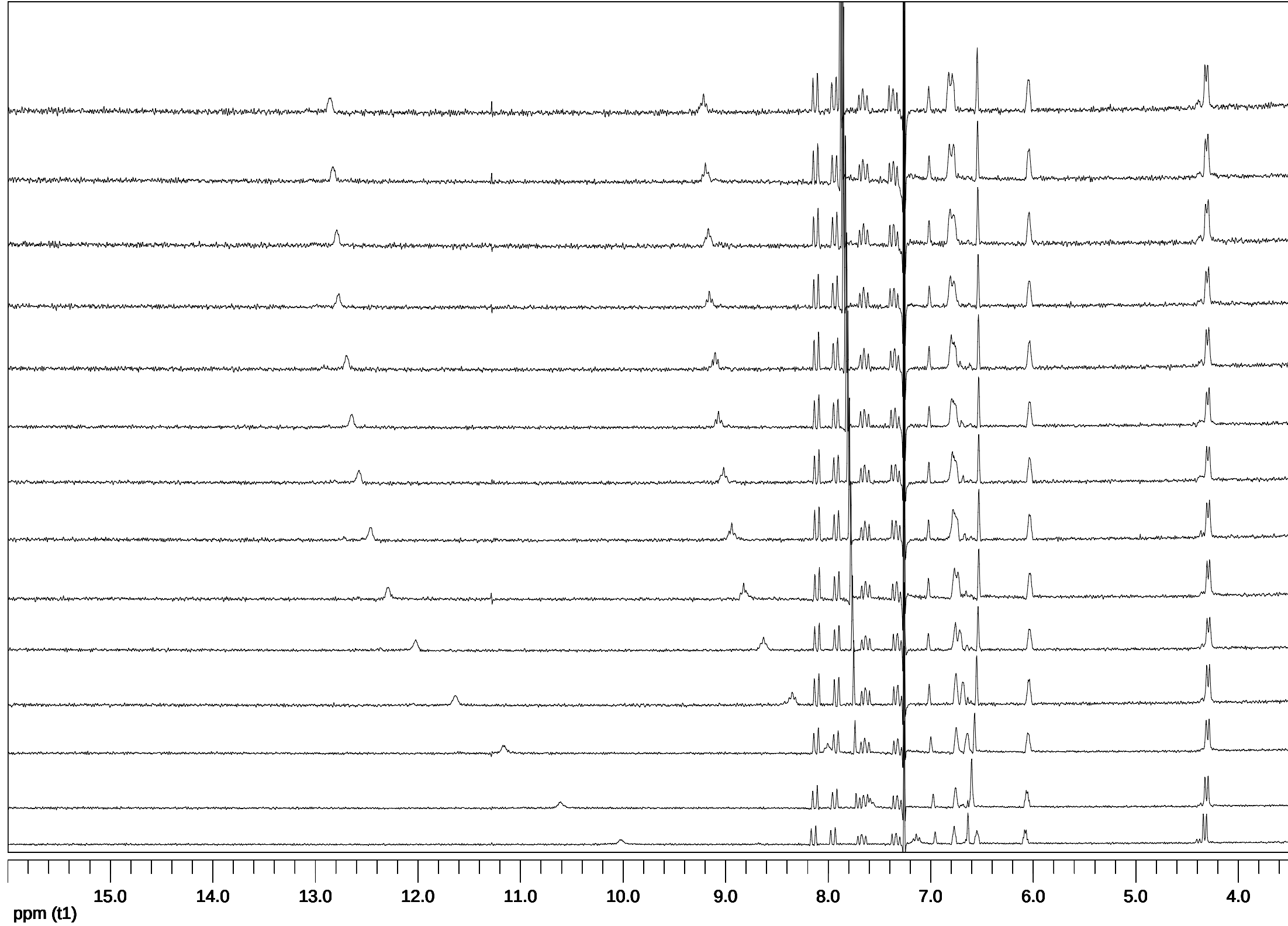
3.5. Terphthalate











4 a.- Titration curves of **1** with:

4.1. Succinate

4.2. Glutarate

4.3. Adipate

4.4. Pimelate

4.5. Suberate

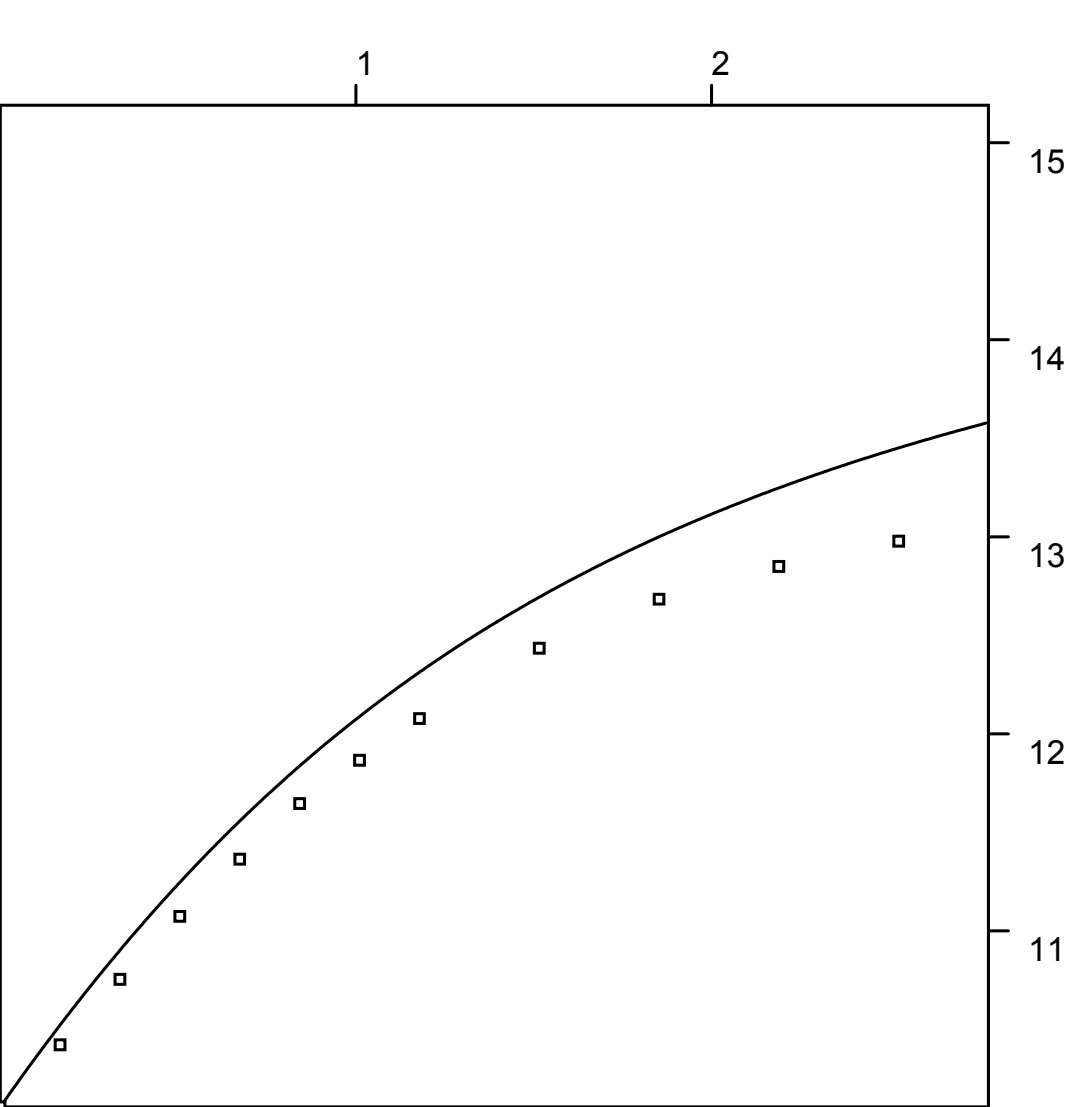
4.6. Isophthalate

4.7. Terphthalate

Constante de Asociación  
Constante: 2.5e+02 1/M  
Despl. Max.: 15.191

Host: receptor Id  
Peso molecular: 572  
Peso puesto (mg): 1.2  
Volumen total (ml): 0.5  
Volumen puesto (ml): 0.5

Guest: succinato cloroformo-DMSO  
Peso molecular: 600  
Peso puesto(mg): 10.6  
Volumen puesto(ml): 1



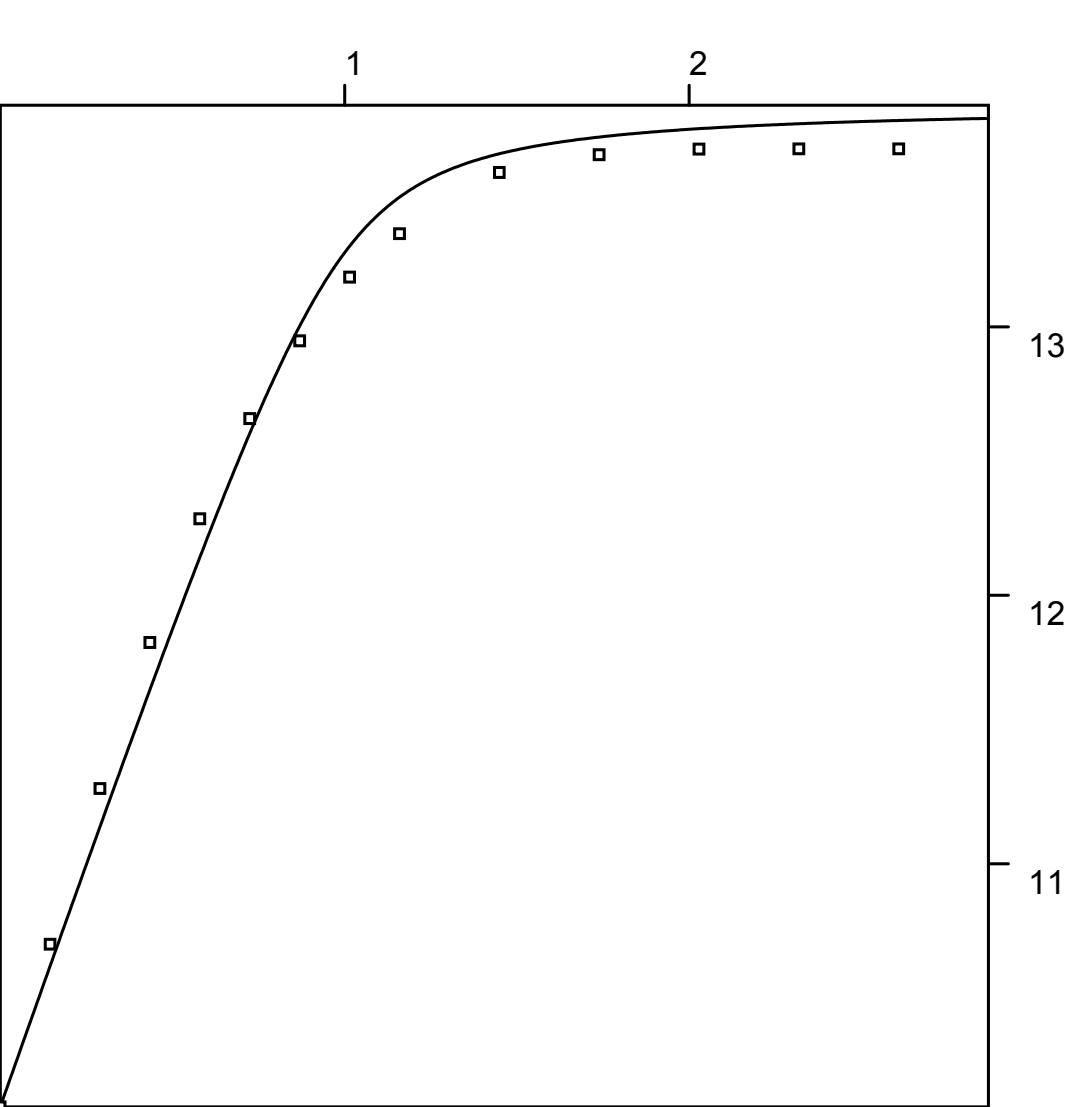
| Desplazamiento | Volumen |
|----------------|---------|
| 10.106         | 0       |
| 10.421         | 0.02    |
| 10.753         | 0.02    |
| 11.073         | 0.02    |
| 11.363         | 0.02    |
| 11.646         | 0.02    |
| 11.866         | 0.02    |
| 12.077         | 0.02    |
| 12.434         | 0.04    |
| 12.683         | 0.04    |
| 12.849         | 0.04    |
| 12.977         | 0.04    |



Constante de Asociación  
Constante: 8.9e+03 1/M  
Despl. Max.: 13.826

Host: Id  
Peso molecular: 572  
Peso puesto (mg): 1.26  
Volumen total (ml): 0.5  
Volumen puesto (ml): 0.5

Guest: Glutarato  
Peso molecular: 614  
Peso puesto(mg): 9.8  
Volumen puesto(ml): 1

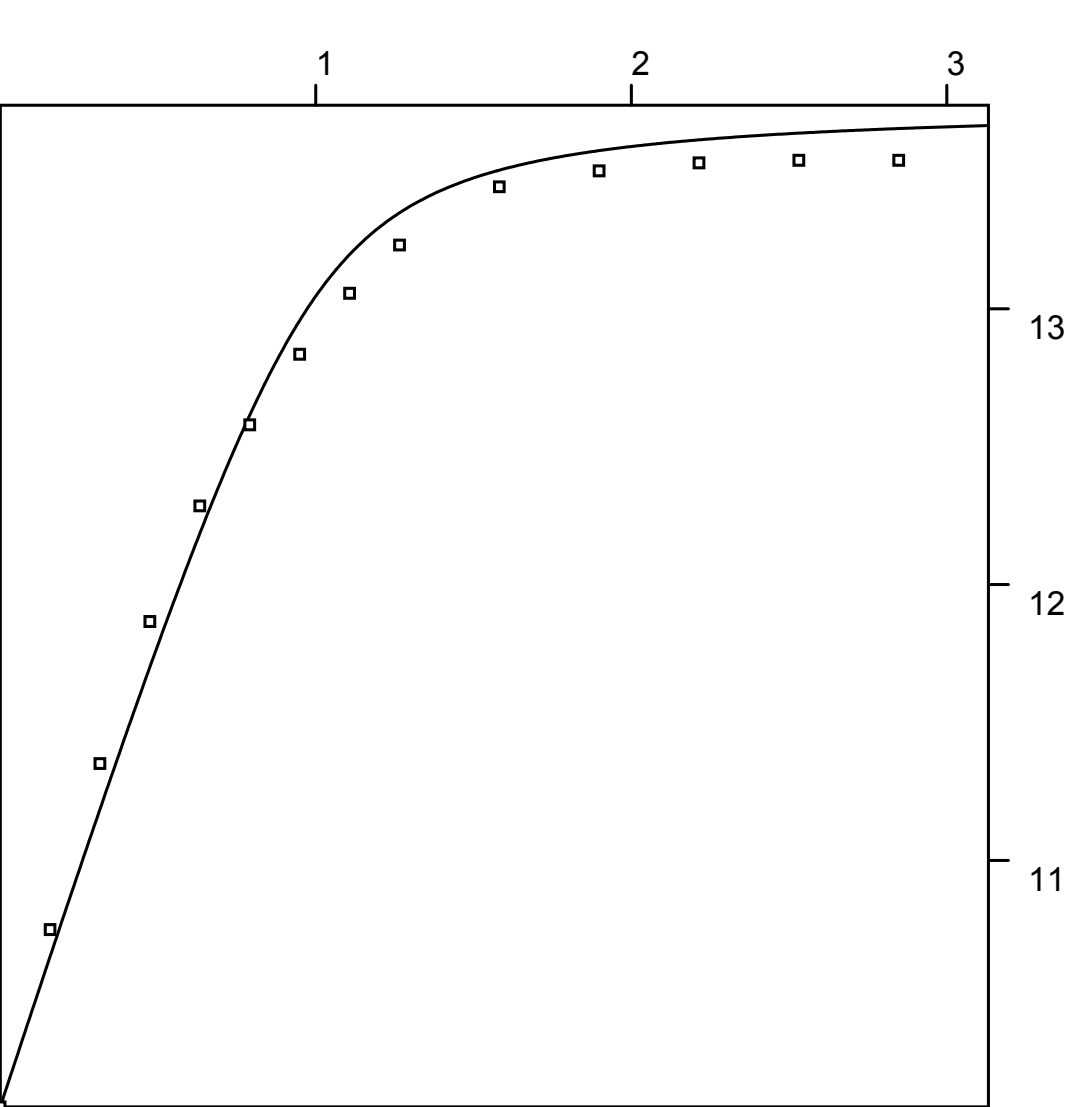


| Desplazamiento | Volumen |
|----------------|---------|
| 10.094         | 0       |
| 10.7           | 0.02    |
| 11.28          | 0.02    |
| 11.824         | 0.02    |
| 12.285         | 0.02    |
| 12.658         | 0.02    |
| 12.948         | 0.02    |
| 13.185         | 0.02    |
| 13.347         | 0.02    |
| 13.575         | 0.04    |
| 13.641         | 0.04    |
| 13.662         | 0.04    |
| 13.663         | 0.04    |
| 13.663         | 0.04    |

Constante de Asociación  
Constante: 5.6e+03 1/M  
Despl. Max.: 13.739

Host: Id  
Peso molecular: 572  
Peso puesto (mg): 1.14  
Volumen total (ml): 0.5  
Volumen puesto (ml): 0.5

Guest: Adipato  
Peso molecular: 628  
Peso puesto(mg): 9.9  
Volumen puesto(ml): 1

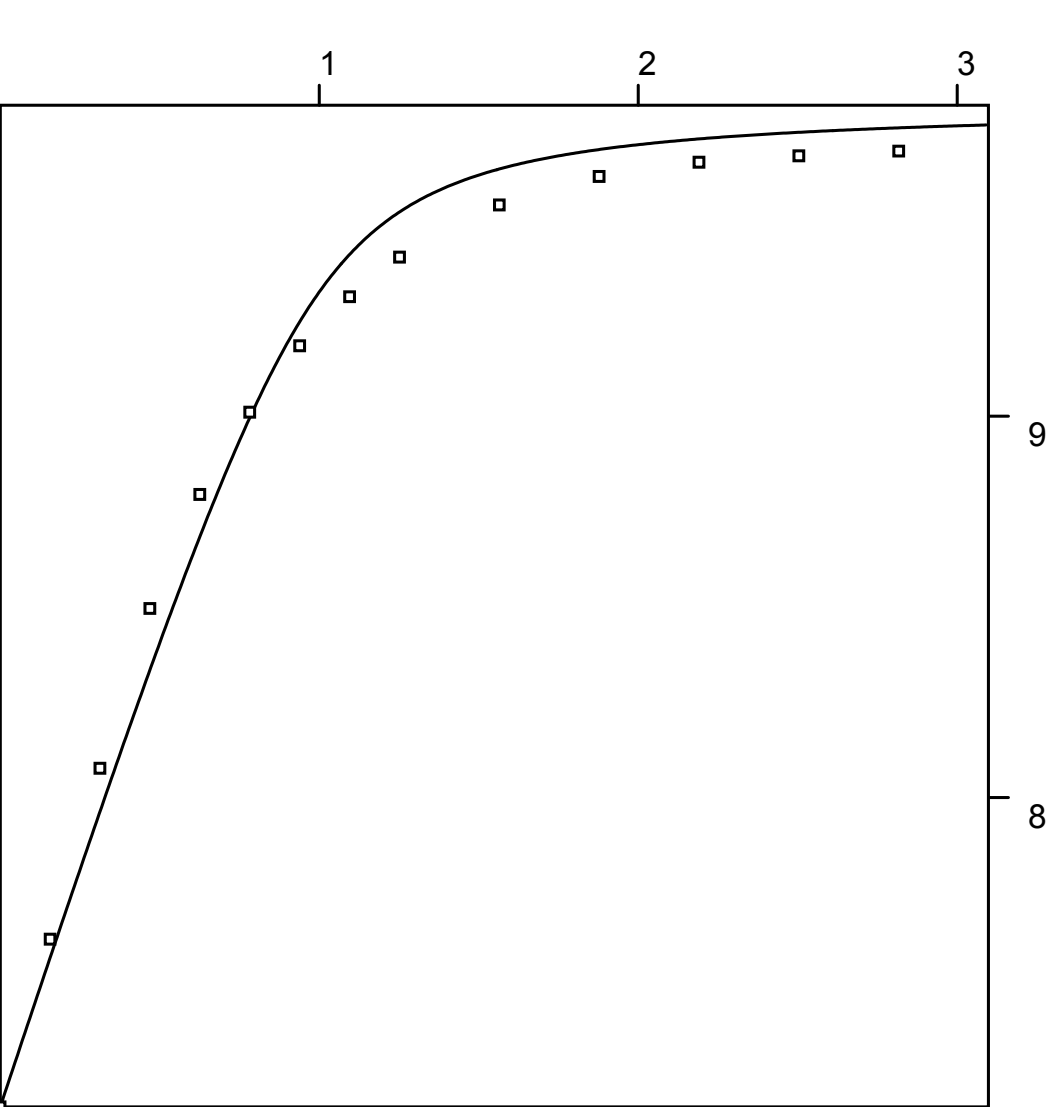


| Desplazamiento | Volumen |
|----------------|---------|
| 10.106         | 0       |
| 10.749         | 0.02    |
| 11.351         | 0.02    |
| 11.866         | 0.02    |
| 12.285         | 0.02    |
| 12.579         | 0.02    |
| 12.835         | 0.02    |
| 13.056         | 0.02    |
| 13.231         | 0.02    |
| 13.442         | 0.04    |
| 13.5           | 0.04    |
| 13.529         | 0.04    |
| 13.538         | 0.04    |
| 13.538         | 0.04    |

Constante de Asociación  
Constante: 5.3e+03 1/M  
Despl. Max.: 9.8159

Host: receptor Id  
Peso molecular: 572  
Peso puesto (mg): 1.26  
Volumen total (ml): 0.5  
Volumen puesto (ml): 0.5

Guest: pimelato cloroformo-DMSO  
Peso molecular: 644  
Peso puesto(mg): 11.1  
Volumen puesto(ml): 1

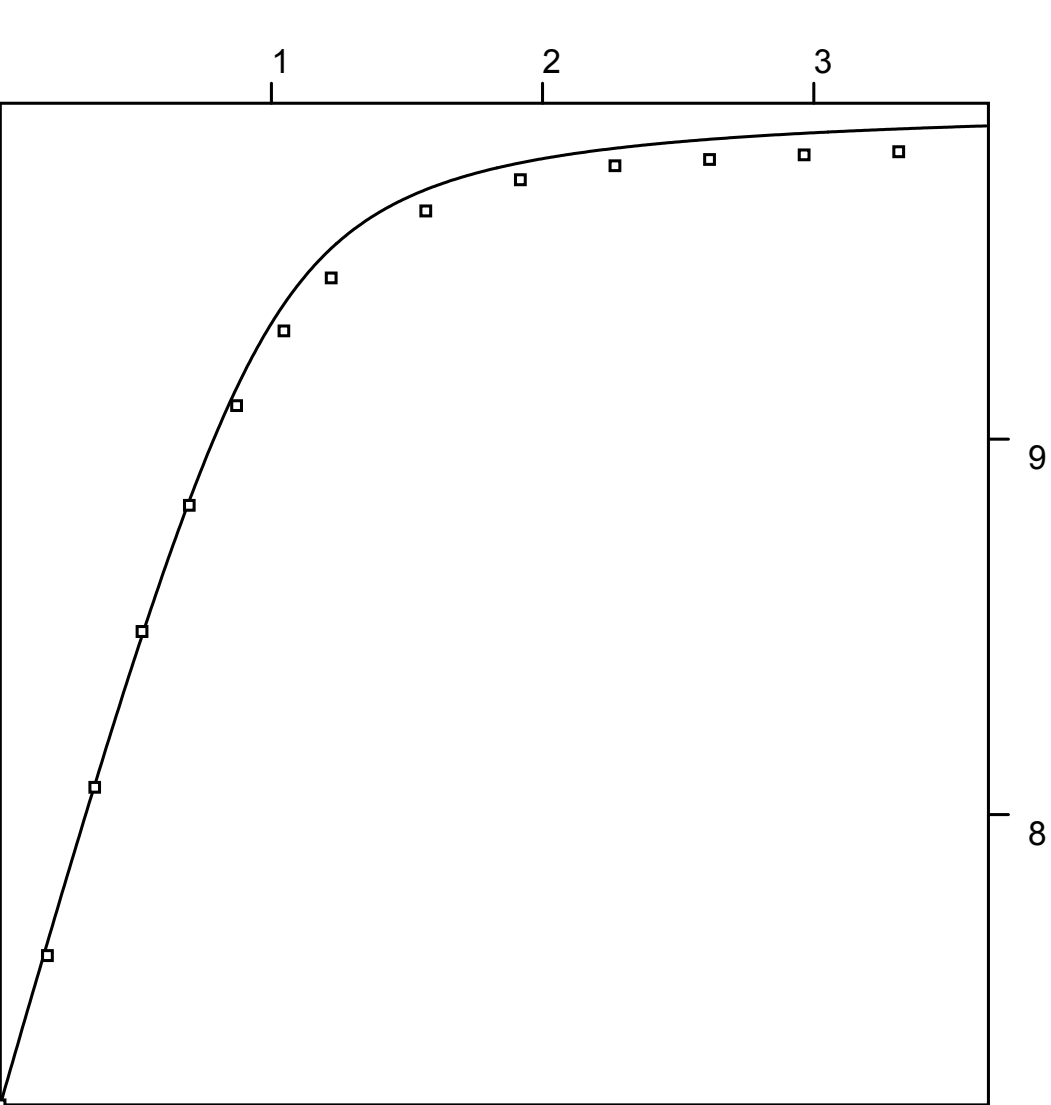


| Desplazamiento | Volumen |
|----------------|---------|
| 7.1887         | 0       |
| 7.6285         | 0.02    |
| 8.0766         | 0.02    |
| 8.4957         | 0.02    |
| 8.7945         | 0.02    |
| 9.0102         | 0.02    |
| 9.1845         | 0.02    |
| 9.3131         | 0.02    |
| 9.4169         | 0.02    |
| 9.5538         | 0.04    |
| 9.6285         | 0.04    |
| 9.6658         | 0.04    |
| 9.6824         | 0.04    |
| 9.6949         | 0.04    |

Constante de Asociación  
Constante: 4e+03 1/M  
Despl. Max.: 9.8952

Host: receptor Id  
Peso molecular: 572  
Peso puesto (mg): 1.14  
Volumen total (ml): 0.5  
Volumen puesto (ml): 0.5

Guest: suberato cloroformo-DMSO  
Peso molecular: 656  
Peso puesto(mg): 11.4  
Volumen puesto(ml): 1

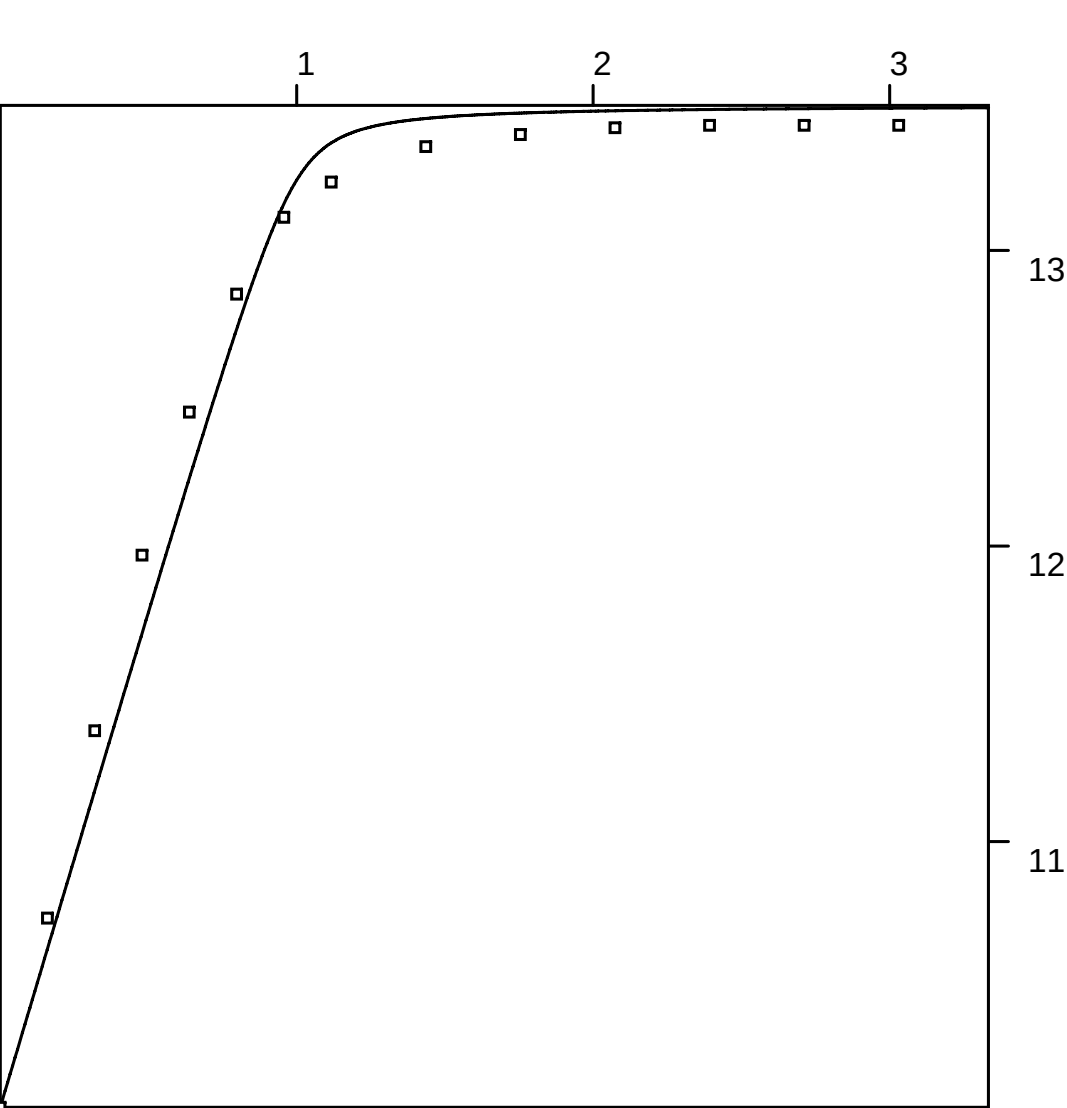


| Desplazamiento | Volumen |
|----------------|---------|
| 7.2266         | 0       |
| 7.6243         | 0.02    |
| 8.0725         | 0.02    |
| 8.4874         | 0.02    |
| 8.8235         | 0.02    |
| 9.0891         | 0.02    |
| 9.2882         | 0.02    |
| 9.4293         | 0.02    |
| 9.6077         | 0.04    |
| 9.6907         | 0.04    |
| 9.7281         | 0.04    |
| 9.7446         | 0.04    |
| 9.7571         | 0.04    |
| 9.7654         | 0.04    |

Constante de Asociación  
Constante: 4.2e+04 1/M  
Despl. Max.: 13.491

Host: receptor Id  
Peso molecular: 572  
Peso puesto (mg): 1.14  
Volumen total (ml): 0.5  
Volumen puesto (ml): 0.5

Guest: isoftalato  
Peso molecular: 648  
Peso puesto(mg): 10.3  
Volumen puesto(ml): 1

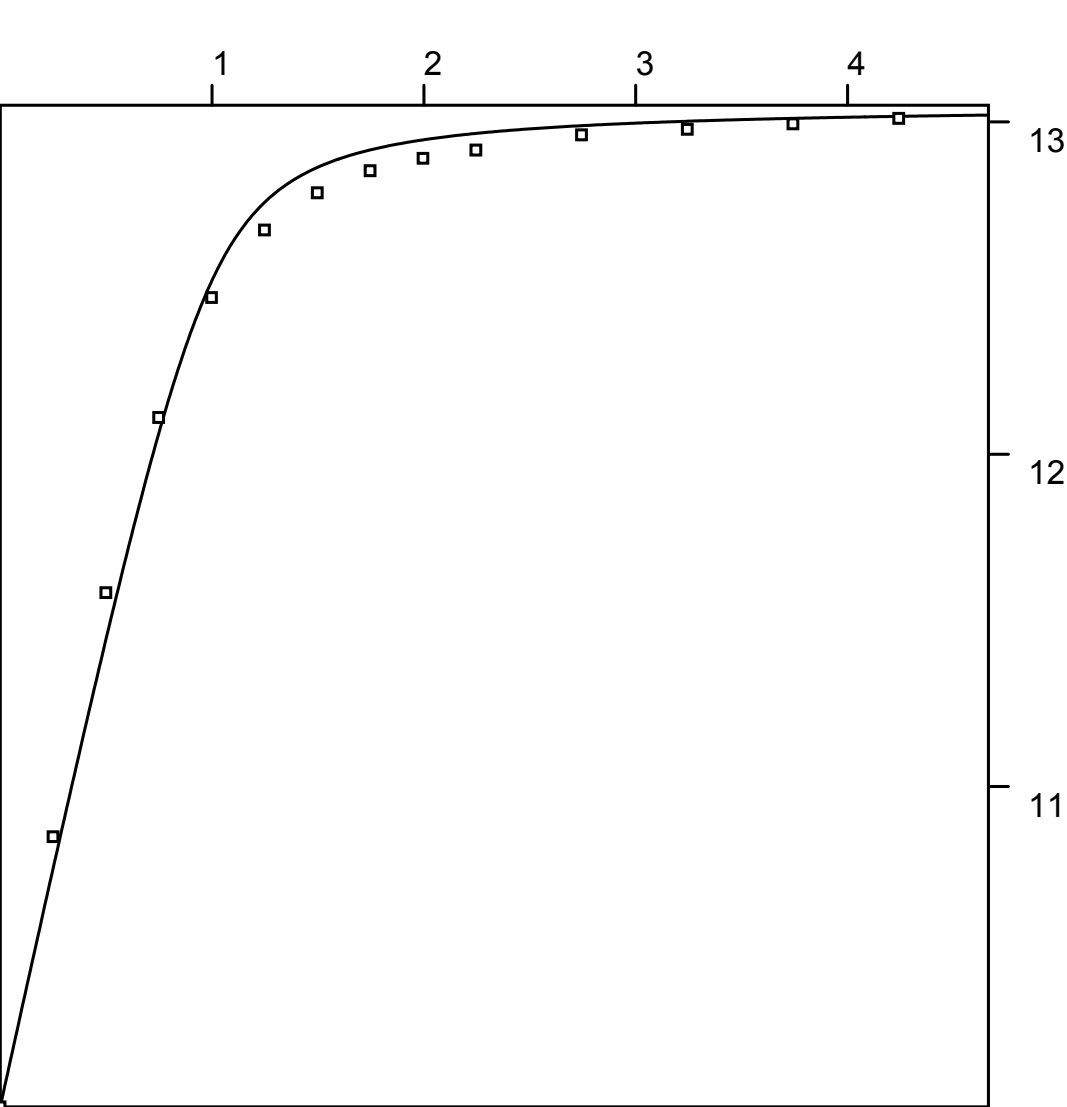


| Desplazamiento | Volumen |
|----------------|---------|
| 0              | 10.101  |
| 0.02           | 10.741  |
| 0.02           | 11.375  |
| 0.02           | 11.969  |
| 0.02           | 12.453  |
| 0.02           | 12.852  |
| 0.02           | 13.112  |
| 0.02           | 13.231  |
| 0.04           | 13.351  |
| 0.04           | 13.392  |
| 0.04           | 13.415  |
| 0.04           | 13.423  |
| 0.04           | 13.423  |
| 0.04           | 13.423  |

Constante de Asociación  
Constante: 1e+04 1/M  
Despl. Max.: 13.051

Host: receptor Id  
Peso molecular: 572  
Peso puesto (mg): 0.75  
Volumen total (ml): 0.5  
Volumen puesto (ml): 0.5

Guest: tereftalato cloroformo-DMSO  
Peso molecular: 648  
Peso puesto(mg): 10.6  
Volumen puesto(ml): 1



| Desplazamiento | Volumen |
|----------------|---------|
| 10.036         | 0       |
| 10.849         | 0.02    |
| 11.583         | 0.02    |
| 12.11          | 0.02    |
| 12.471         | 0.02    |
| 12.675         | 0.02    |
| 12.787         | 0.02    |
| 12.853         | 0.02    |
| 12.89          | 0.02    |
| 12.915         | 0.02    |
| 12.961         | 0.04    |
| 12.977         | 0.04    |
| 12.994         | 0.04    |
| 13.011         | 0.04    |

4 b.- Titration curves of **2** with:

4.1. Succinate

4.2. Glutarate

4.3. Adipate

4.4. Pimelate

4.5. Suberate

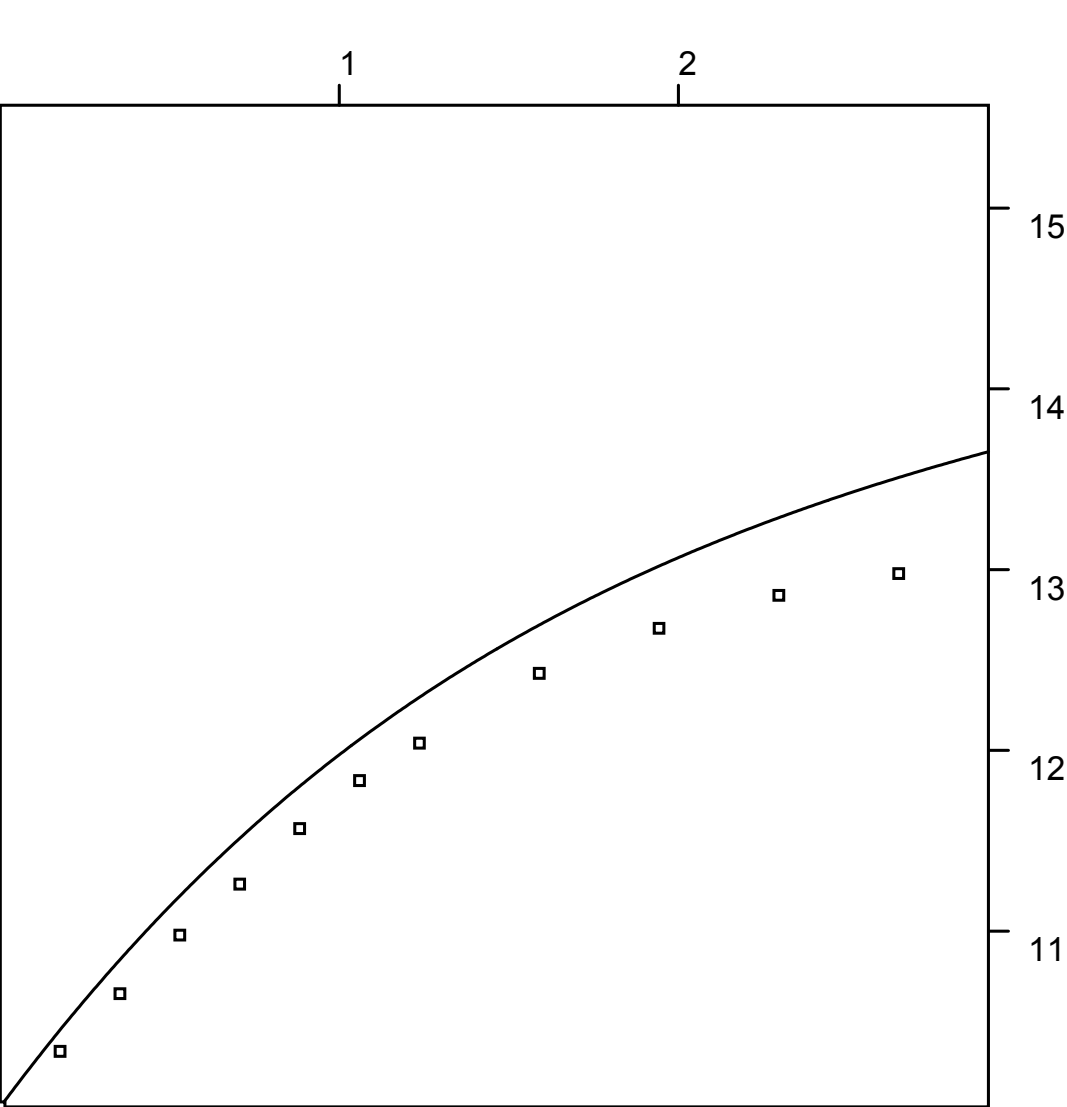
4.6. Isophthalate

4.7. Terphthalate

Constante de Asociación  
Constante: 2.1e+02 1/M  
Despl. Max.: 15.57

Host: receptor Ia  
Peso molecular: 515  
Peso puesto (mg): 1.03  
Volumen total (ml): 0.5  
Volumen puesto (ml): 0.5

Guest: succinato cloroformo-DMSO  
Peso molecular: 600  
Peso puesto(mg): 10.6  
Volumen puesto(ml): 1



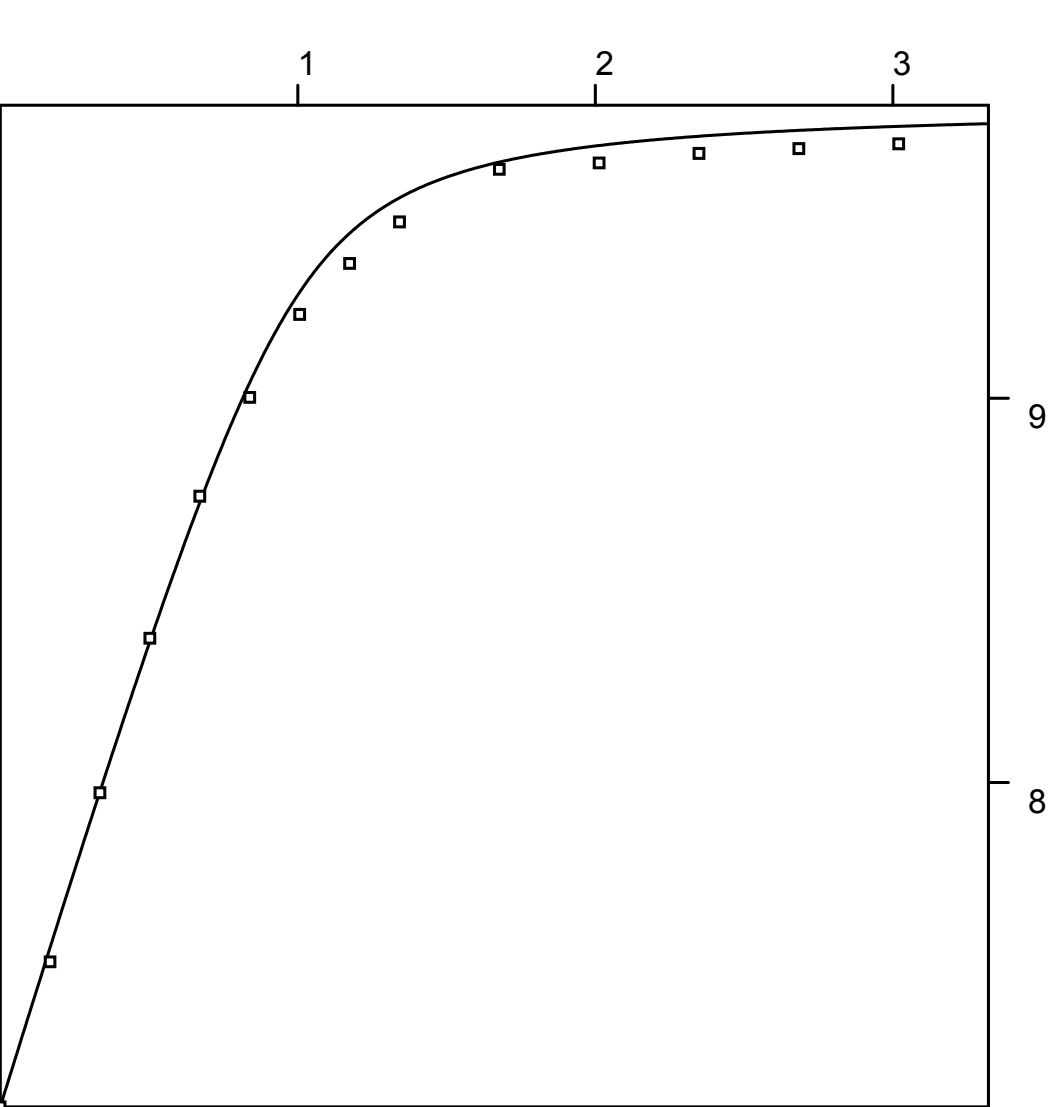
| Desplazamiento | Volumen |
|----------------|---------|
| 10.027         | 0       |
| 10.335         | 0.02    |
| 10.654         | 0.02    |
| 10.978         | 0.02    |
| 11.26          | 0.02    |
| 11.567         | 0.02    |
| 11.832         | 0.02    |
| 12.04          | 0.02    |
| 12.426         | 0.04    |
| 12.675         | 0.04    |
| 12.857         | 0.04    |
| 12.978         | 0.04    |



Constante de Asociación  
Constante: 5.8e+03 1/M  
Despl. Max.: 9.763

Host: receptor Ia  
Peso molecular: 515  
Peso puesto (mg): 1  
Volumen total (ml): 0.5  
Volumen puesto (ml): 0.5

Guest: glutarato cloroformo- DMSO  
Peso molecular: 614  
Peso puesto(mg): 10  
Volumen puesto(ml): 1

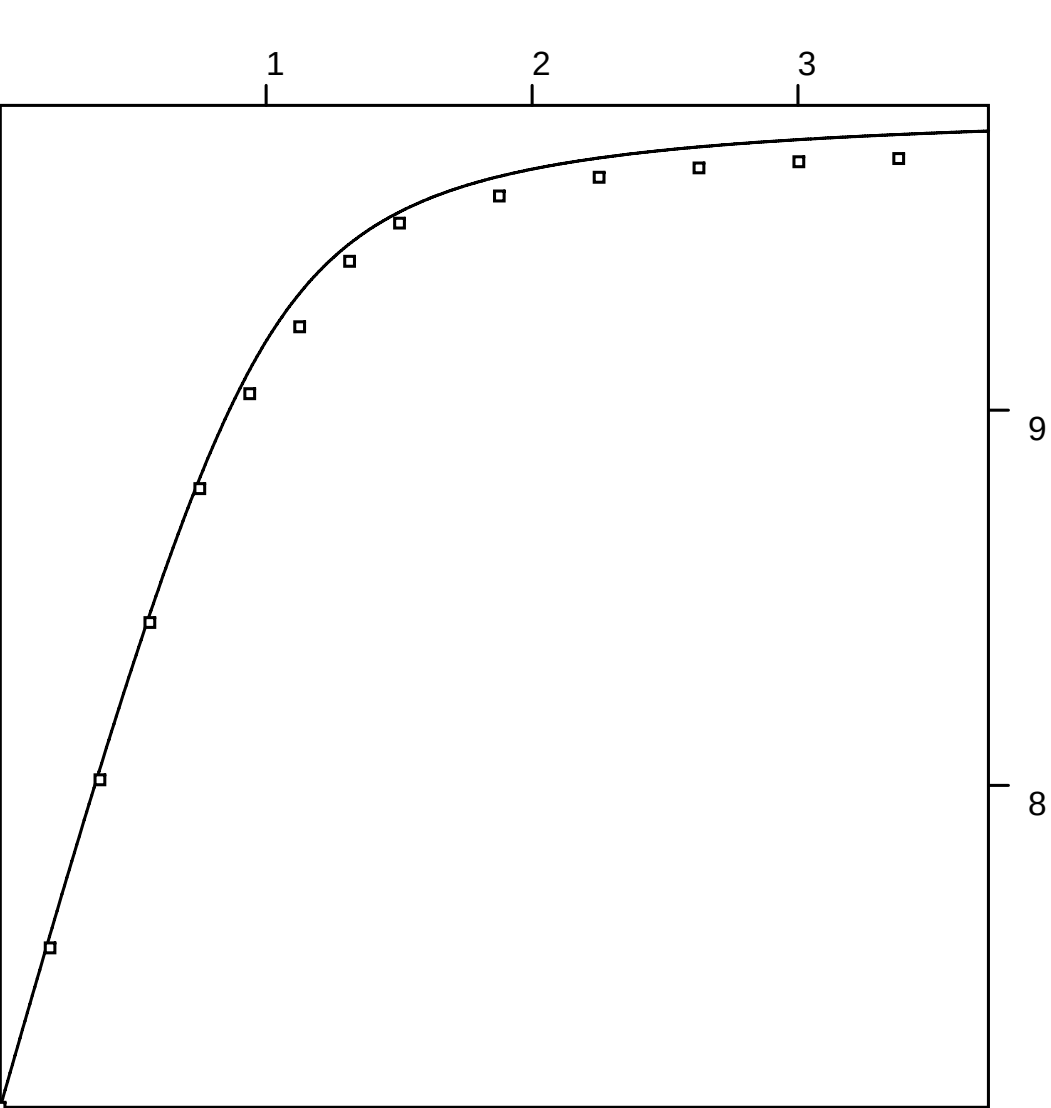


| Desplazamiento | Volumen |
|----------------|---------|
| 7.1557         | 0       |
| 7.5333         | 0.02    |
| 7.9731         | 0.02    |
| 8.3753         | 0.02    |
| 8.7449         | 0.02    |
| 9.0021         | 0.02    |
| 9.2179         | 0.02    |
| 9.3507         | 0.02    |
| 9.4586         | 0.02    |
| 9.5955         | 0.04    |
| 9.6121         | 0.04    |
| 9.637          | 0.04    |
| 9.6494         | 0.04    |
| 9.6619         | 0.04    |

Constante de Asociación  
Constante: 3.9e+03 1/M  
Despl. Max.: 9.8127

Host: ia  
Peso molecular: 515  
Peso puesto (mg): 0.9  
Volumen total (ml): 0.5  
Volumen puesto (ml): 0.5

Guest: adipato  
Peso molecular: 628  
Peso puesto(mg): 10.3  
Volumen puesto(ml): 1

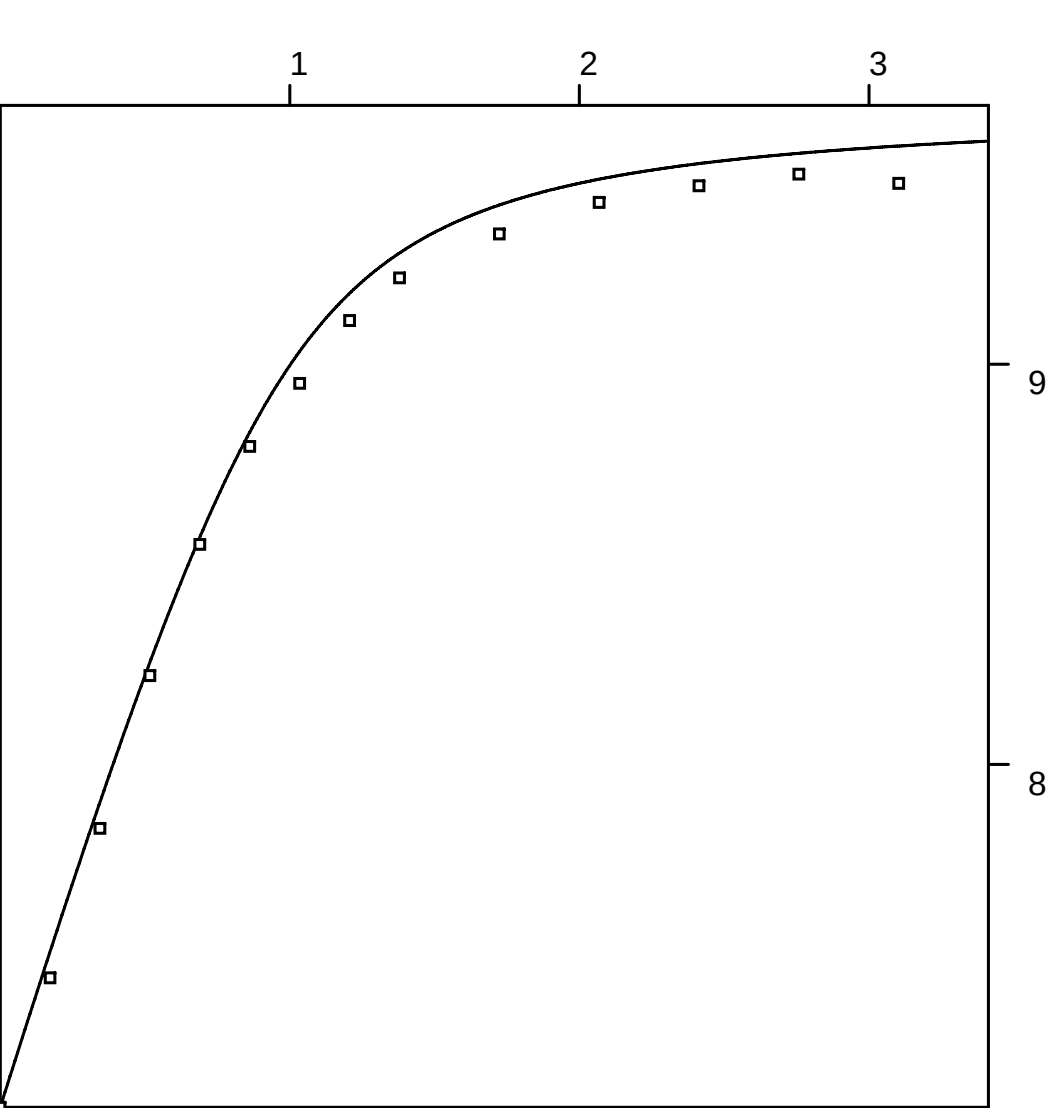


| Desplazamiento | Volumen |
|----------------|---------|
| 7.1417         | 0       |
| 7.5665         | 0.02    |
| 8.0146         | 0.02    |
| 8.4337         | 0.02    |
| 8.7905         | 0.02    |
| 9.0436         | 0.02    |
| 9.222          | 0.02    |
| 9.3965         | 0.02    |
| 9.4982         | 0.02    |
| 9.5706         | 0.04    |
| 9.6204         | 0.04    |
| 9.6453         | 0.04    |
| 9.6619         | 0.04    |
| 9.6702         | 0.04    |

Constante de Asociación  
Constante: 3.1e+03 1/M  
Despl. Max.: 9.6474

Host: ia  
Peso molecular: 515  
Peso puesto (mg): 0.9  
Volumen total (ml): 0.5  
Volumen puesto (ml): 0.5

Guest: pimelato  
Peso molecular: 644  
Peso puesto(mg): 9.7  
Volumen puesto(ml): 1

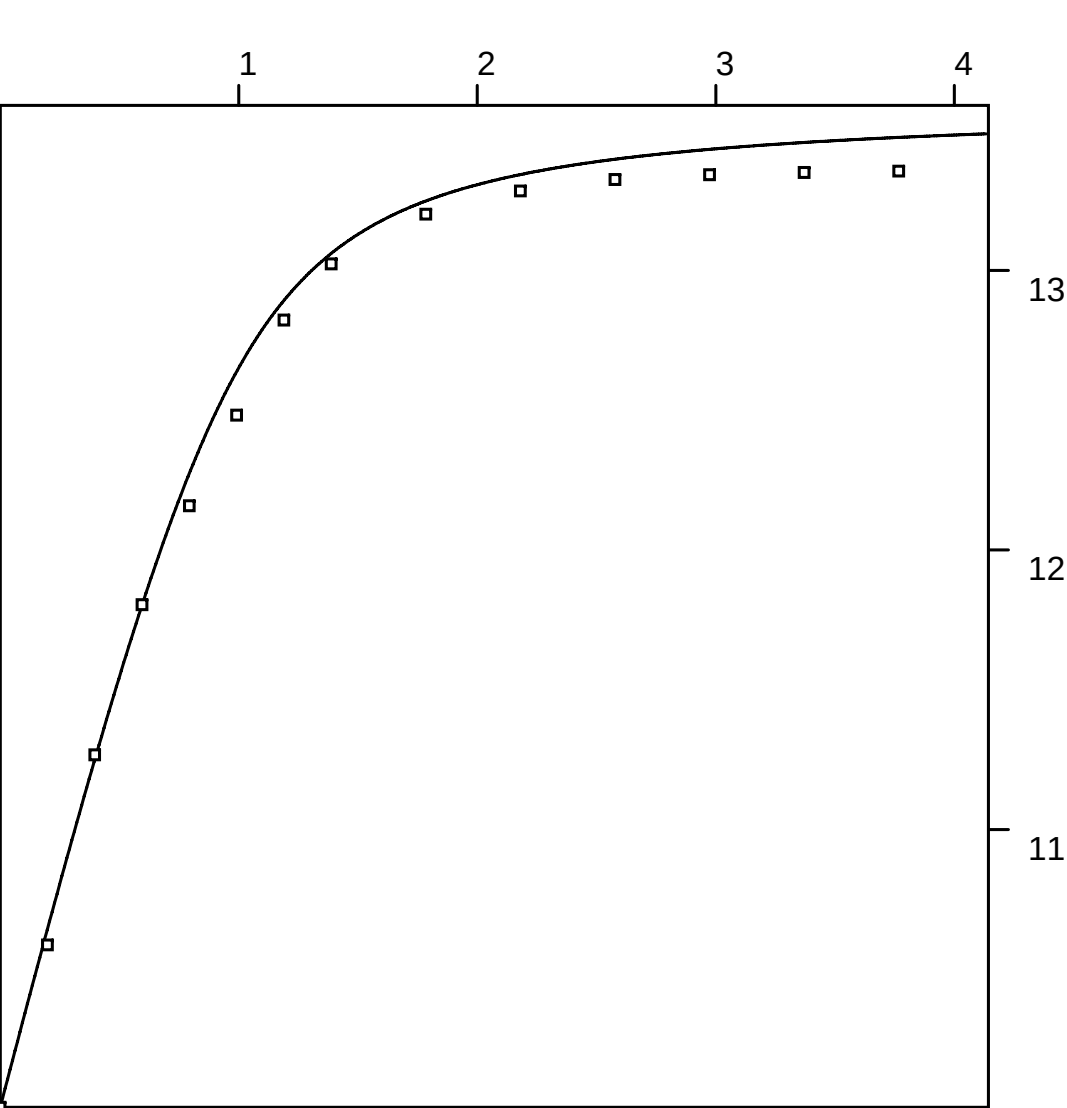


| Desplazamiento | Volumen |
|----------------|---------|
| 7.143          | 0       |
| 7.4667         | 0.02    |
| 7.8401         | 0.02    |
| 8.2219         | 0.02    |
| 8.5496         | 0.02    |
| 8.7945         | 0.02    |
| 8.9521         | 0.02    |
| 9.1091         | 0.02    |
| 9.2157         | 0.02    |
| 9.3256         | 0.04    |
| 9.4044         | 0.04    |
| 9.4459         | 0.04    |
| 9.4749         | 0.04    |
| 9.4519         | 0.04    |

Constante de Asociación  
Constante: 2.8e+03 1/M  
Despl. Max.: 13.591

Host: ia  
Peso molecular: 515  
Peso puesto (mg): 0.99  
Volumen total (ml): 0.5  
Volumen puesto (ml): 0.5

Guest: suberato  
Peso molecular: 656  
Peso puesto(mg): 12.5  
Volumen puesto(ml): 1

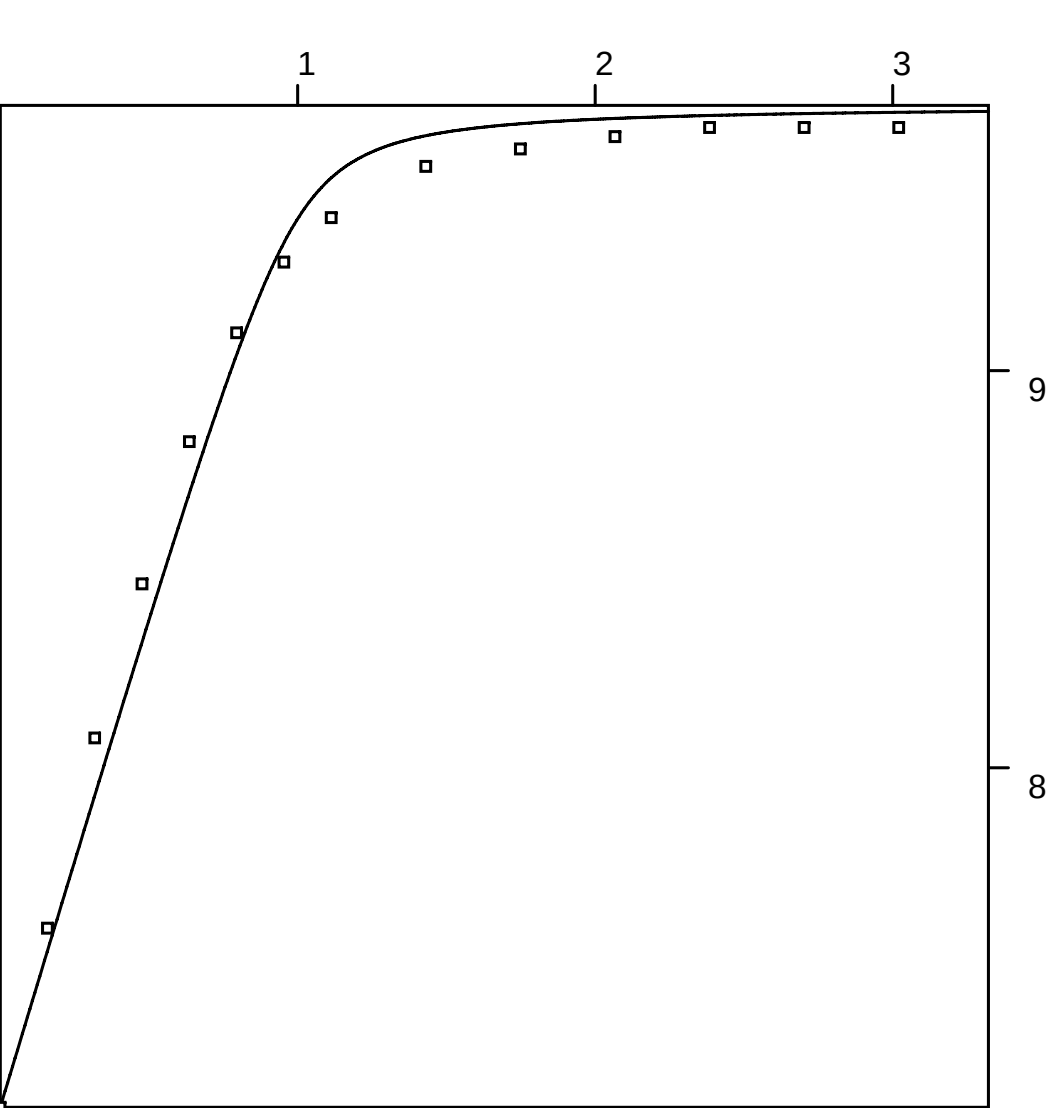


| Desplazamiento | Volumen |
|----------------|---------|
| 10.006         | 0       |
| 10.587         | 0.02    |
| 11.267         | 0.02    |
| 11.804         | 0.02    |
| 12.158         | 0.02    |
| 12.482         | 0.02    |
| 12.822         | 0.02    |
| 13.023         | 0.02    |
| 13.201         | 0.04    |
| 13.284         | 0.04    |
| 13.325         | 0.04    |
| 13.342         | 0.04    |
| 13.35          | 0.04    |
| 13.355         | 0.04    |

Constante de Asociación  
Constante: 1.7e+04 1/M  
Despl. Max.: 9.6683

Host: receptor Ia  
Peso molecular: 515  
Peso puesto (mg): 1.03  
Volumen total (ml): 0.5  
Volumen puesto (ml): 0.5

Guest: isoftalato  
Peso molecular: 648  
Peso puesto(mg): 10.3  
Volumen puesto(ml): 1

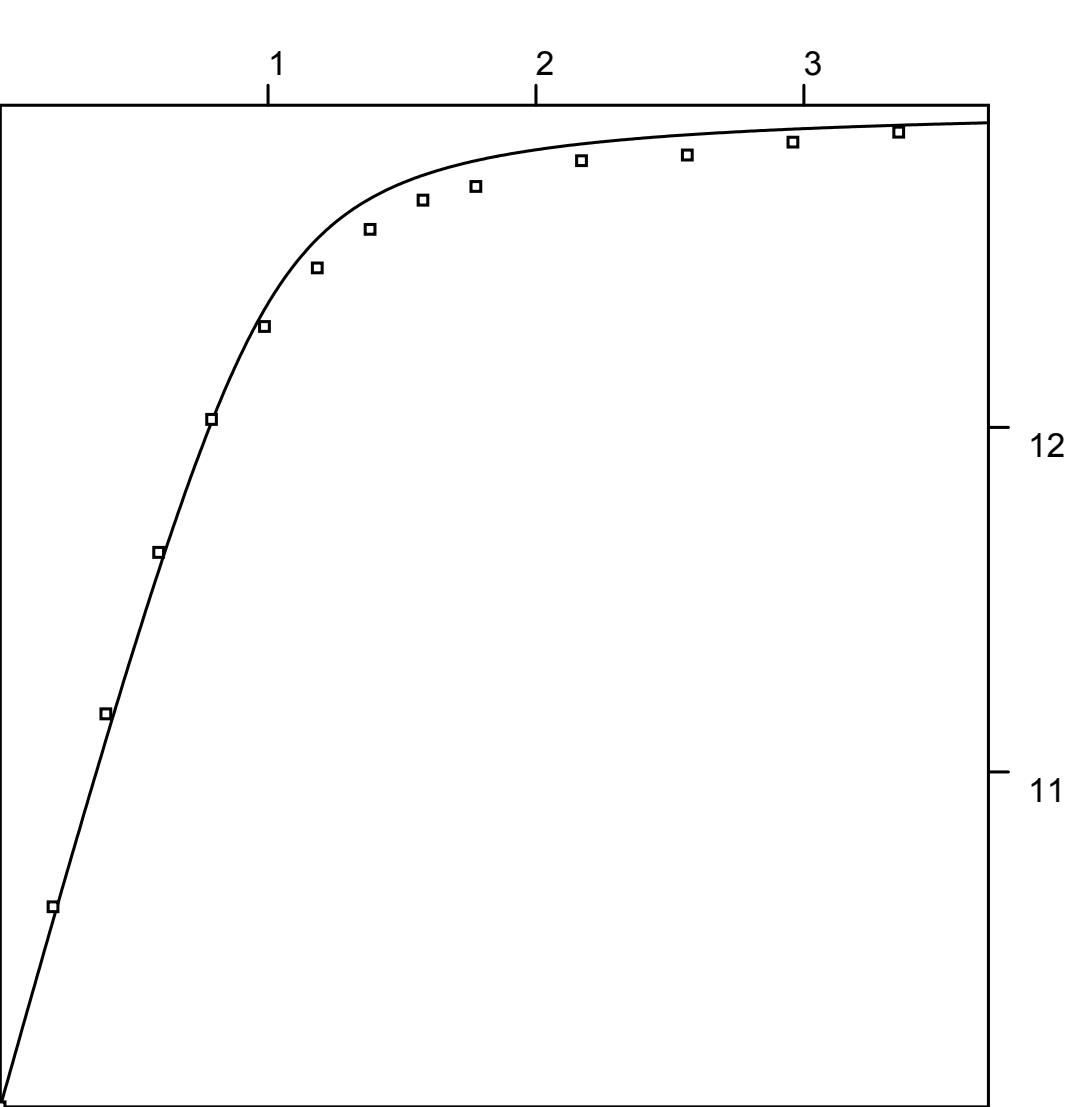


| Desplazamiento | Volumen |
|----------------|---------|
| 7.145          | 0       |
| 7.596          | 0.02    |
| 8.075          | 0.02    |
| 8.463          | 0.02    |
| 8.821          | 0.02    |
| 9.095          | 0.02    |
| 9.273          | 0.02    |
| 9.385          | 0.02    |
| 9.514          | 0.04    |
| 9.558          | 0.04    |
| 9.589          | 0.04    |
| 9.612          | 0.04    |
| 9.612          | 0.04    |
| 9.612          | 0.04    |

Constante de Asociación  
Constante: 6.2e+03 1/M  
Despl. Max.: 12.936

Host: receptor Ia  
Peso molecular: 515  
Peso puesto (mg): 0.85  
Volumen total (ml): 0.5  
Volumen puesto (ml): 0.5

Guest: tereftalato cloroformo-DMSO  
Peso molecular: 648  
Peso puesto(mg): 10.6  
Volumen puesto(ml): 1



| Desplazamiento | Volumen |
|----------------|---------|
| 0              | 10.027  |
| 0.02           | 10.608  |
| 0.02           | 11.168  |
| 0.02           | 11.637  |
| 0.02           | 12.023  |
| 0.02           | 12.293  |
| 0.02           | 12.463  |
| 0.02           | 12.575  |
| 0.02           | 12.66   |
| 0.02           | 12.7    |
| 0.04           | 12.774  |
| 0.04           | 12.791  |
| 0.04           | 12.828  |
| 0.04           | 12.857  |

## 5.- Fluorescence experiments of **1** with glutarate TBA-salt

