

# Supporting Information

## Preparation of Cp-functionalized N-heterocyclic carbene complexes of Ruthenium. Purification of chiral complexes and catalytic studies

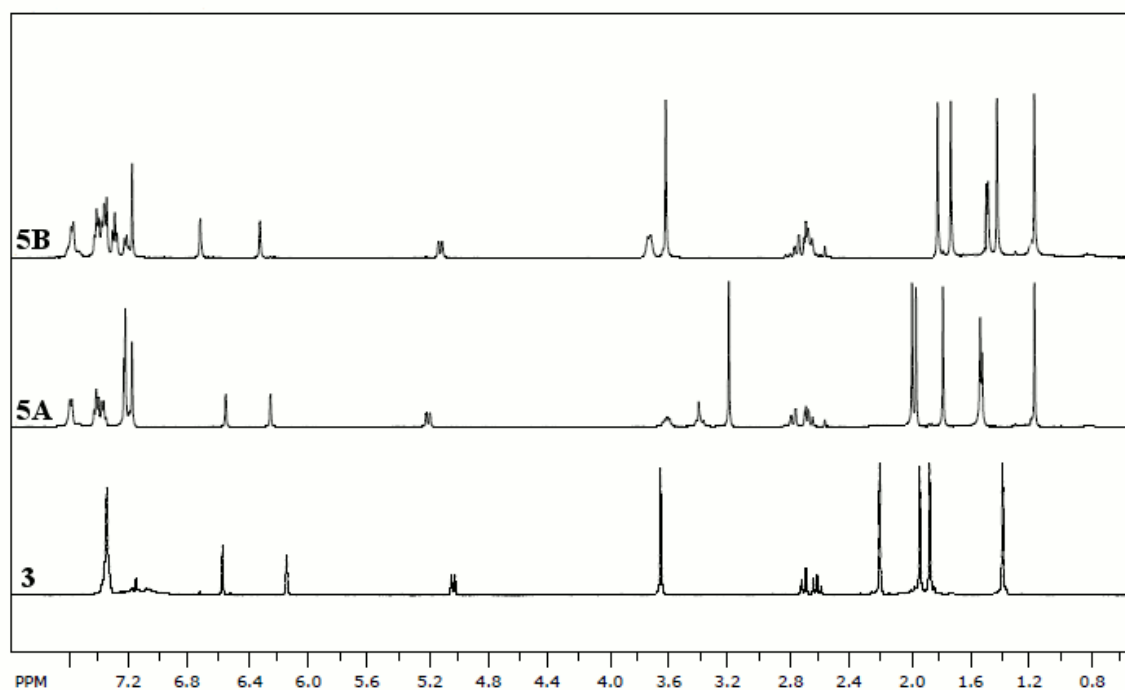
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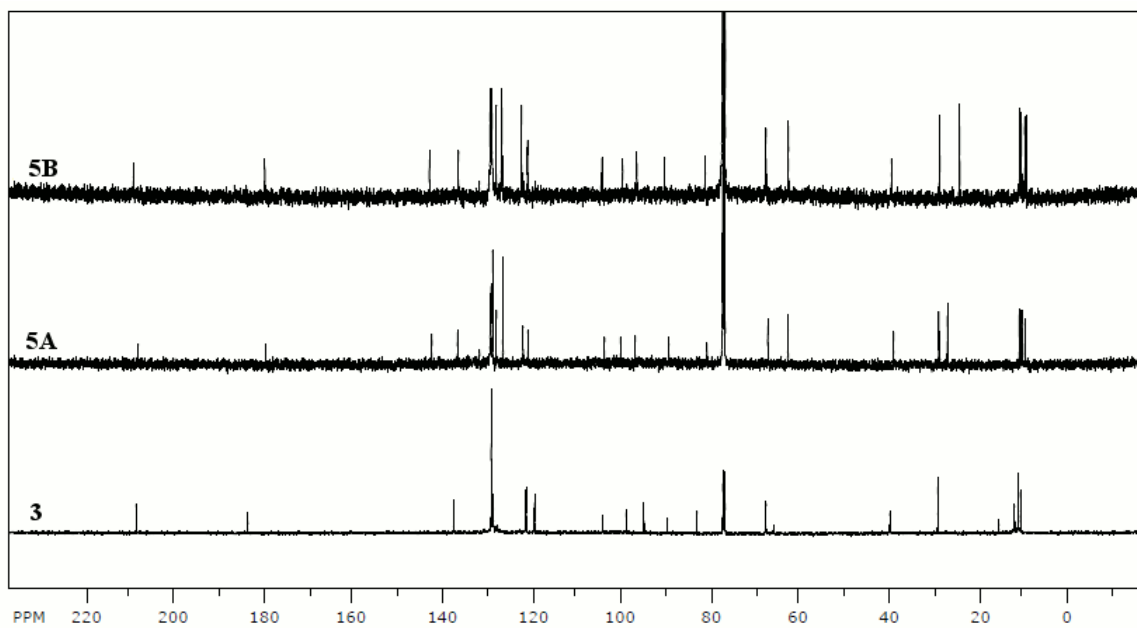
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- 1** – <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) of **3**, **5A** and **5B**
- 2** – <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) of **3**, **5A** and **5B**
- 3** – <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) of **4**
- 4** – <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) of **6A** and **6B**
- 5** – <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) of **4**
- 6** – <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) of **6A**
- 7** – Preparative TLCs for separation of **5** and **6**
- 8** – HRMS (ESI-TOF) of **3**
- 9** – HRMS (ESI-TOF) of **4**
- 10** – HRMS (ESI-TOF) of **5A**
- 11** – HRMS (ESI-TOF) of **5B**
- 12** – HRMS (ESI-TOF) of **6A**
- 13** – HRMS (ESI-TOF) of **6B**

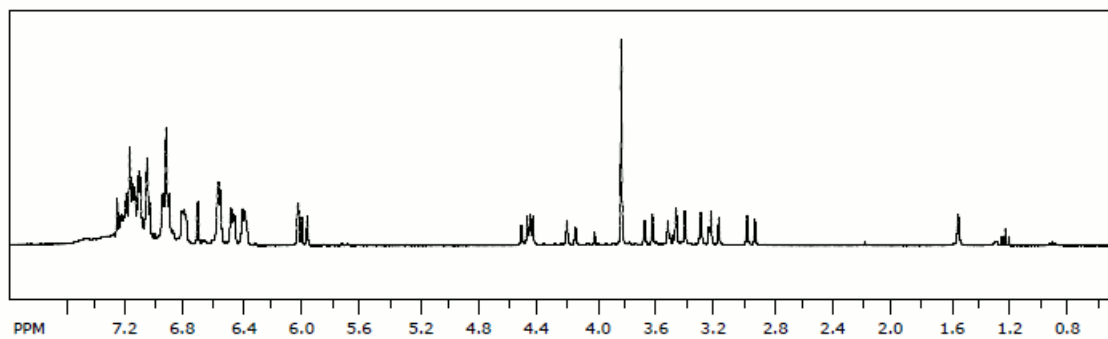
**1 –  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) of **3**, **5A** and **5B****



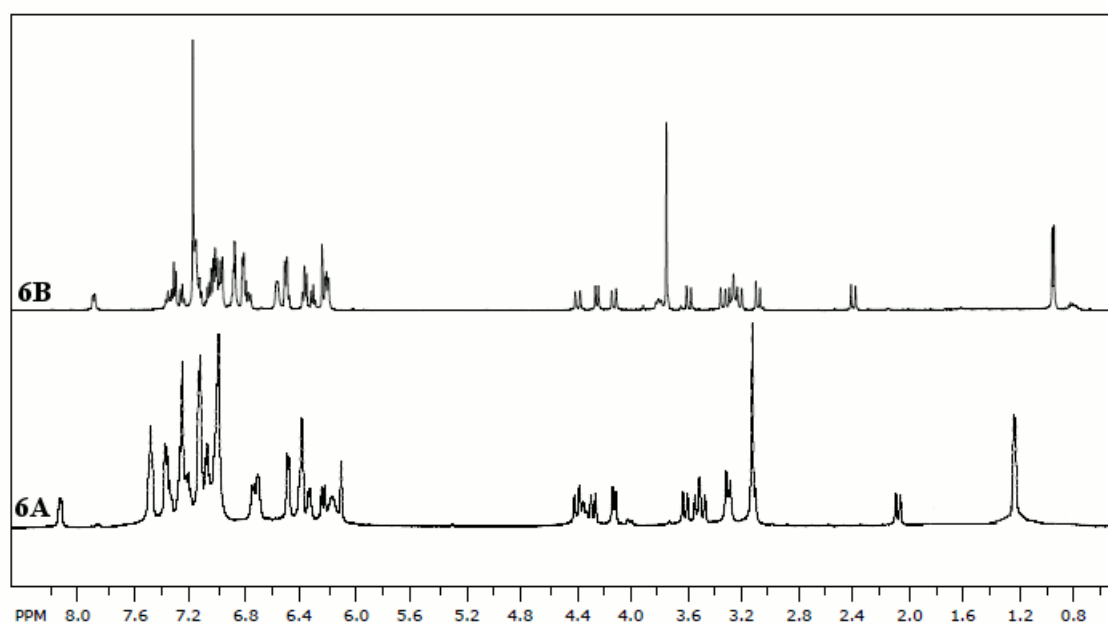
**2 –  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) of **3**, **5A** and **5B****



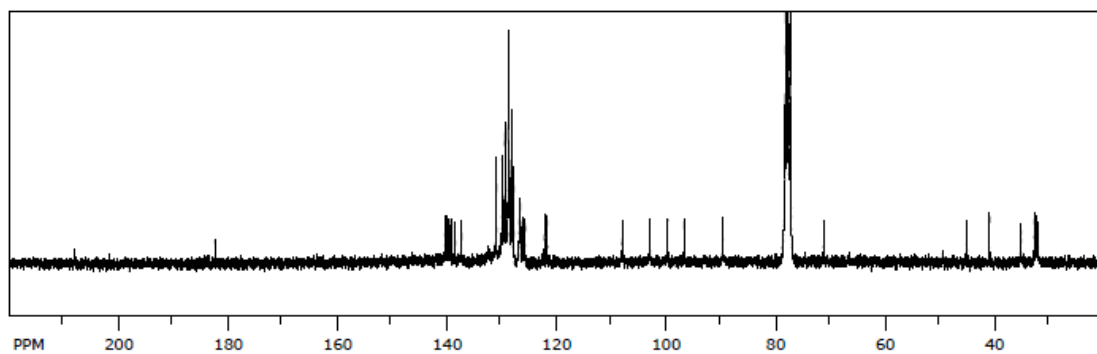
**3** –  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) of **4**



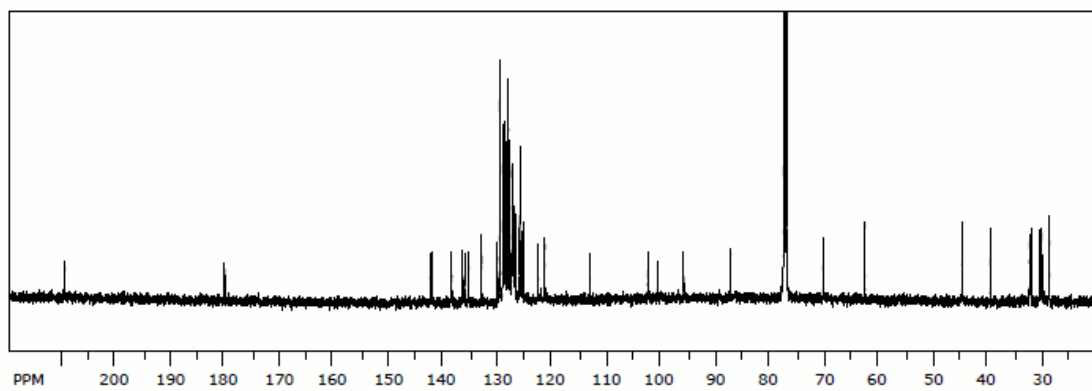
**4** –  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) of **6A** and **6B**



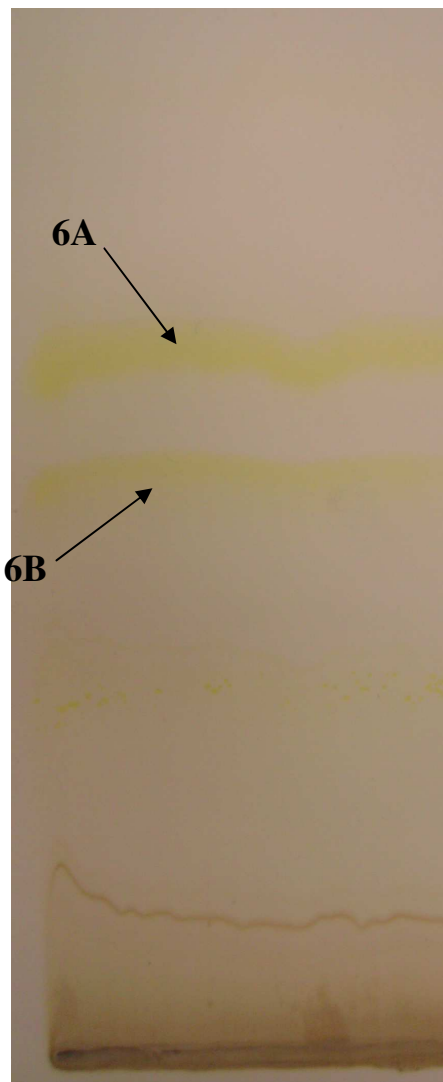
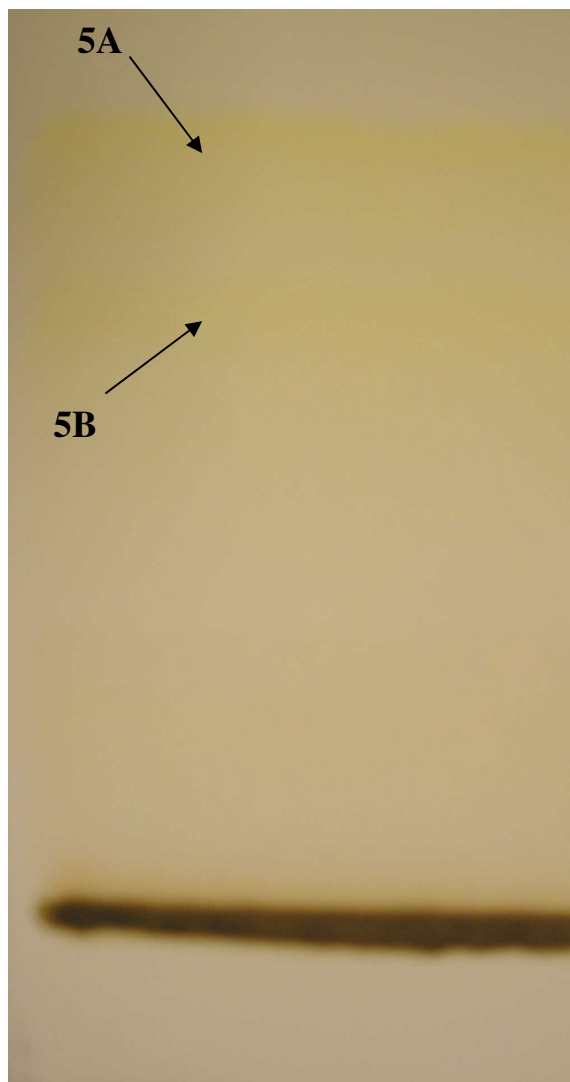
**5** –  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) of **4**



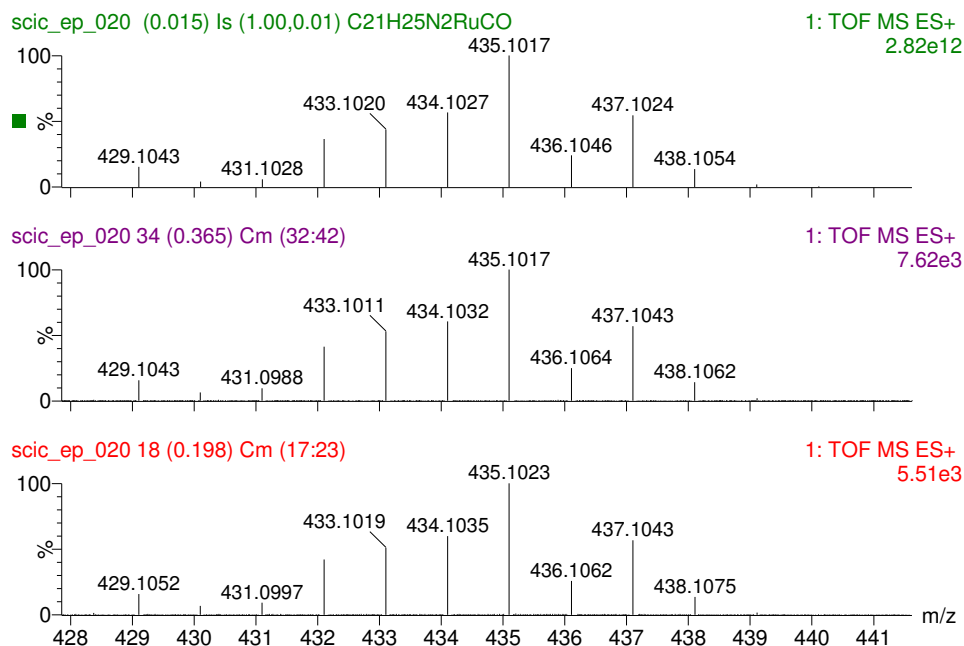
**6** –  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) of **6A**



**7** – Preparative TLCs for separation of **5** and **6**

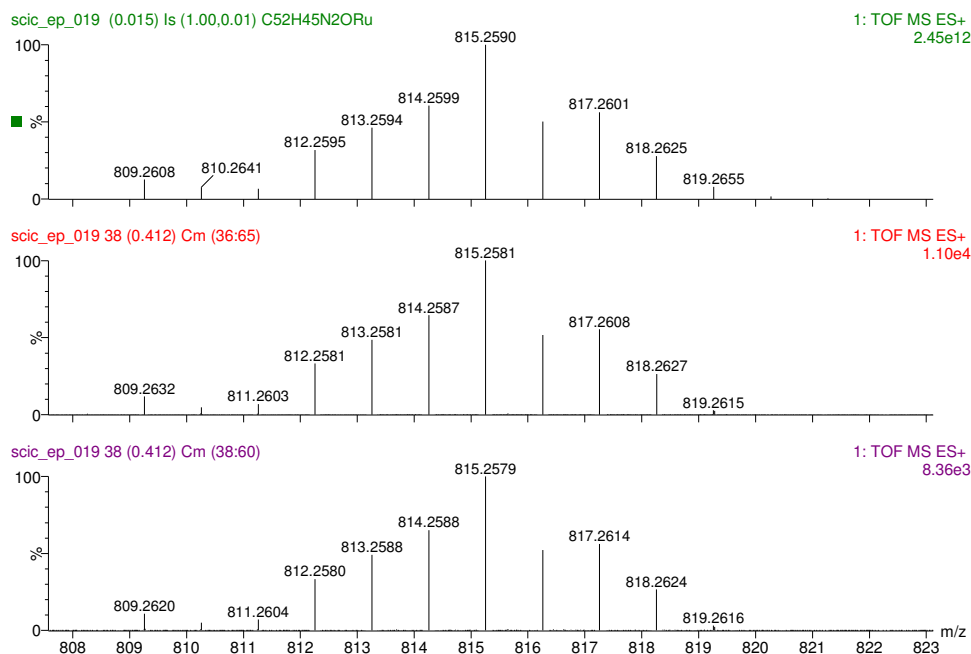


## 8 – HRMS (ESI-TOF) of 3



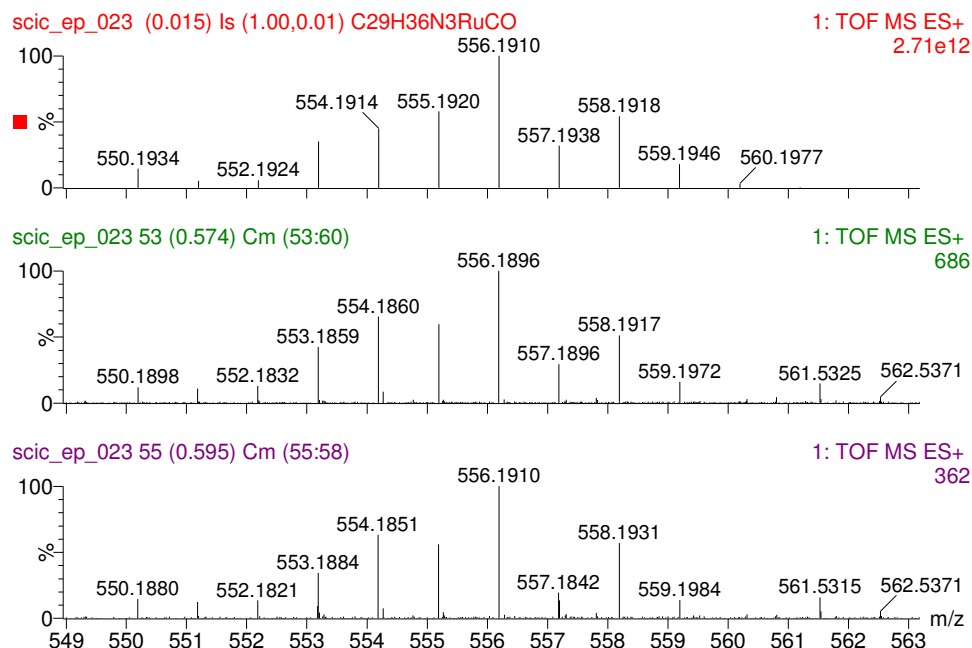
| Peak (m/z) | Experimental mass | Theoretical mass | Relative error (ppm) |
|------------|-------------------|------------------|----------------------|
| 435.1      | 435.1017          | 435.1017         | -                    |
| 435.1      | 435.1023          | 435.1017         | 1.4                  |

## 9 – HRMS (ESI-TOF) of 4



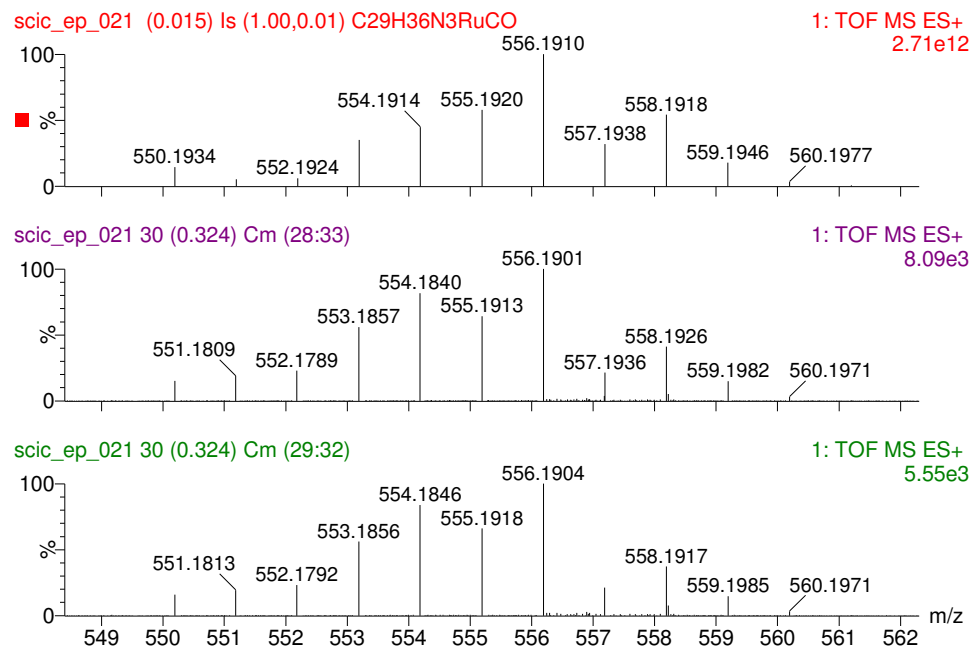
| Peak (m/z) | Experimental mass | Theoretical mass | Relative error (ppm) |
|------------|-------------------|------------------|----------------------|
| 815.3      | 815.2581          | 815.2590         | 1.1                  |
| 815.3      | 815.2579          | 815.2590         | 1.4                  |

## 10 – HRMS (ESI-TOF) of 5A



| Peak (m/z) | Experimental mass | Theoretical mass | Relative error (ppm) |
|------------|-------------------|------------------|----------------------|
| 556.2      | 556.1896          | 556.1910         | 2.5                  |
| 556.2      | 556.1910          | 556.1910         | -                    |

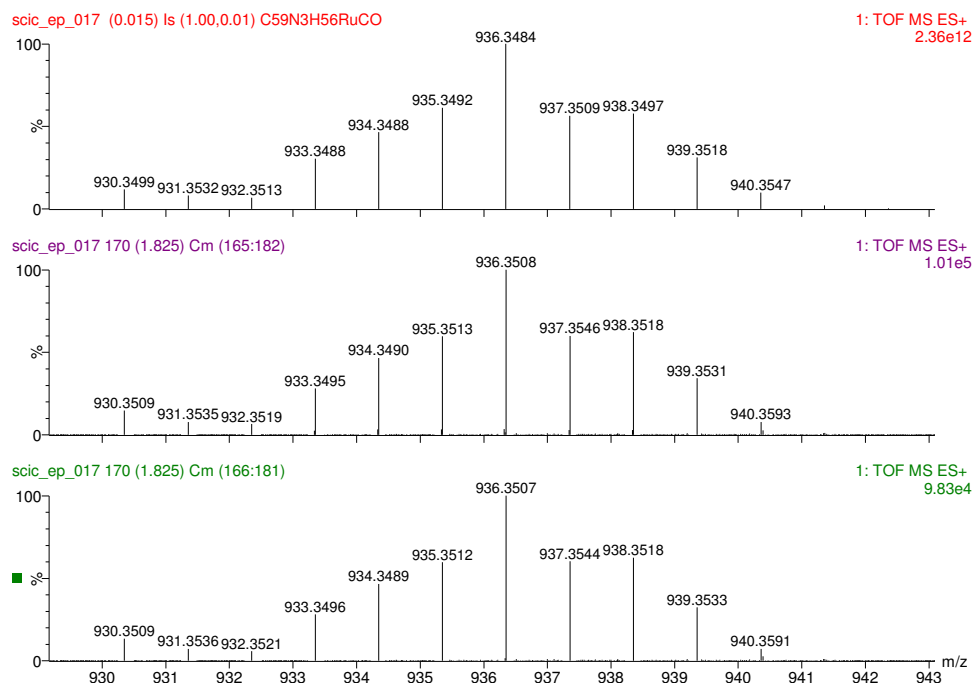
## 11 – HRMS (ESI-TOF) of 5B



| Peak (m/z) | Experimental mass | Theoretical mass | Relative error (ppm) |
|------------|-------------------|------------------|----------------------|
| 556.2      | 936.1901          | 556.1910         | 1.6                  |

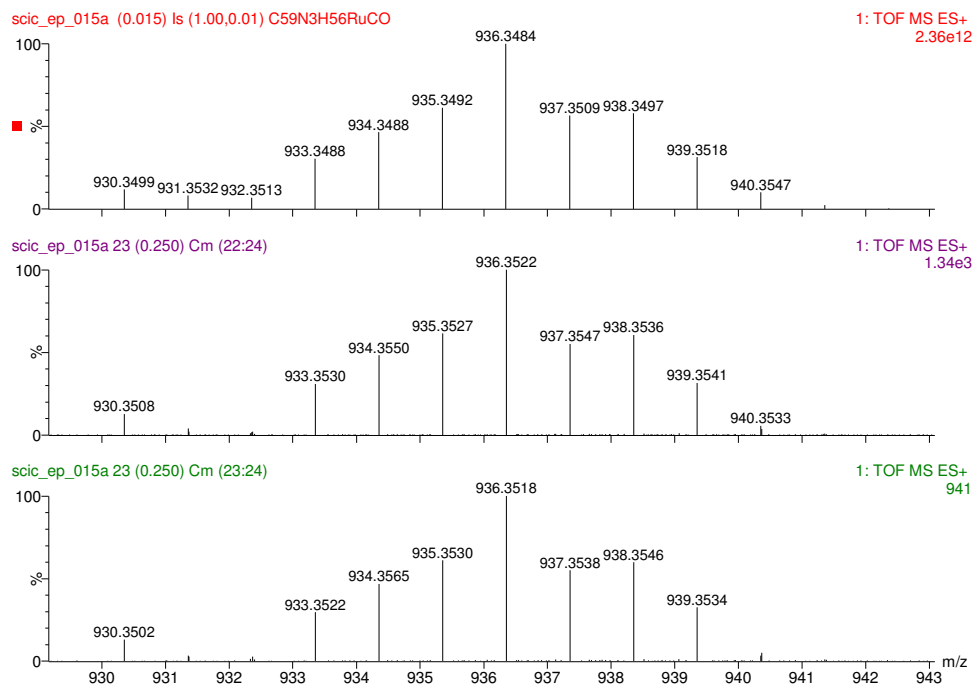
|       |          |          |     |
|-------|----------|----------|-----|
| 556.2 | 936.1904 | 556.1910 | 1.1 |
|-------|----------|----------|-----|

## 12 – HRMS (ESI-TOF) of **6A**



| Peak (m/z) | Experimental mass | Theoretical mass | Relative error (ppm) |
|------------|-------------------|------------------|----------------------|
| 936.4      | 936.3508          | 936.3484         | 2.6                  |
| 936.4      | 936.3507          | 936.3484         | 2.5                  |

## 13 – HRMS (ESI-TOF) of **6B**



| Peak (m/z) | Experimental mass | Theoretical mass | Relative error (ppm) |
|------------|-------------------|------------------|----------------------|
| 936.4      | 936.3522          | 936.3484         | 4.0                  |
| 936.4      | 936.3518          | 936.3484         | 3.6                  |



