



## Supporting Information

for

### **Metal catalyst-free N-allylation/alkylation of imidazole and benzimidazole with Morita–Baylis–Hillman (MBH) alcohols and acetates**

Olfa Mhasni, Jalloul Bouajila and Farhat Rezgui

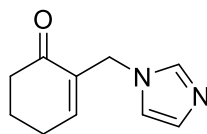
*Beilstein J. Org. Chem.* **2023**, *19*, 1251–1258. [doi:10.3762/bjoc.19.93](https://doi.org/10.3762/bjoc.19.93)

### **$^1\text{H}$ and $^{13}\text{C}$ NMR and HRMS spectra of compounds**

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| ESI-HRMS spectra .....  | S22–S35 |

# $^1\text{H}/^{13}\text{C}$ NMR spectra for compounds 6a–d, 7a–d, 8a–f



6a

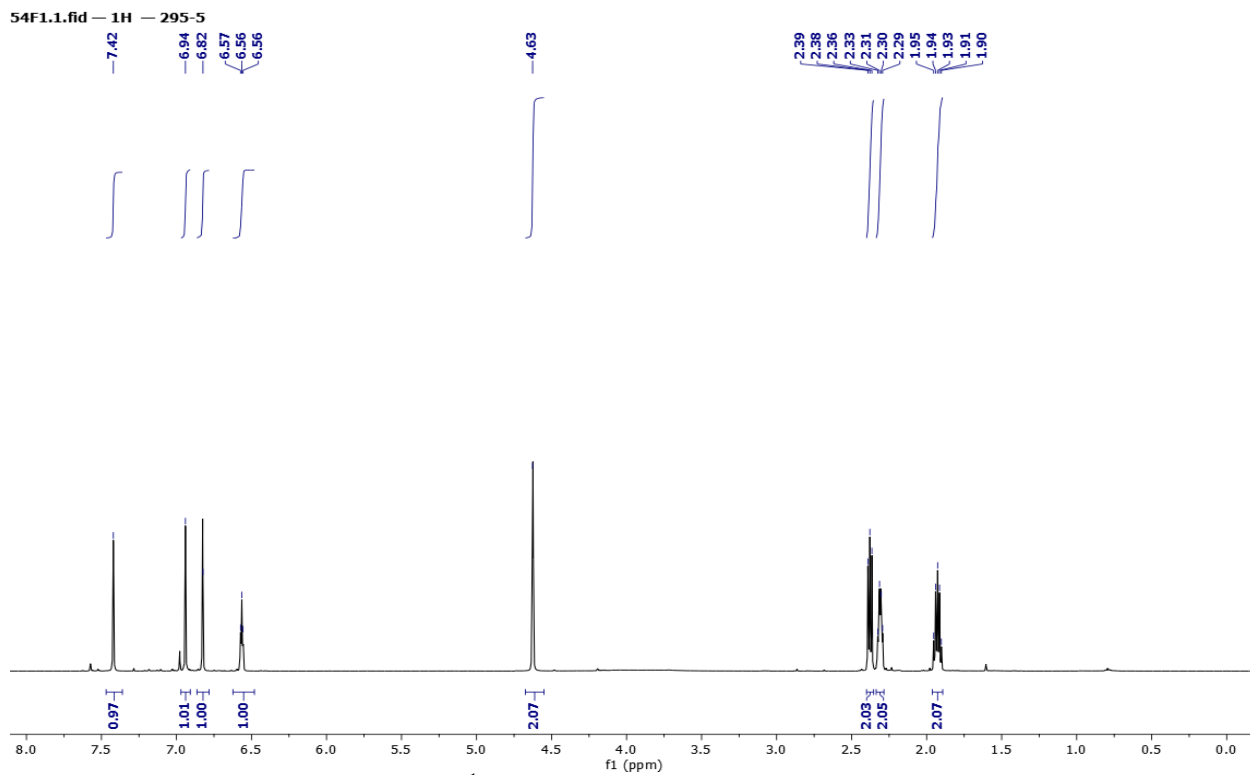


Figure S1.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectra of 6a

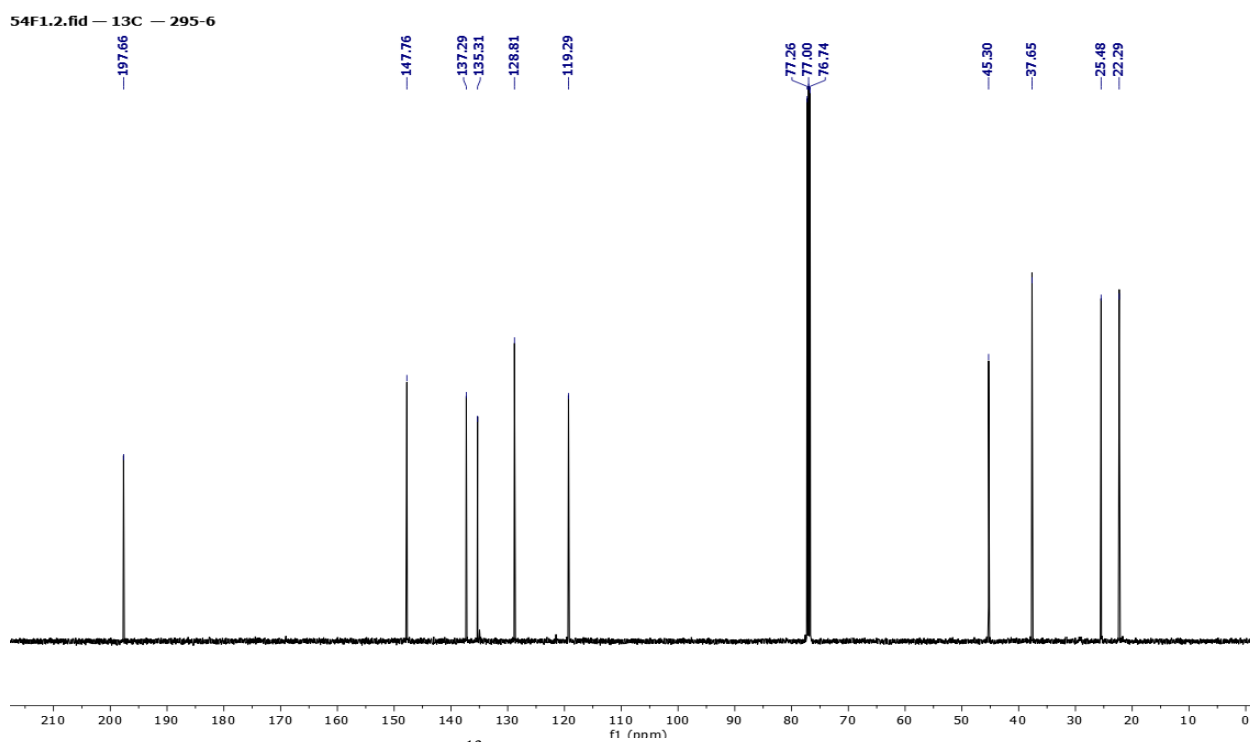


Figure S2.  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectra of 6a

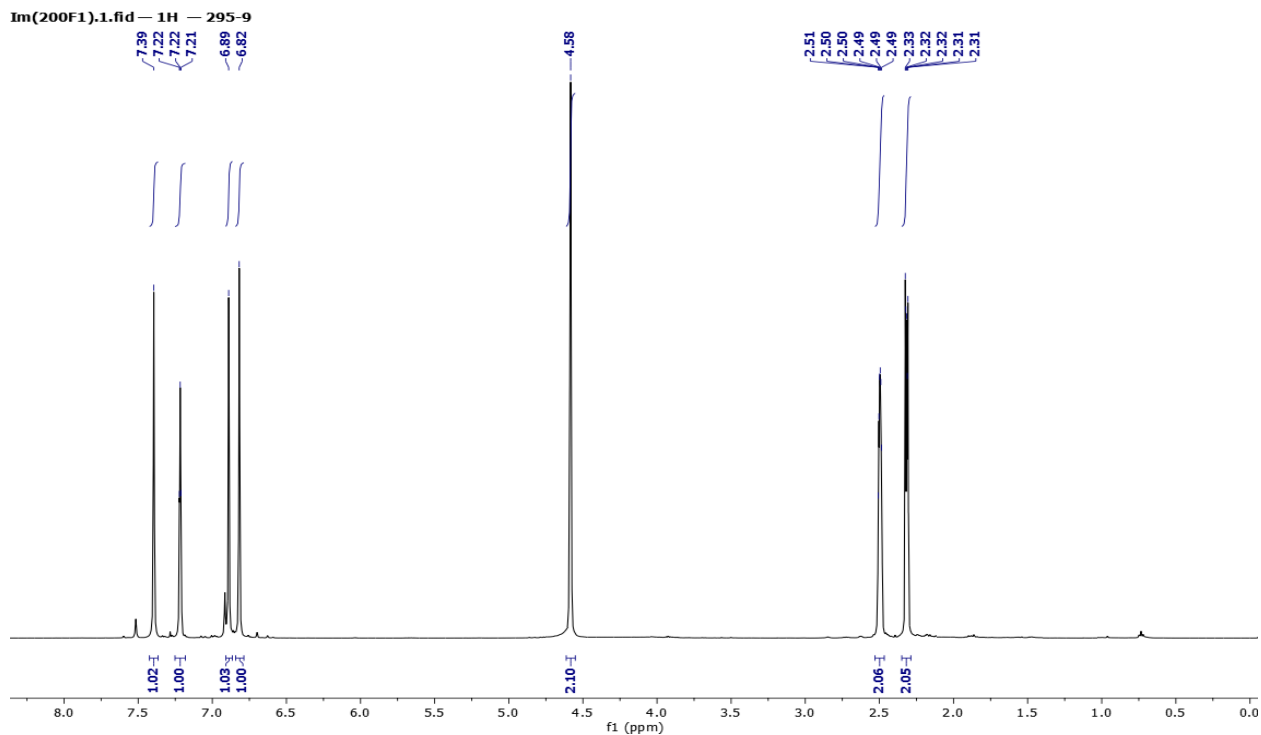
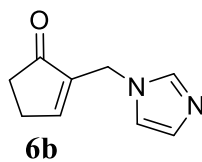


Figure S3.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectra of **6b**

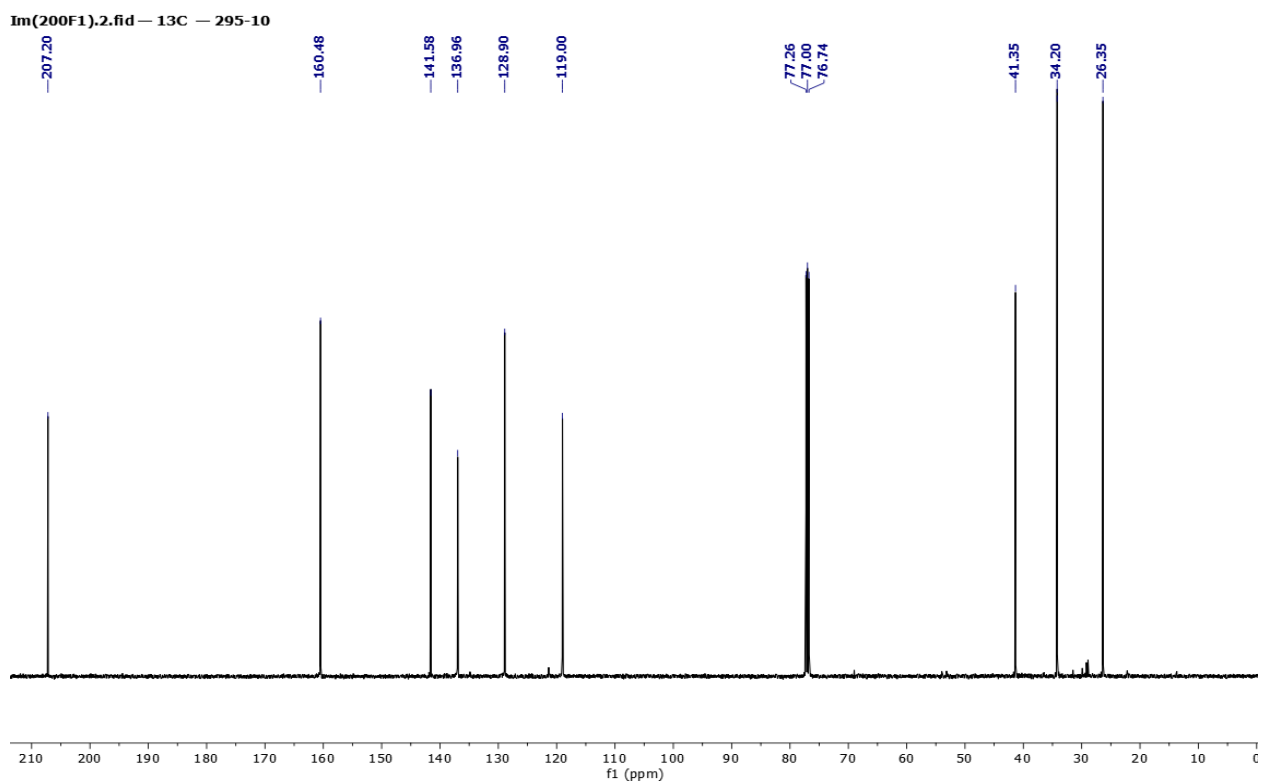
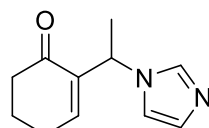
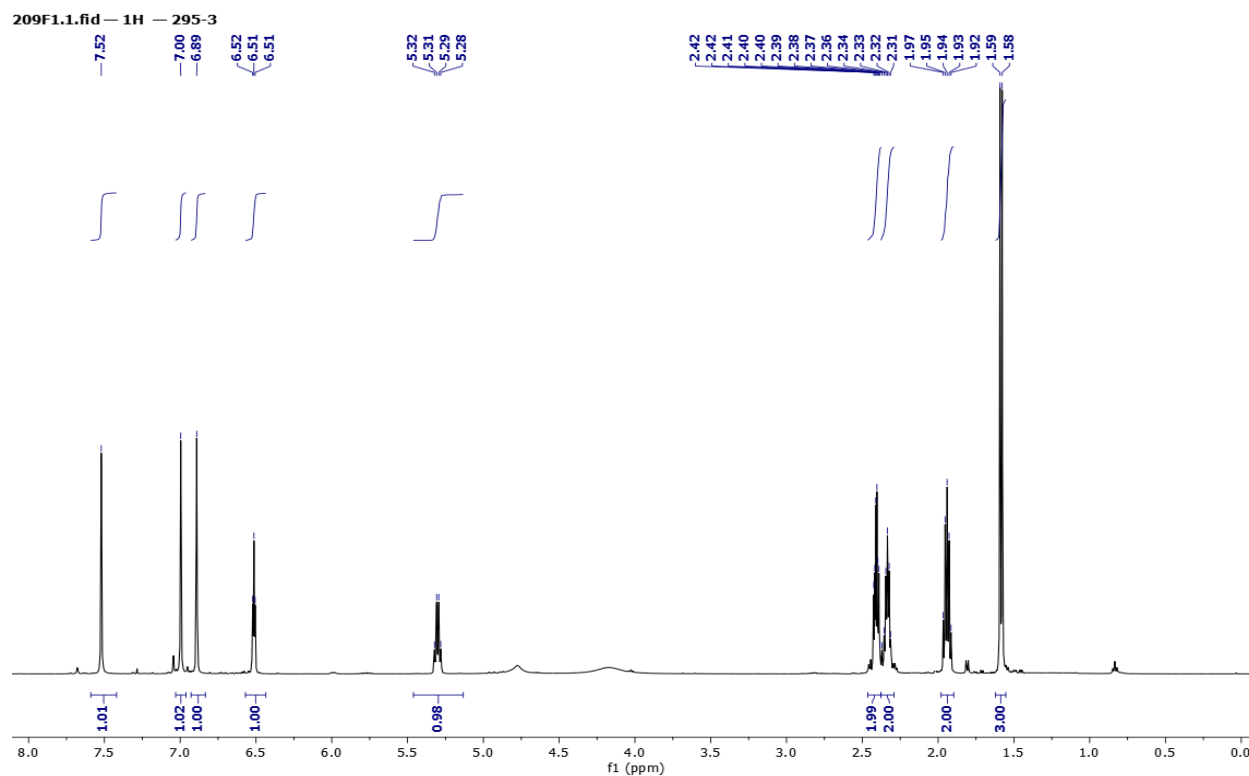


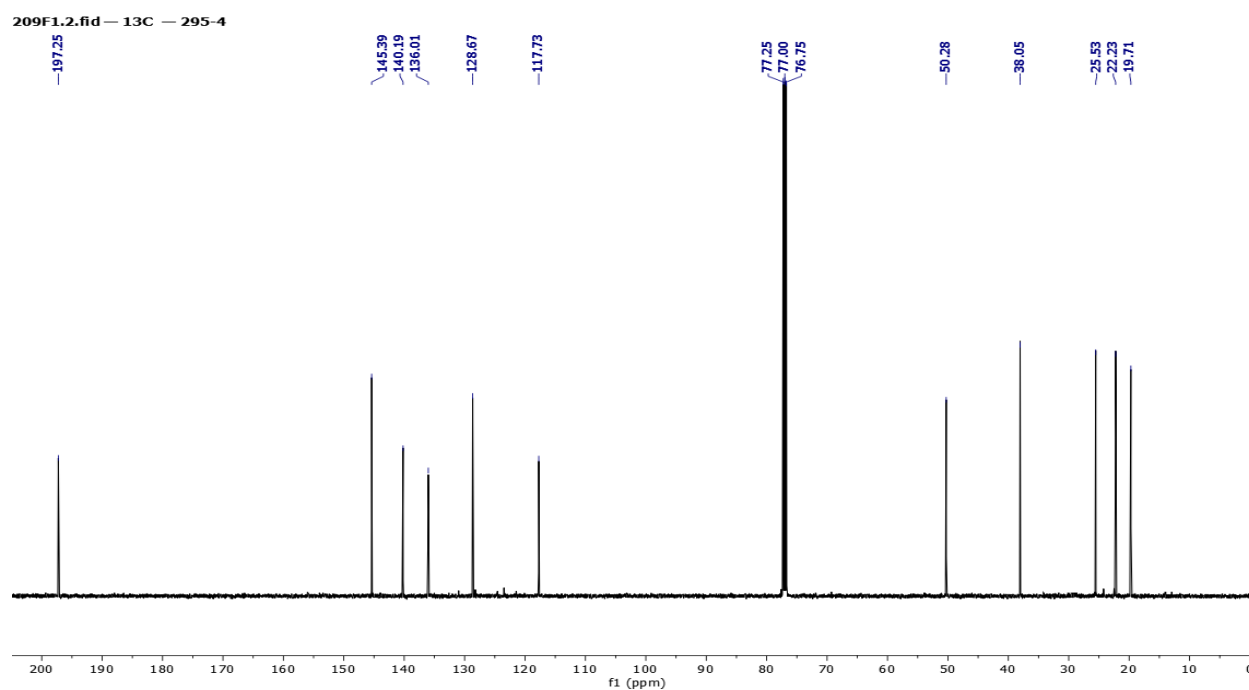
Figure S4.  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectra of **6b**



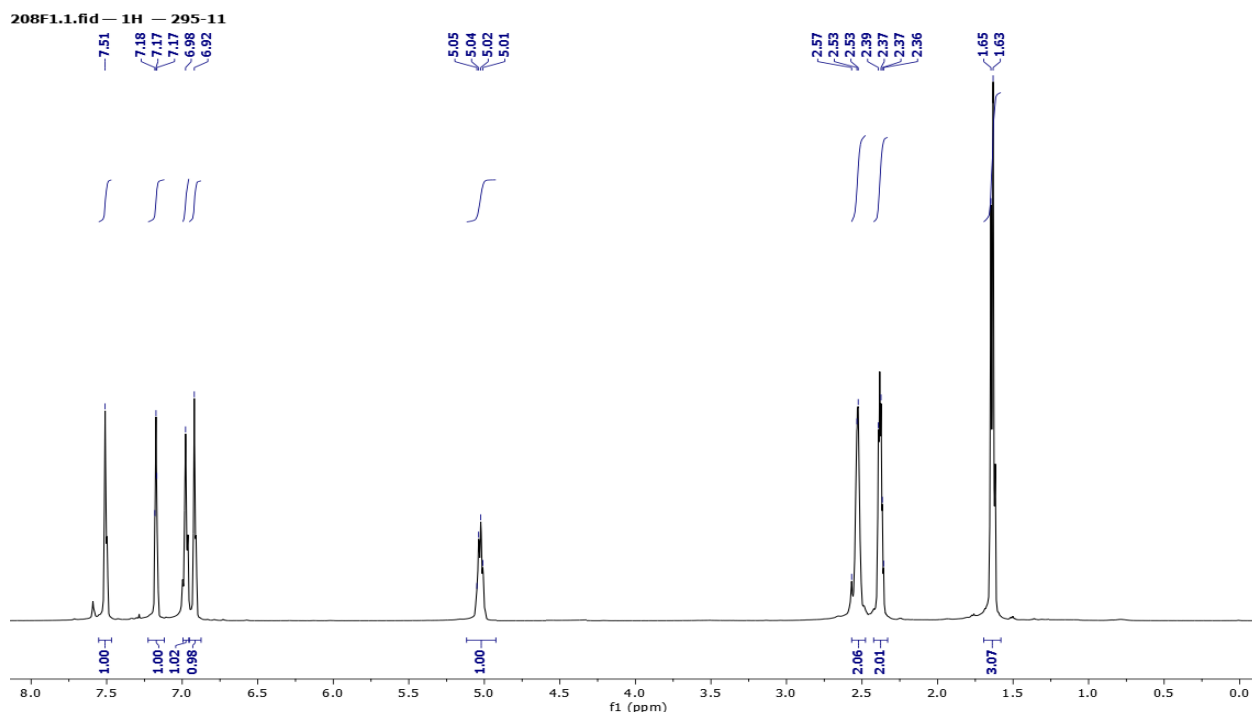
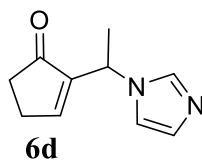
**6c**



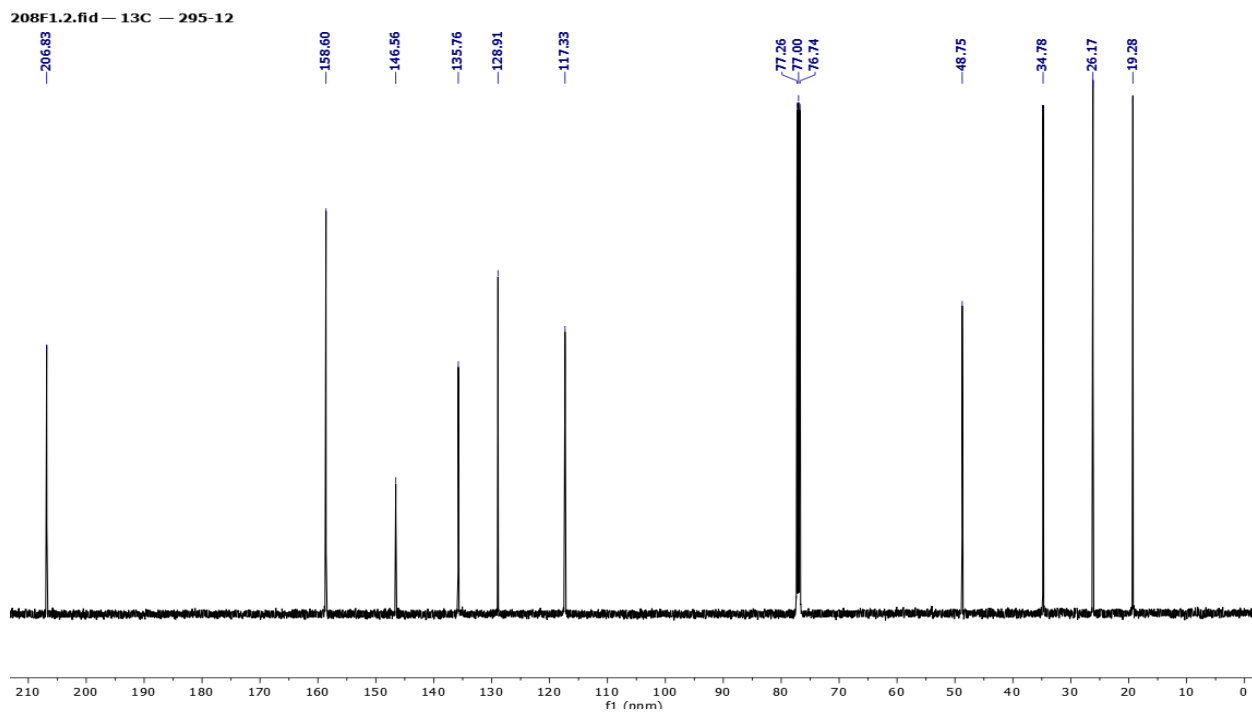
**Figure S5.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectra of **6c**



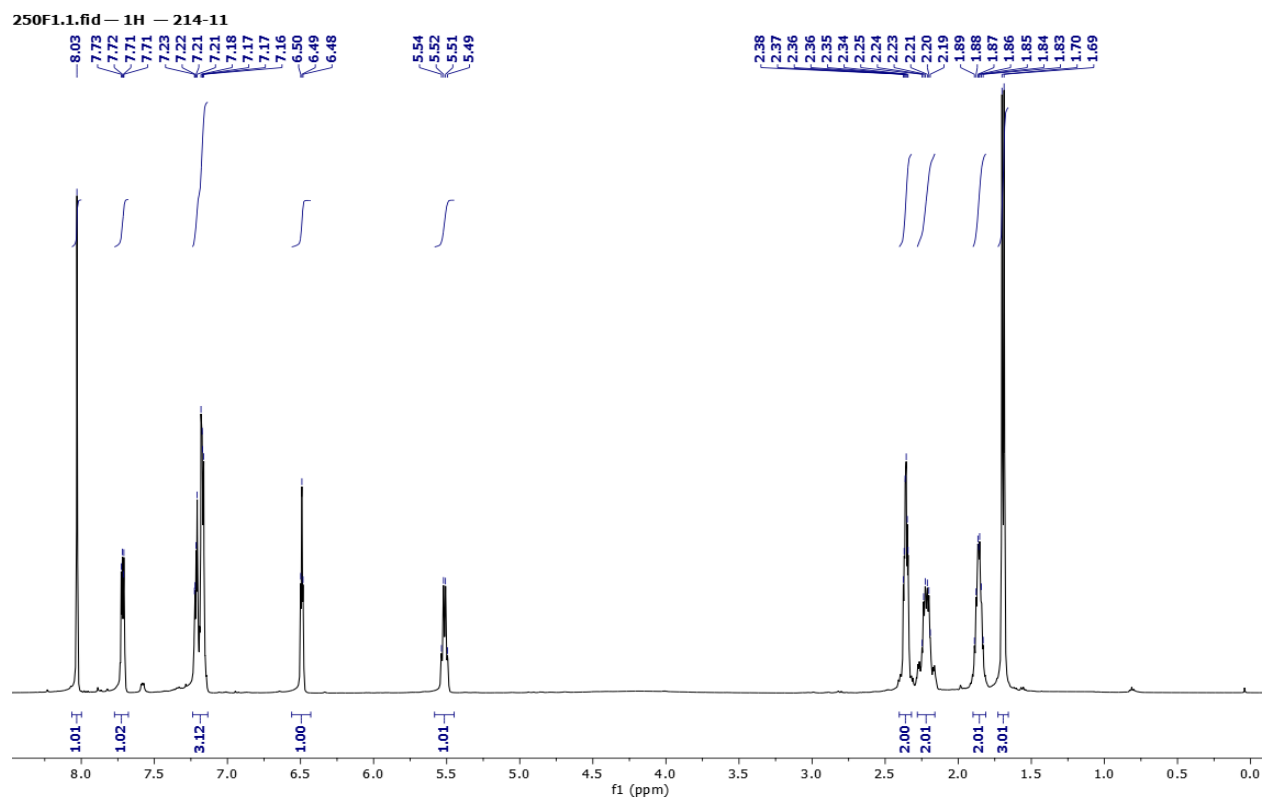
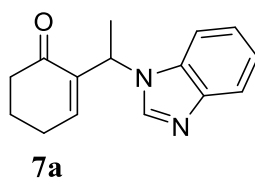
**Figure S6.**  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectra of **6c**



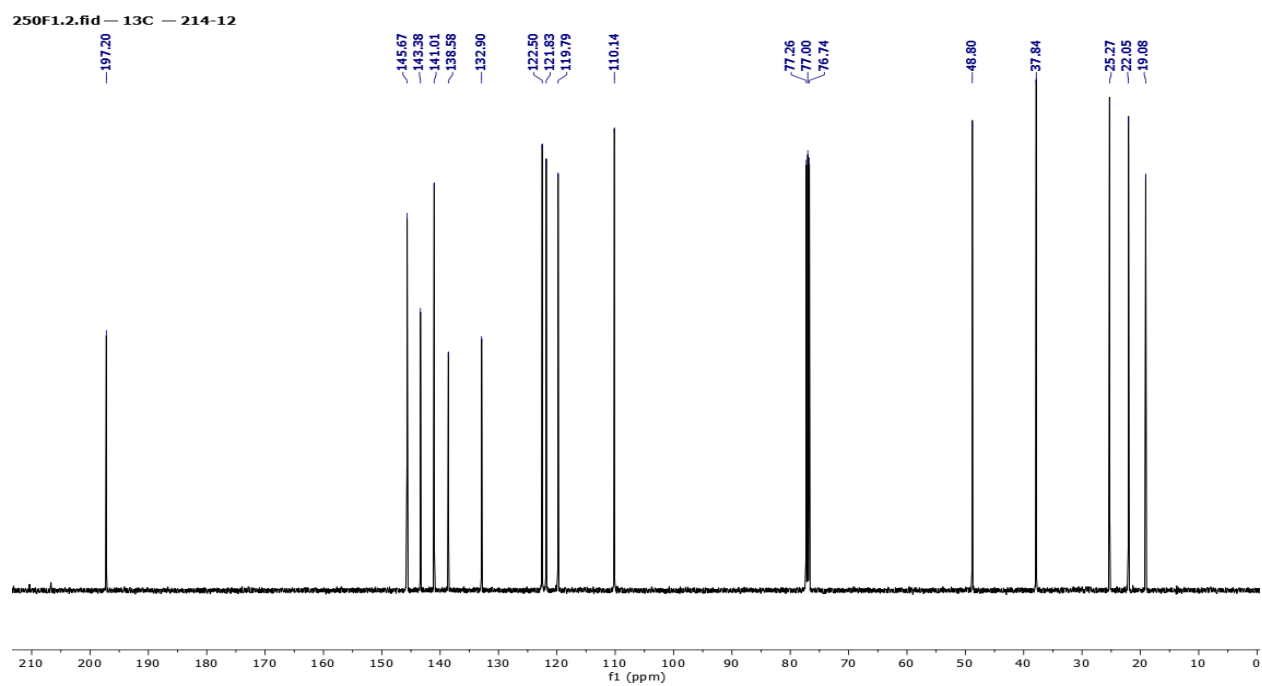
**Figure S7.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectra of **6d**



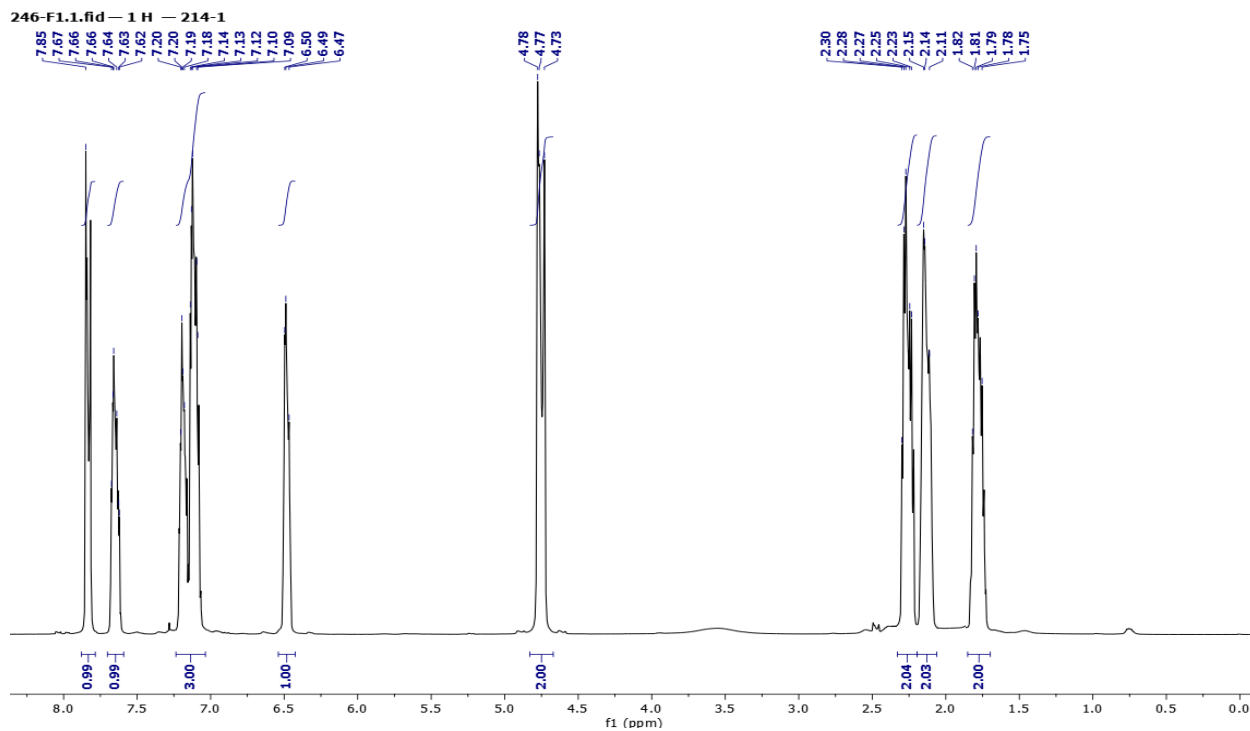
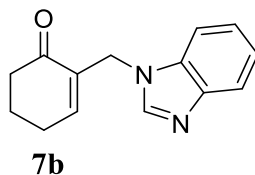
**Figure S8.**  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectra of **6d**



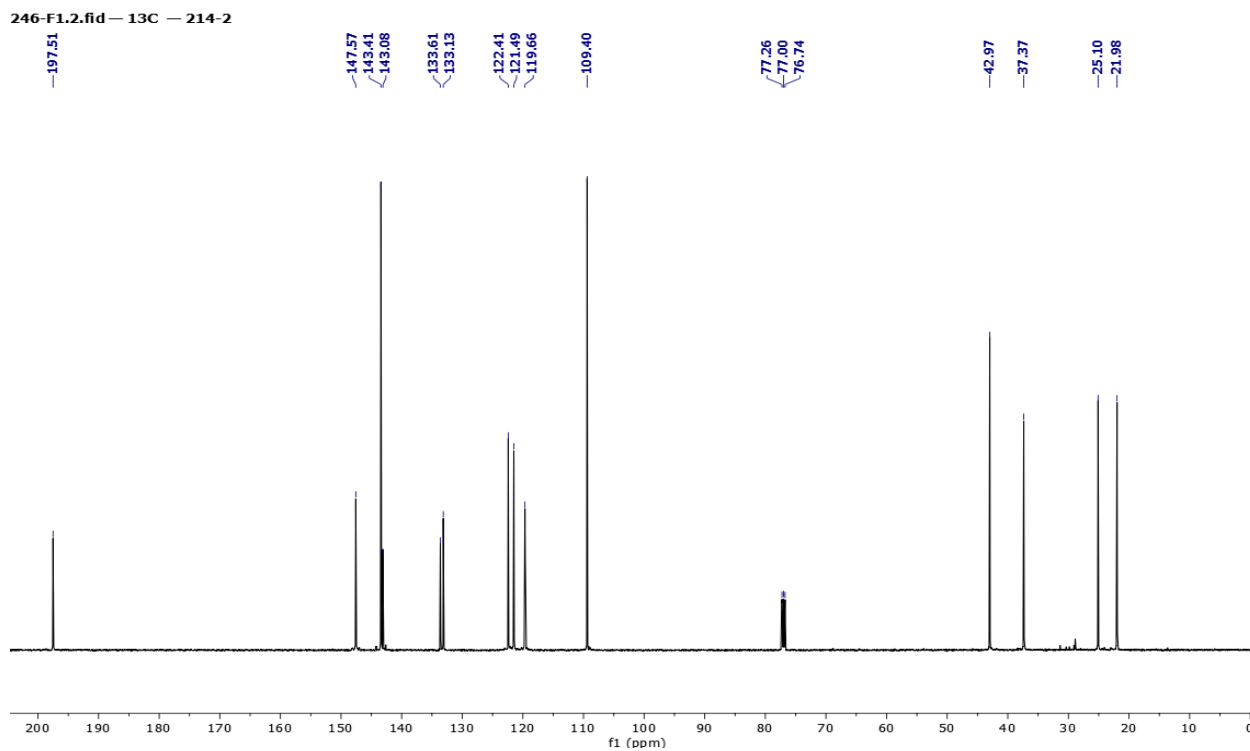
**Figure S9.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectra of **7a**



**Figure S10.**  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectra of **7a**

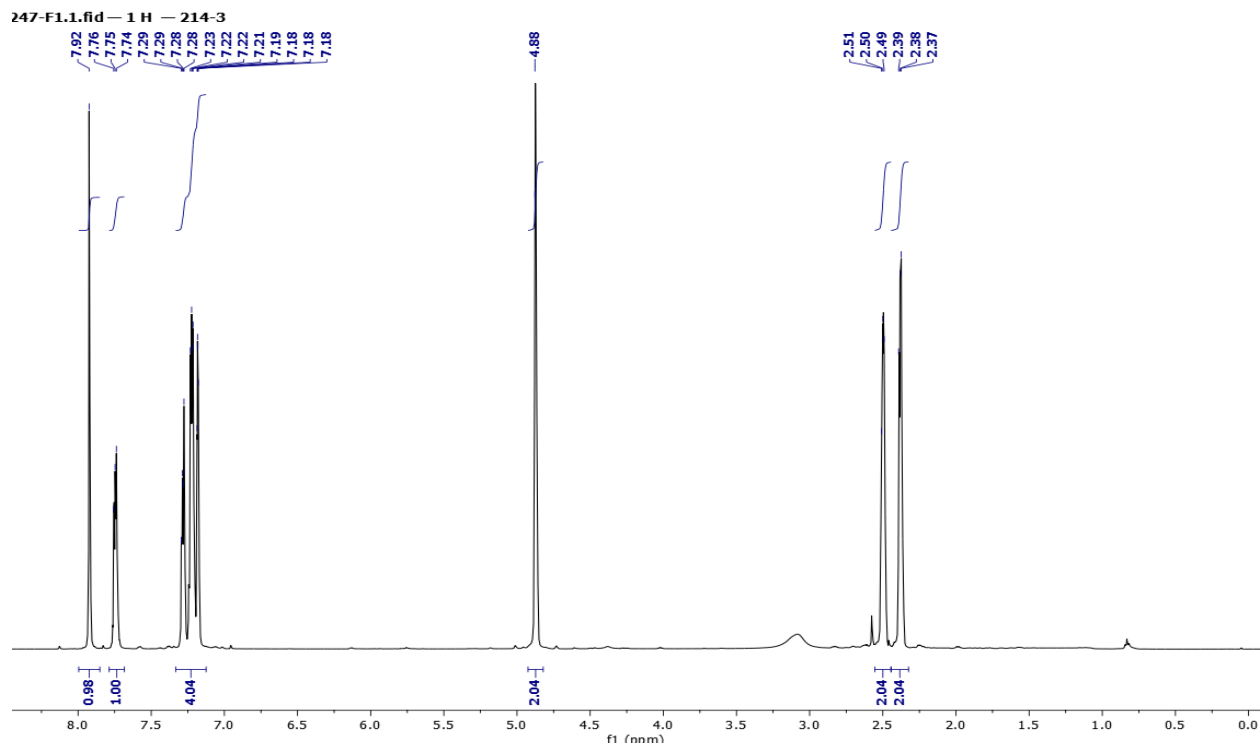
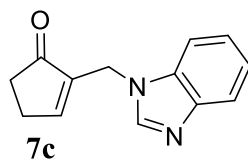


**Figure S11.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectra of **7b**

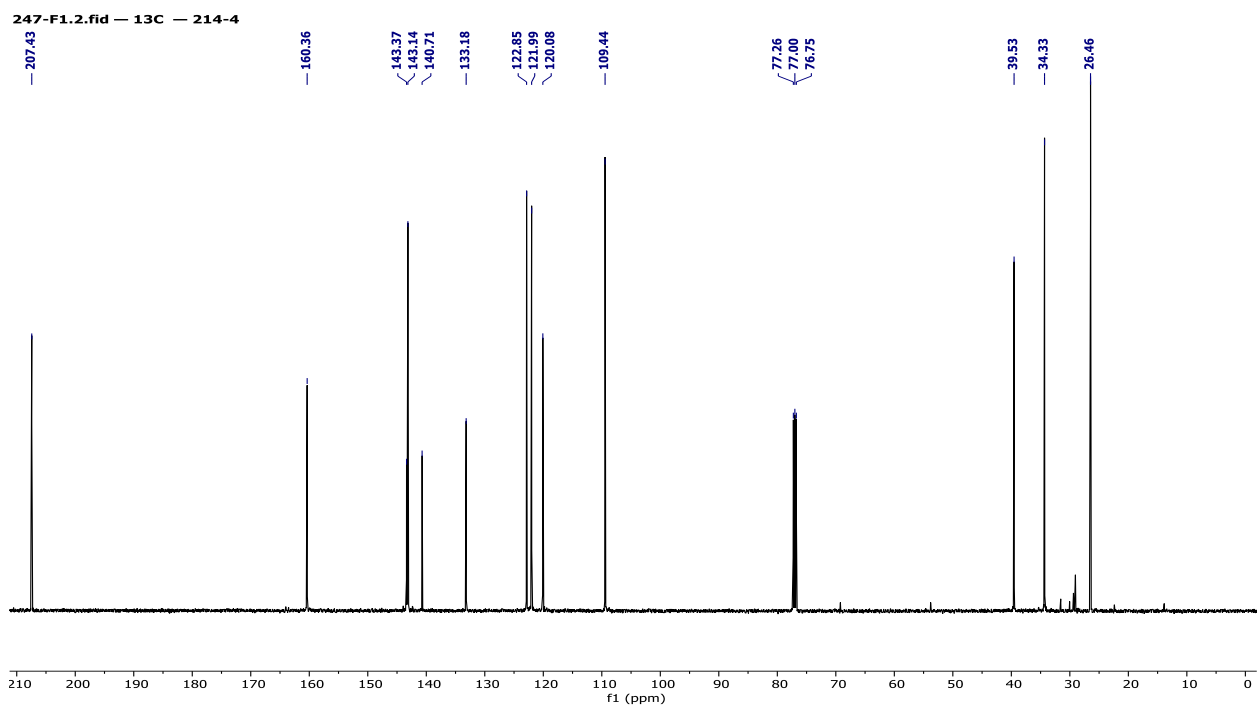


**Figure S12.**  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectra of **7b**

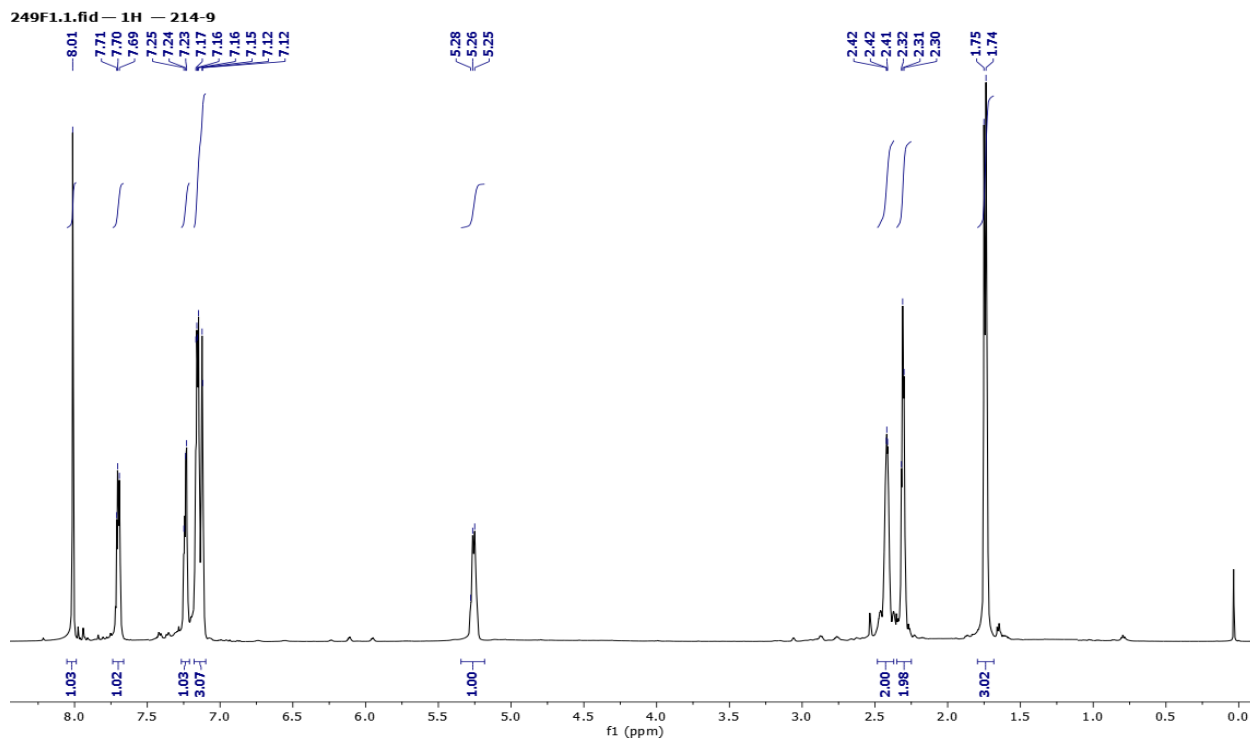
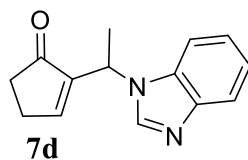




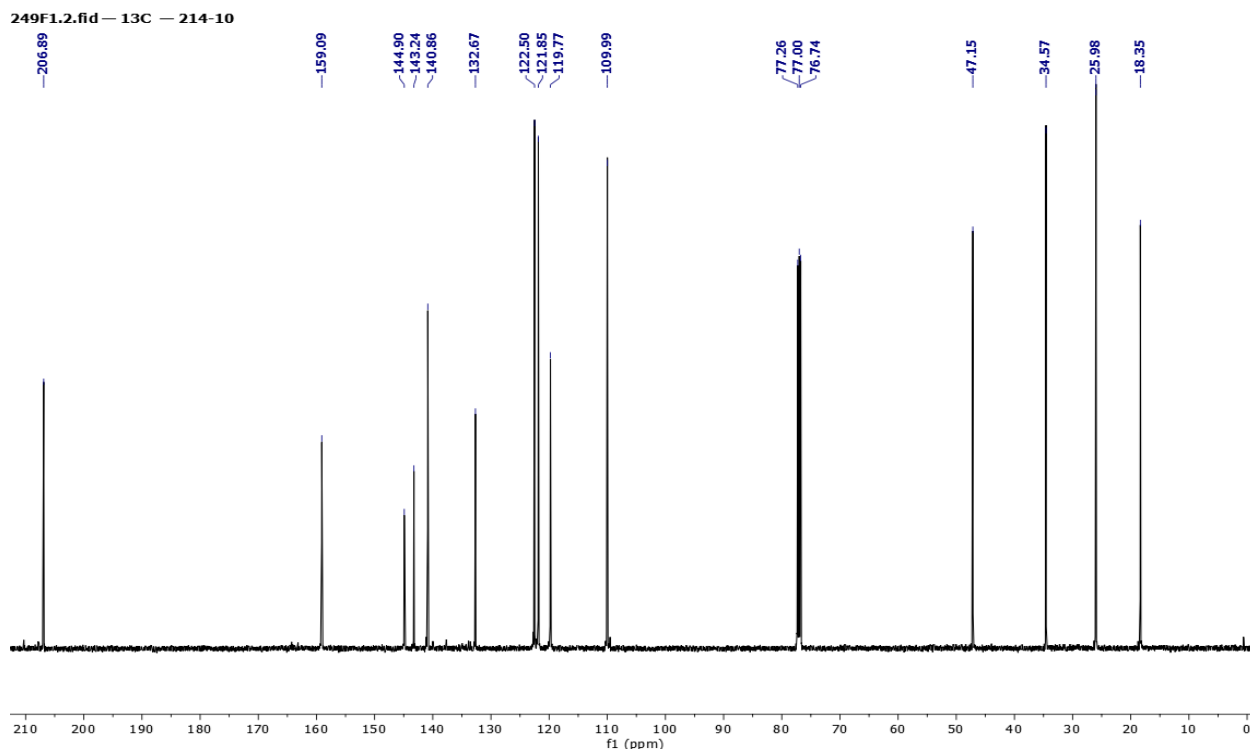
**Figure S13.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectra of **7c**



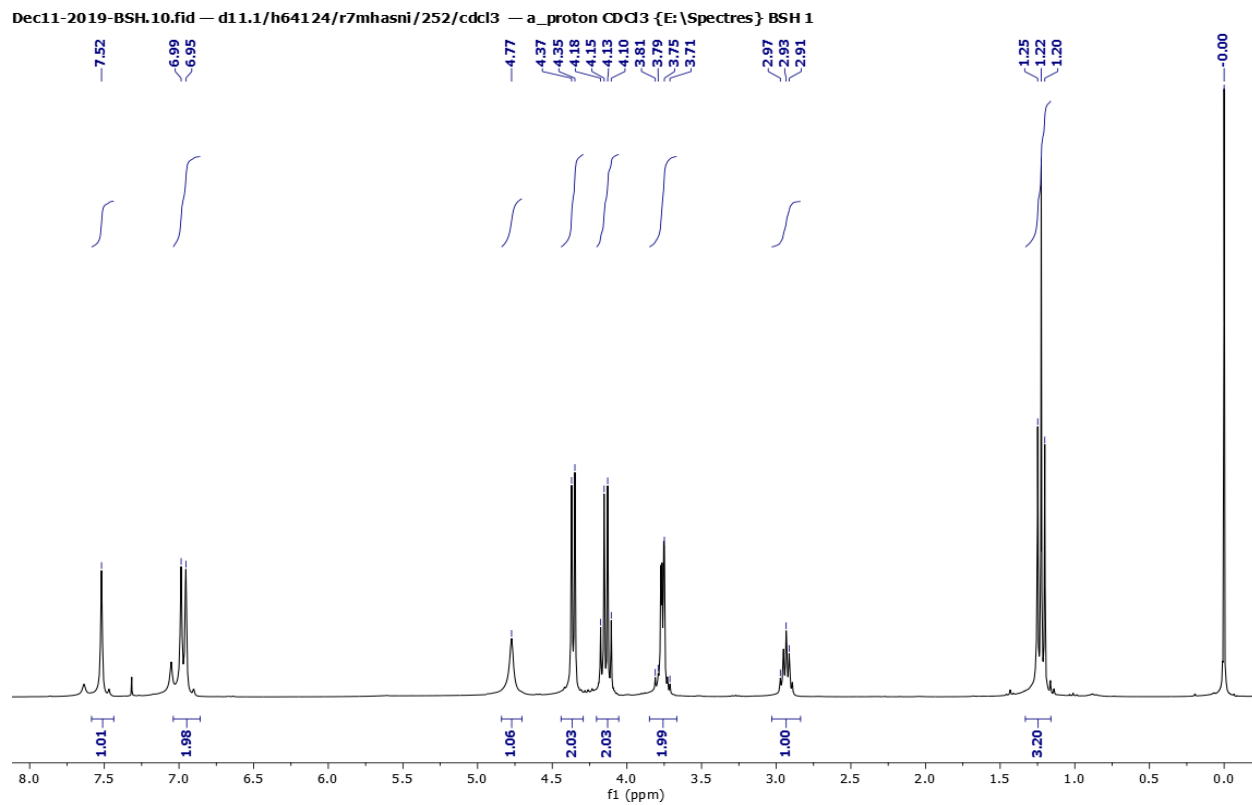
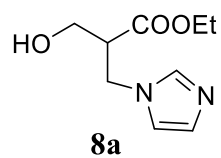
**Figure S14.**  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectra of **7c**



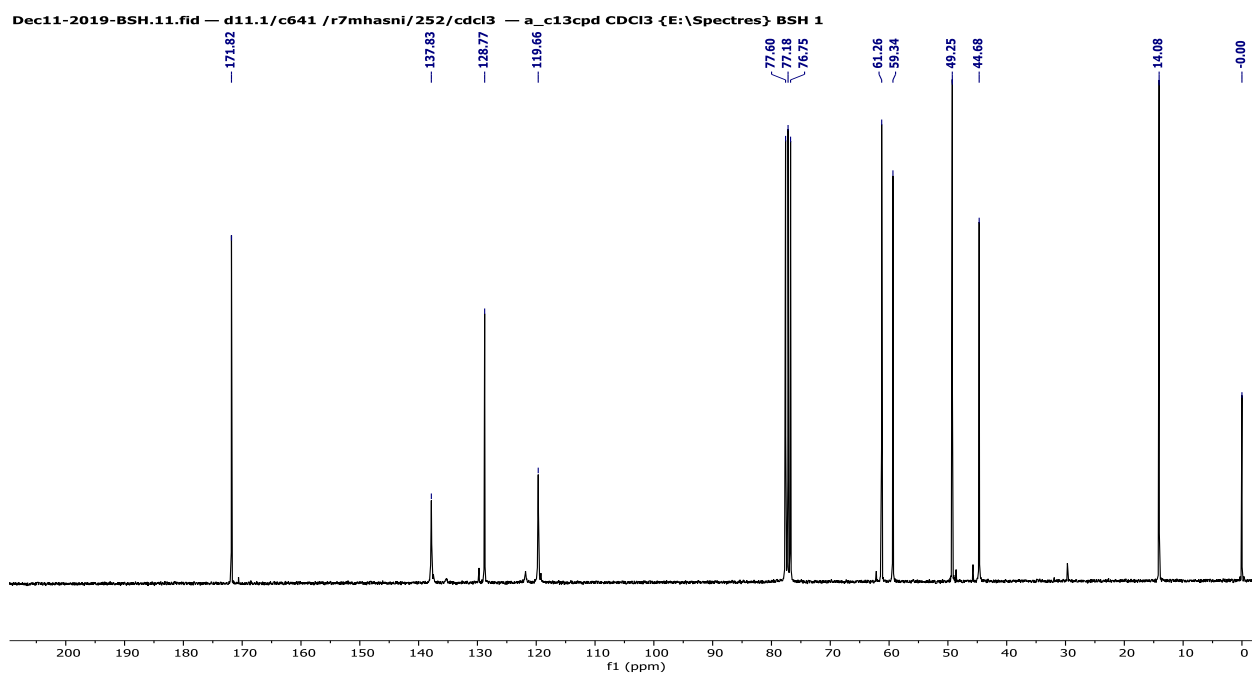
**Figure S15.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectra of **7d**



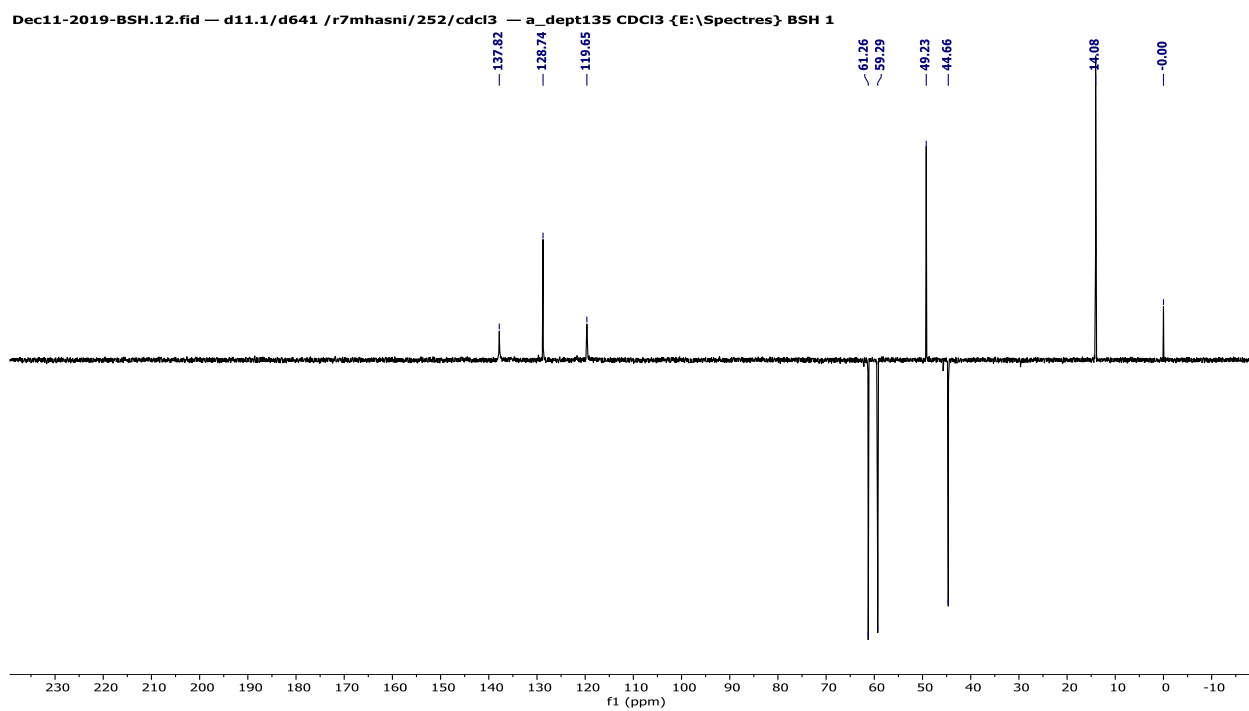
**Figure S16.**  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectra of **7d**



**Figure S17.**  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) spectra of **8a**



**Figure S18.**  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) spectra of **8a**



**Figure S19.** dept 135 NMR (75 MHz, CDCl<sub>3</sub>) spectra of **8a**

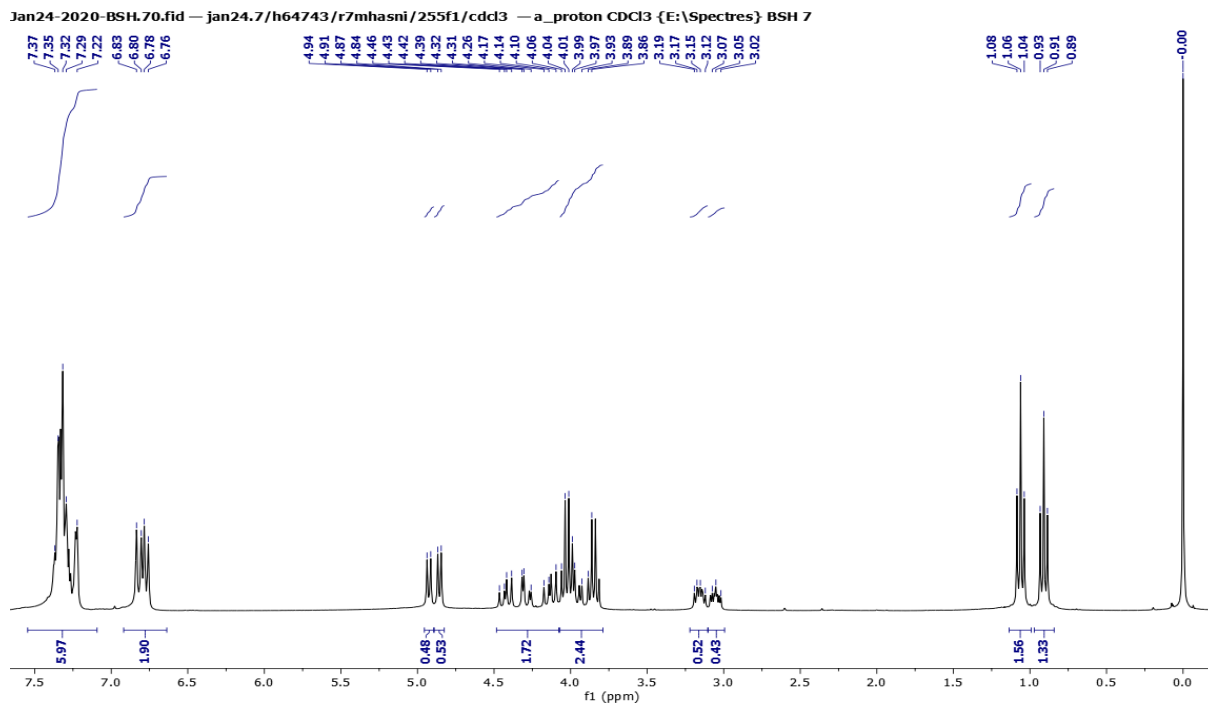
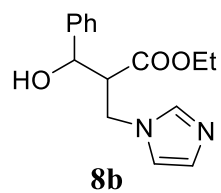


Figure S20. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) spectra of **8b**

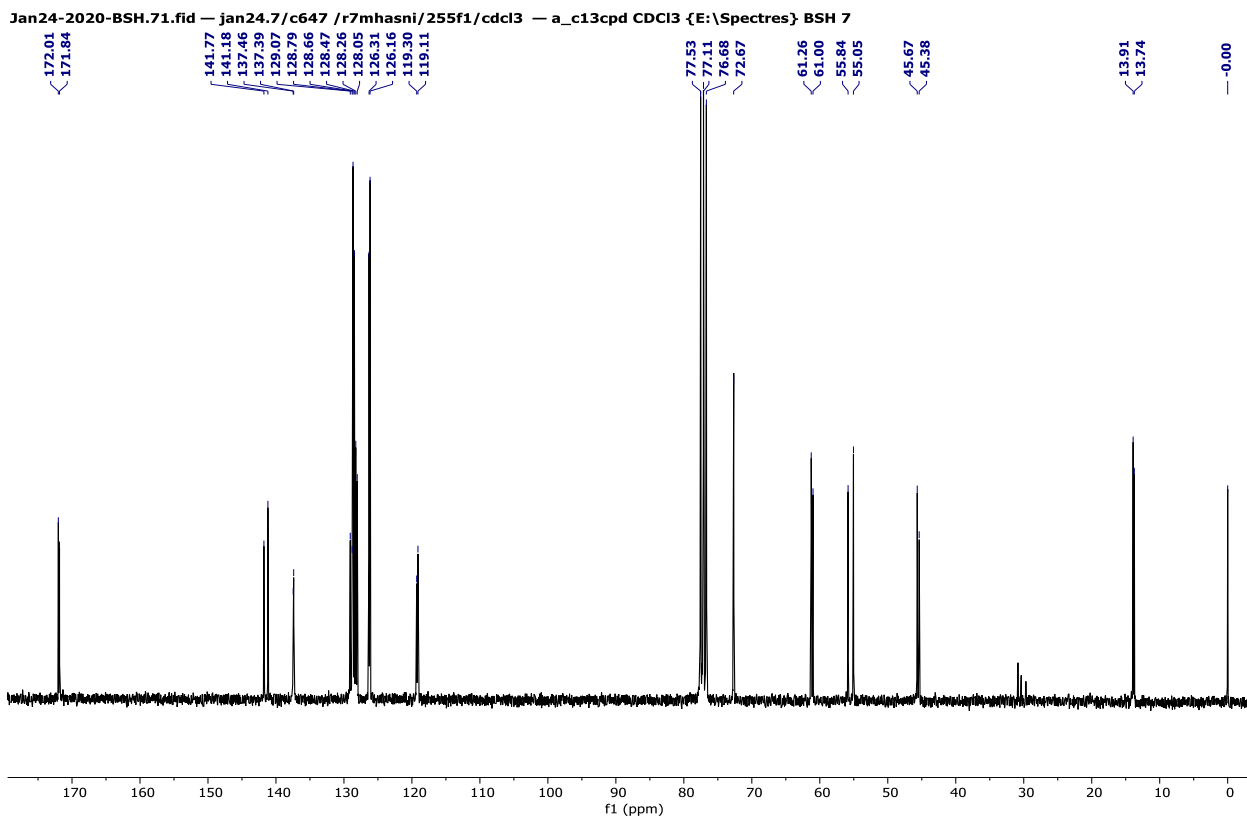


Figure S21. <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) spectra of **8b**



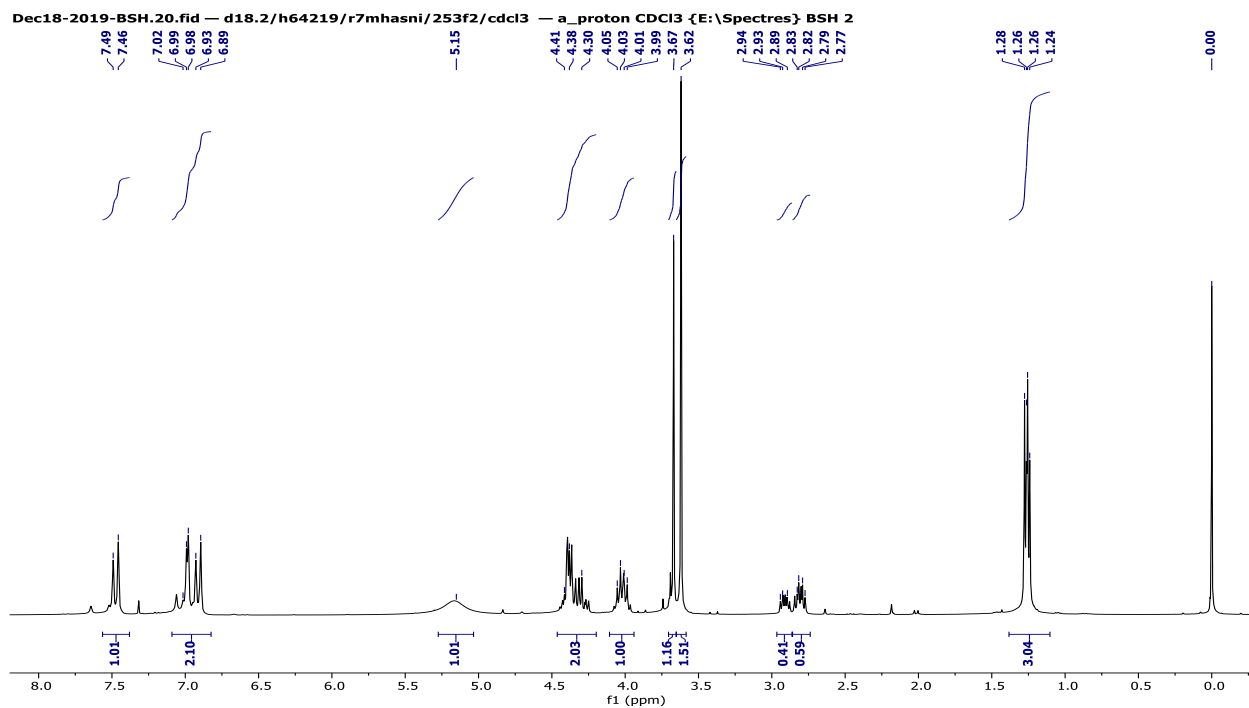
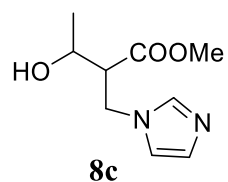


Figure S23.  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) spectra of **8c**

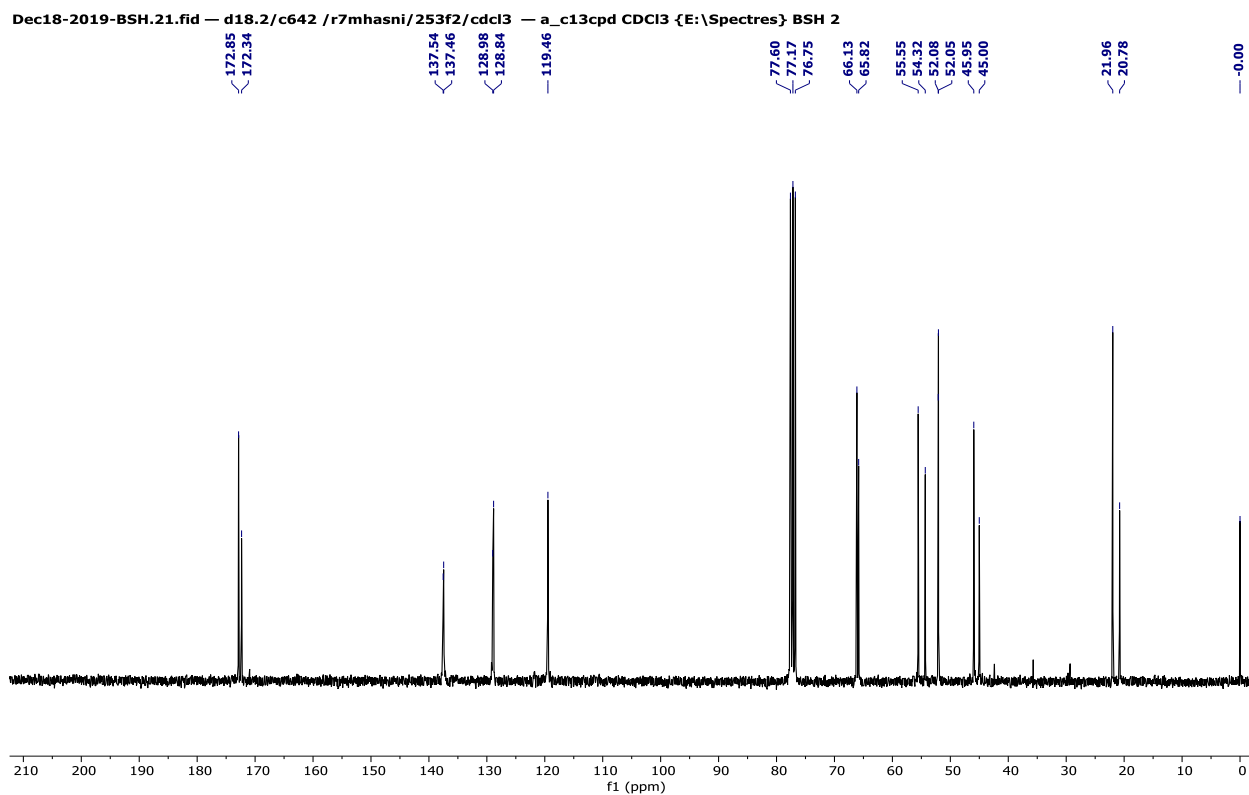
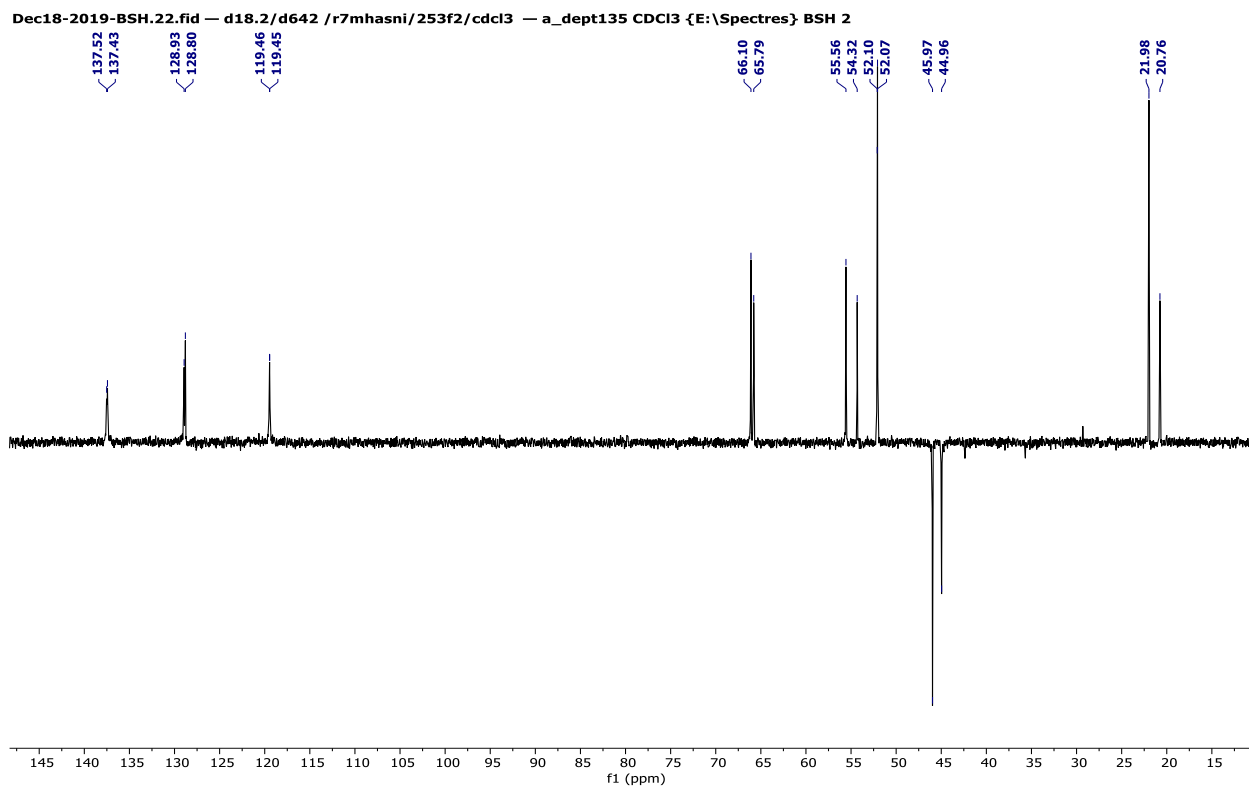
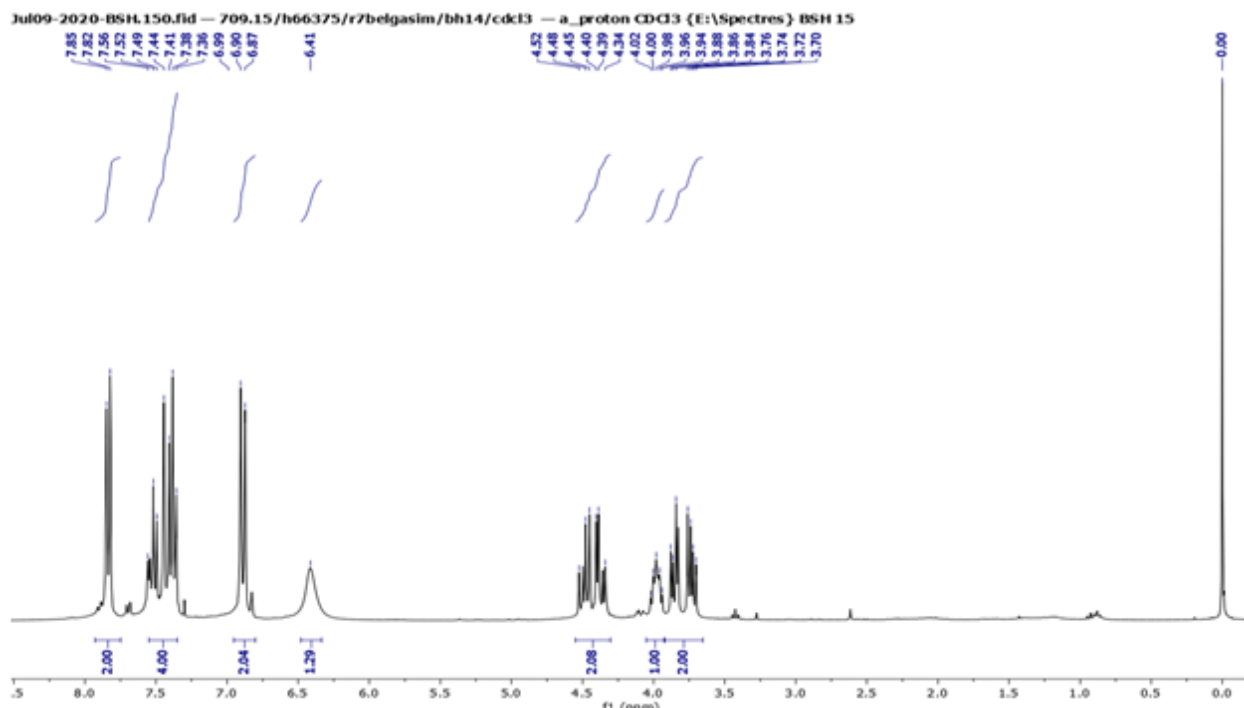
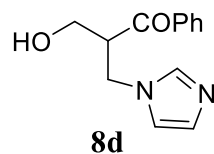


Figure S24.  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) spectra of **8c**

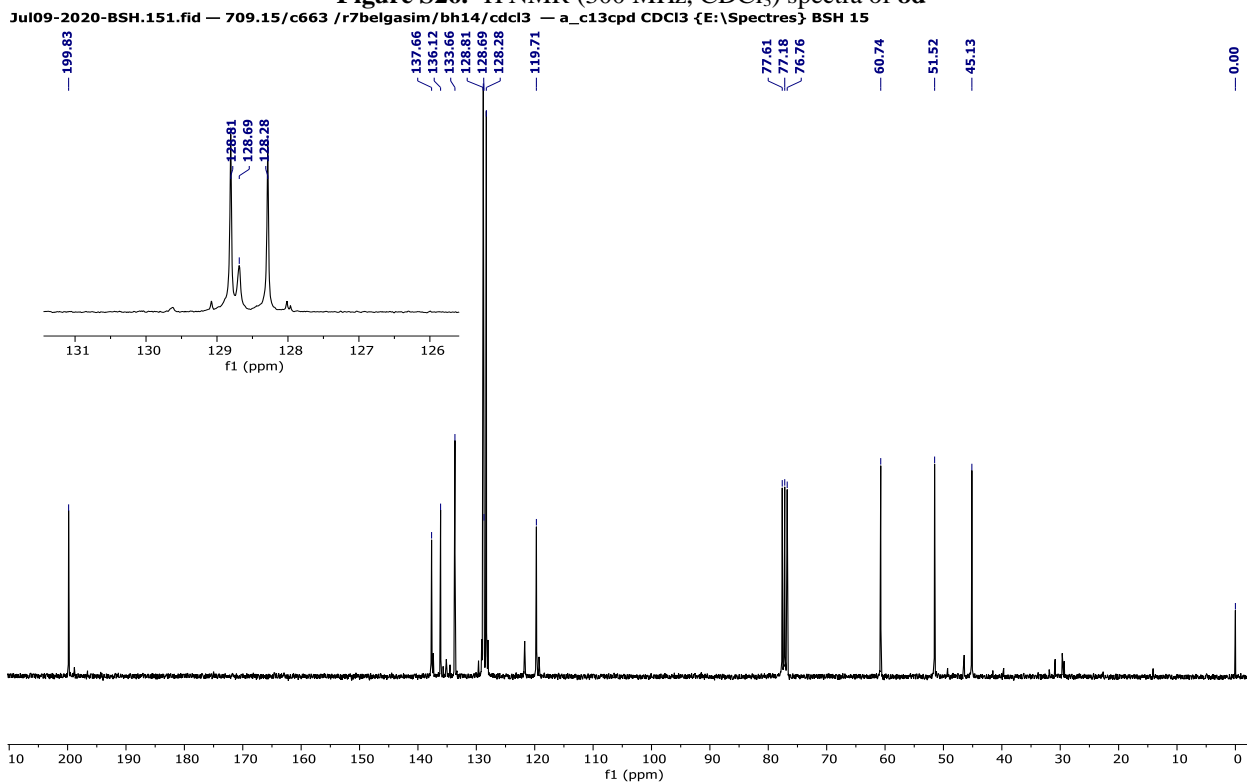


**Figure S25.** dept 135 NMR (75 MHz, CDCl<sub>3</sub>) spectra of **8c**





**Figure S26.**  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) spectra of **8d**



**Figure S27.**  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) spectra of **8d**

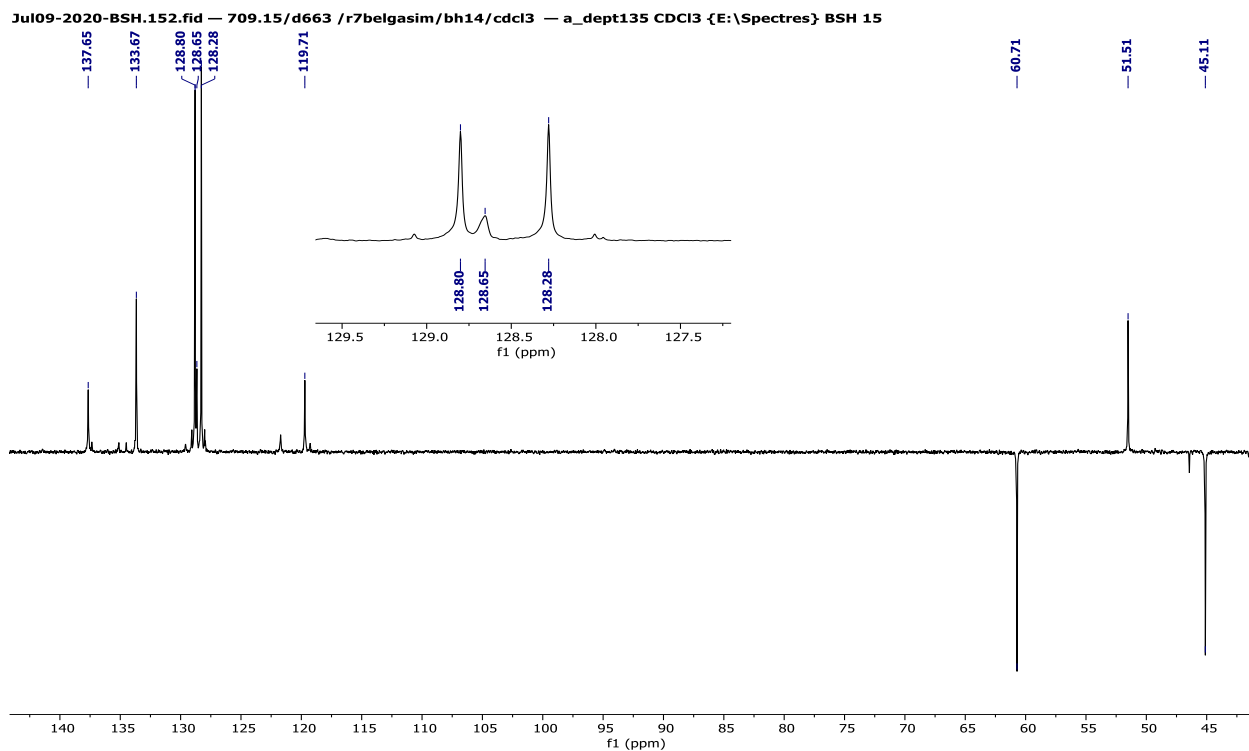


Figure S28. dept 135 NMR (75 MHz,  $\text{CDCl}_3$ ) spectra of **8d**

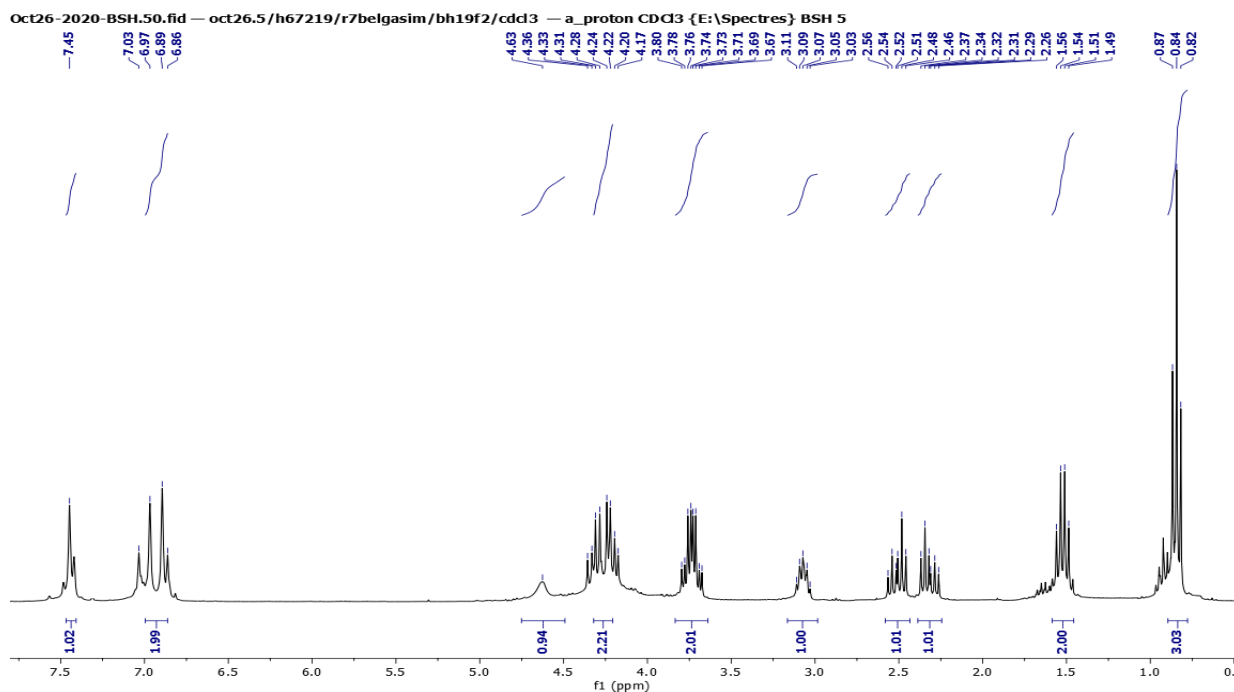
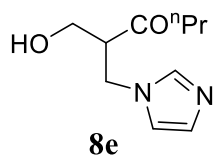


Figure S29. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) spectra of **8e**

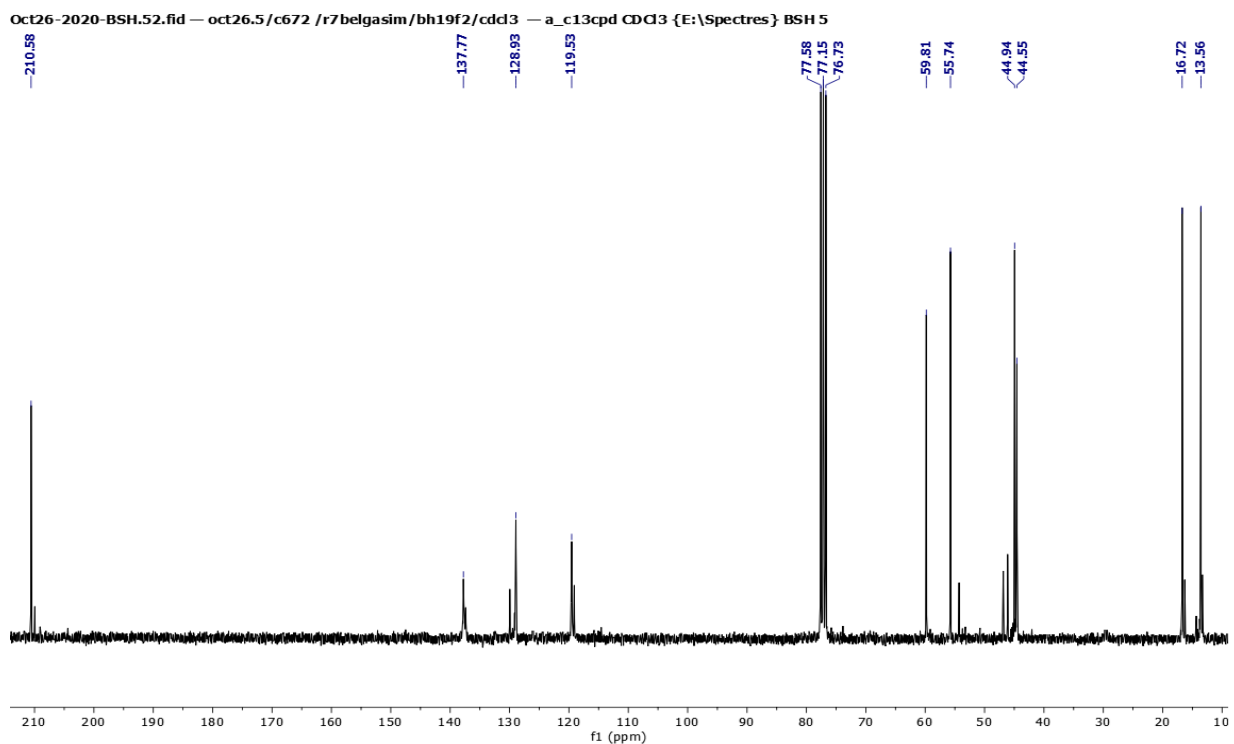
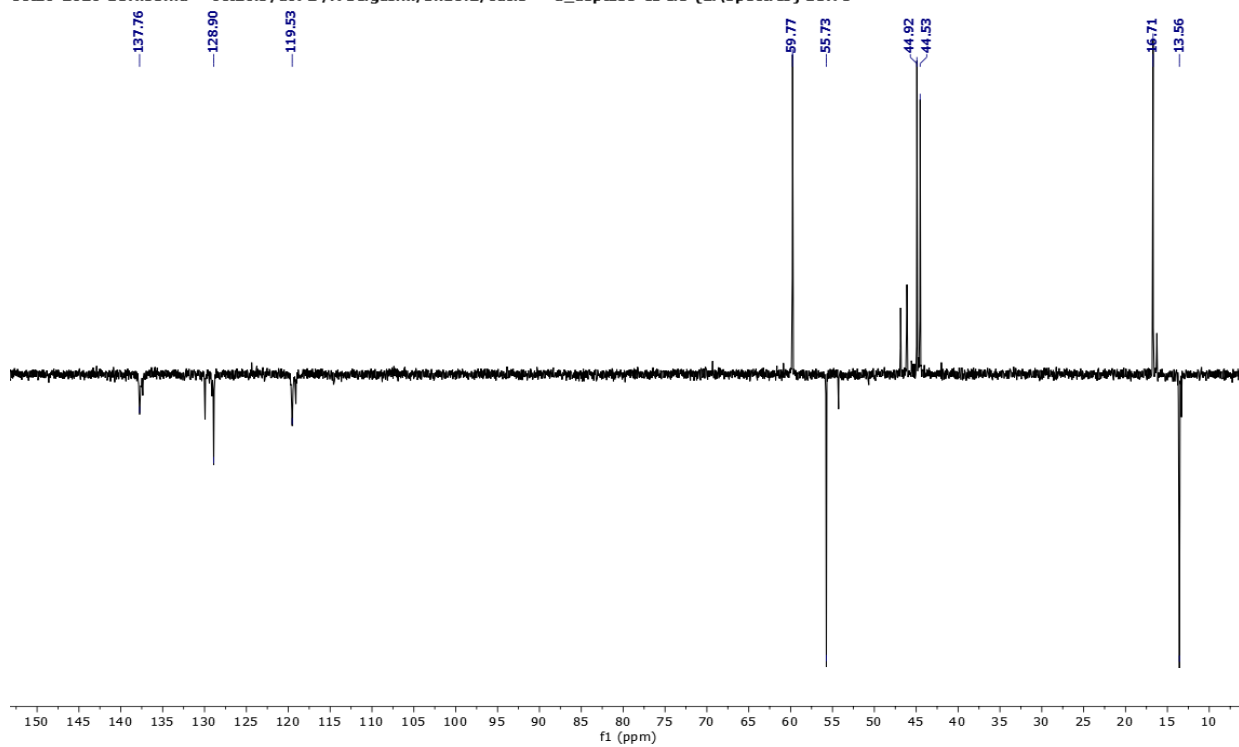
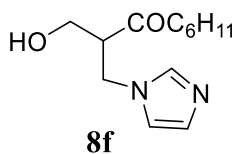


Figure S30. <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) spectra of **8e**

Oct26-2020-BSH,53.fid — oct26.5/d672 /r7belgasim/bh19f2/cdcl3 — a\_dept135 CDCl3 {E:\Spectres} BSH 5



**Figure S31.** dept 135 NMR (75 MHz, CDCl<sub>3</sub>) spectra of **8e**



Jul21-2020-BSH.160.fid — 721.16/h66754/r7mhasni/bh16/cdd3 — a\_proton CDCl3 {E:\Spectres} BSH 16

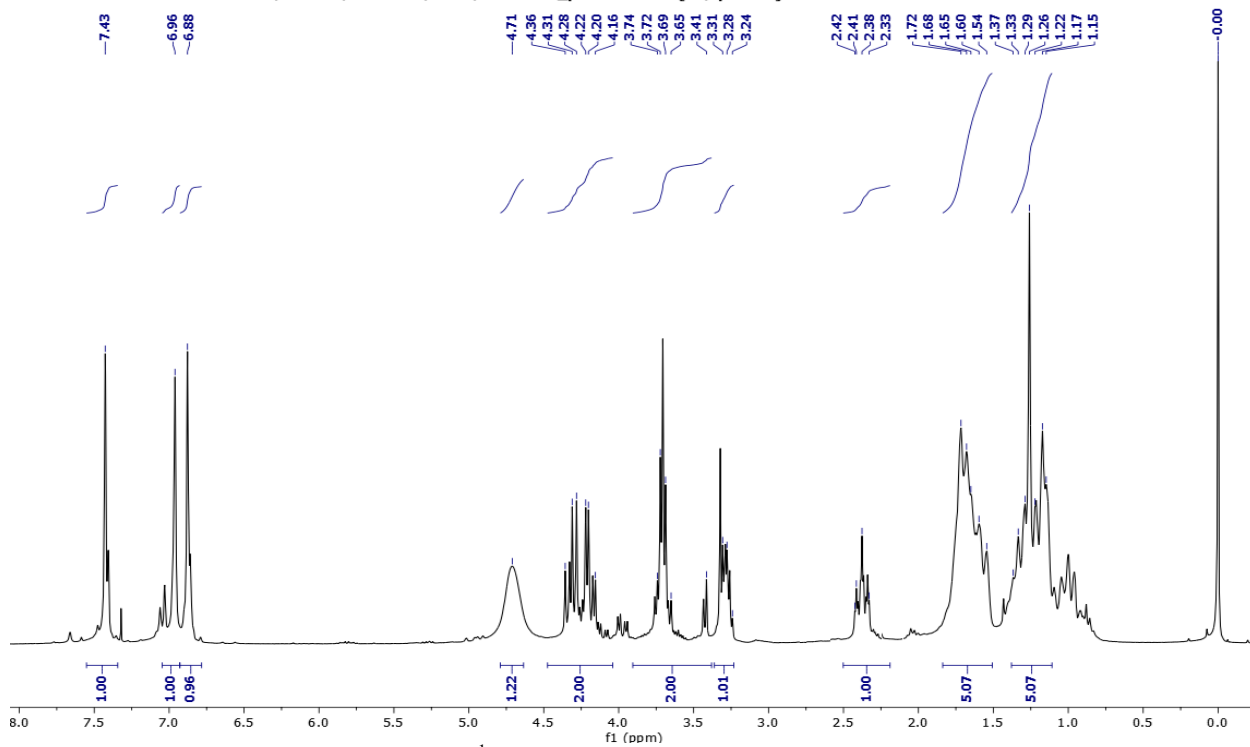


Figure S32. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) spectra of **8f**

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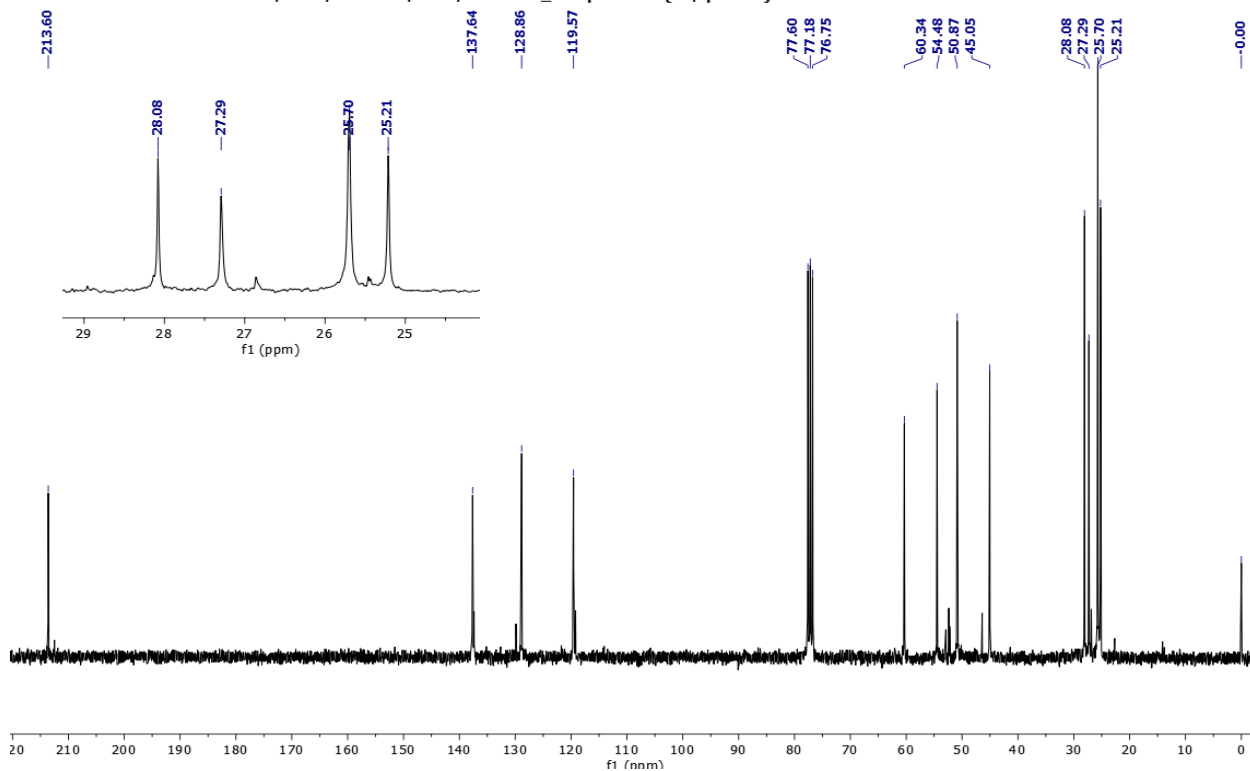
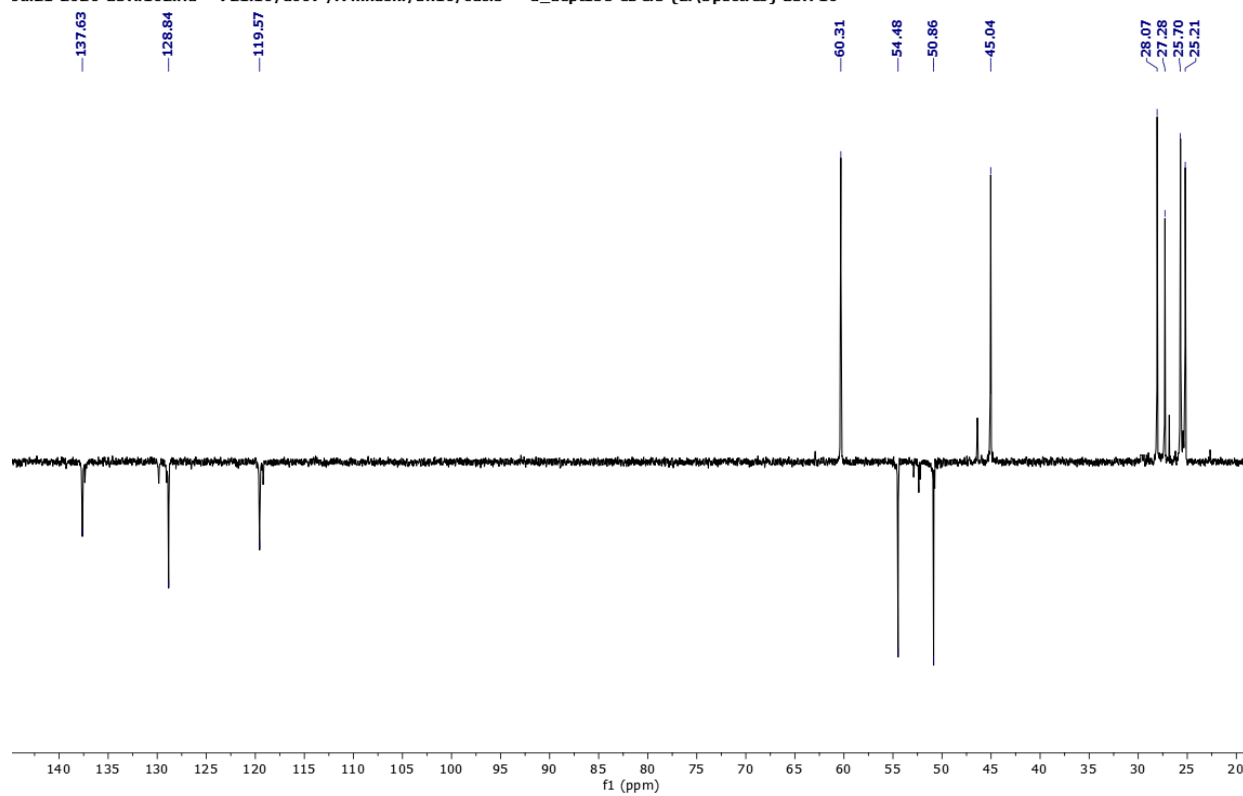


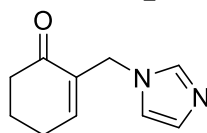
Figure S33. <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) spectra of **8f**

Jul21-2020-BSH.162.fid — 721.16/d667 /r7mhasni/bh16/cdcl3 — a\_dept135 CDCl3 {E:\Spectres} BSH 16



**Figure S34.** dept 135 NMR (75 MHz, CDCl<sub>3</sub>) spectra of **8f**

## ESI-HRMS spectra for compounds 6a–d, 7a–d, 8a–f



**6a**

### Analysis Info

Analysis Name D:\Data\SSO\imen\MO54F1.d  
 Method tune\_low\_LiOH\_pos\_50\_1000.m  
 Sample Name MO54F1  
 Comment

Acquisition Date 3/27/2013 9:23:25 AM

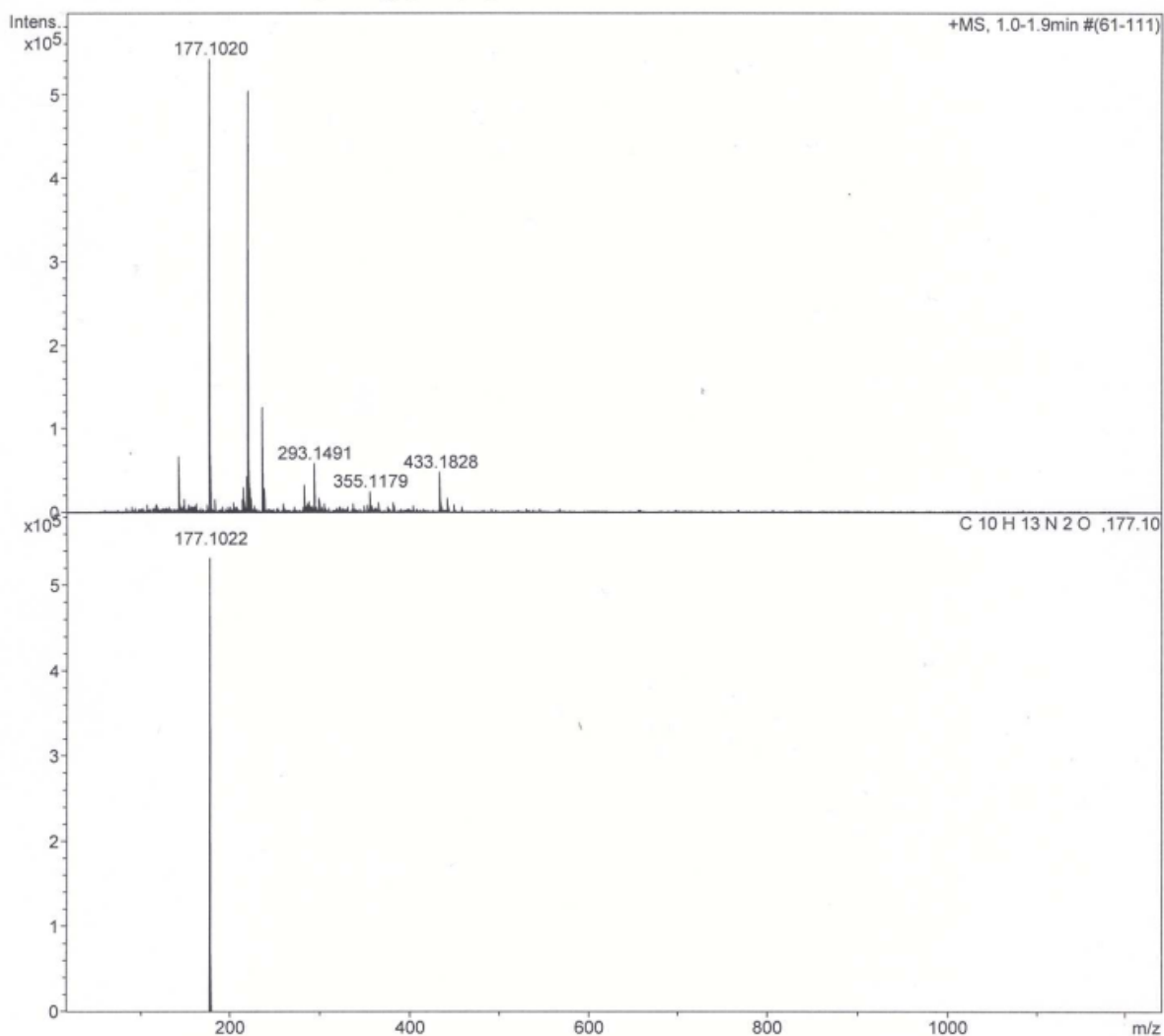
Operator BDAL@DE  
 Instrument / Ser# micrOTOF 235

### Acquisition Parameter

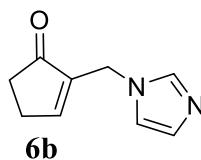
|             |            |                      |          |                  |           |
|-------------|------------|----------------------|----------|------------------|-----------|
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| Focus       | Not active |                      |          | Set Dry Heater   | 180 °C    |
| Scan Begin  | 50 m/z     | Set Capillary        | 3500 V   | Set Dry Gas      | 4.0 l/min |
| Scan End    | 1200 m/z   | Set End Plate Offset | -500 V   | Set Divert Valve | Waste     |

| Meas. m/z | # | Formula         | m/z      | mSigma | err [ppm] | err [mDa] |
|-----------|---|-----------------|----------|--------|-----------|-----------|
| 177.1020  | 1 | C 10 H 13 N 2 O | 177.1022 | 4.0    | 1.6       | 0.3       |

| Meas. m/z | # | Formula | m/z | mSigma | err [ppm] | err [mDa] |
|-----------|---|---------|-----|--------|-----------|-----------|
|-----------|---|---------|-----|--------|-----------|-----------|



**Figure S35.** ESI-HRMS spectra of **6a**



**Analysis Info**

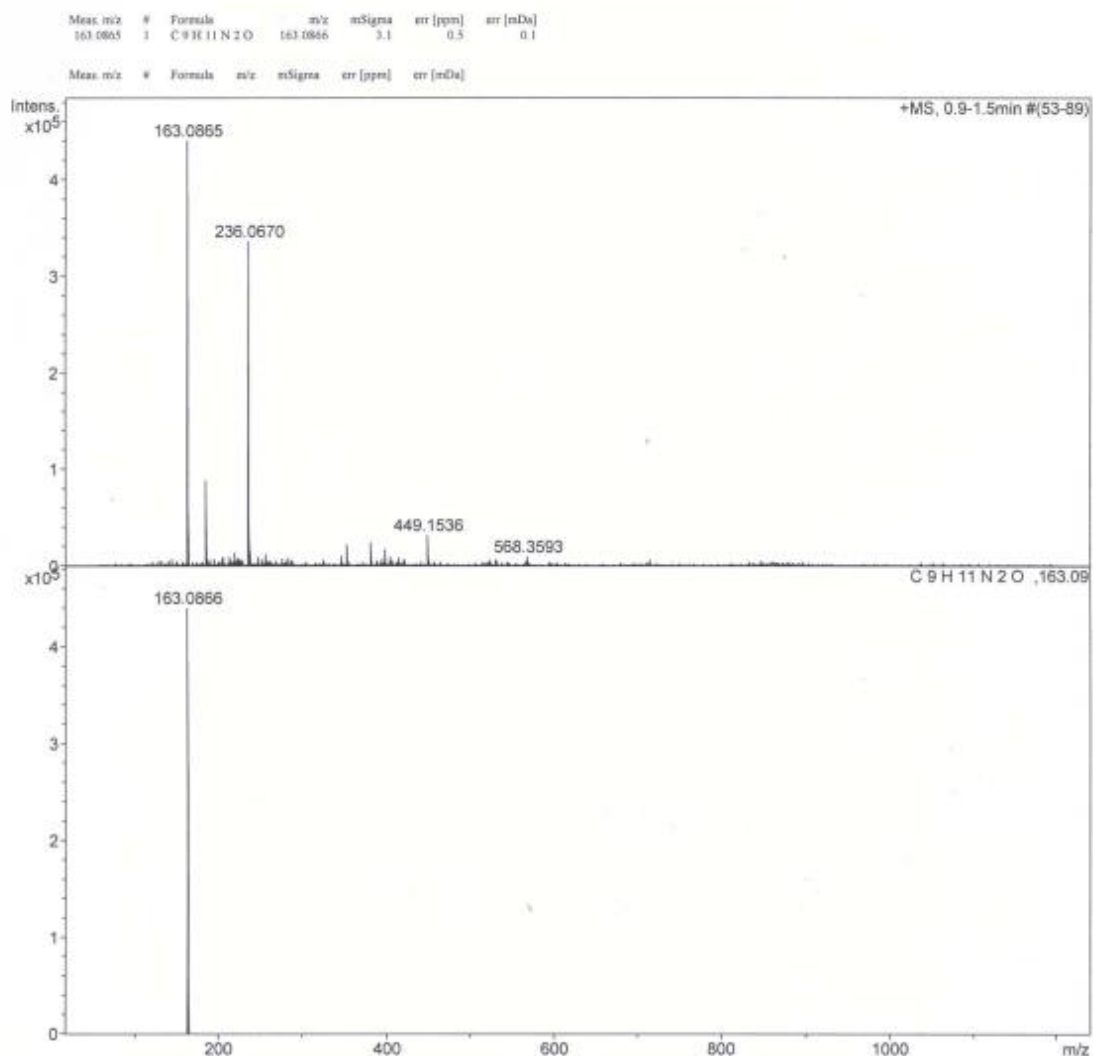
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 Sample Name MO200F2  
 Comment MeOH

Acquisition Date 3/26/2013 12:44:39 PM

Operator BDAL@DE  
 Instrument / Ser# micrOTOF 235

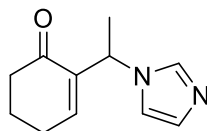
**Acquisition Parameter**

|             |            |                      |          |                  |           |
|-------------|------------|----------------------|----------|------------------|-----------|
| Source Type | ESI        | Ion Polarity         | Positive | Set Nebulizer    | 5.8 psi   |
| Focus       | Not active |                      |          | Set Dry Heater   | 180 °C    |
| Scan Begin  | 50 m/z     | Set Capillary        | 3500 V   | Set Dry Gas      | 4.0 l/min |
| Scan End    | 1200 m/z   | Set End Plate Offset | -500 V   | Set Divert Valve | Waste     |



**Figure S36.** ESI-HRMS spectra of **6b**





**6c**

**Elemental Composition Report**

**Single Mass Analysis**

Tolerance = 3.0 PPM / DBE: min = -5.0, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

226 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-80 H: 0-100 N: 0-10 O: 0-10

Cone voltage =30V

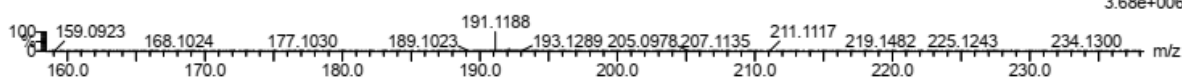
Xevo G2 QTof #YCA210

07-Jul-2022 09:20:01

205F1 75 (0.471) AM2 (Ar,20000.0,0.00,0.00); Cm (67:75-62:65x2.000)

1: TOF MS ES+

3.68e+006



Minimum: -5.0  
Maximum: 3.0 3.0 80.0

| Mass     | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf (%) | Formula      |
|----------|------------|-----|-----|-----|-------|------|----------|--------------|
| 191.1188 | 191.1184   | 0.4 | 2.1 | 5.5 | 700.8 | n/a  | n/a      | C11 H15 N2 O |

Cone voltage =30V

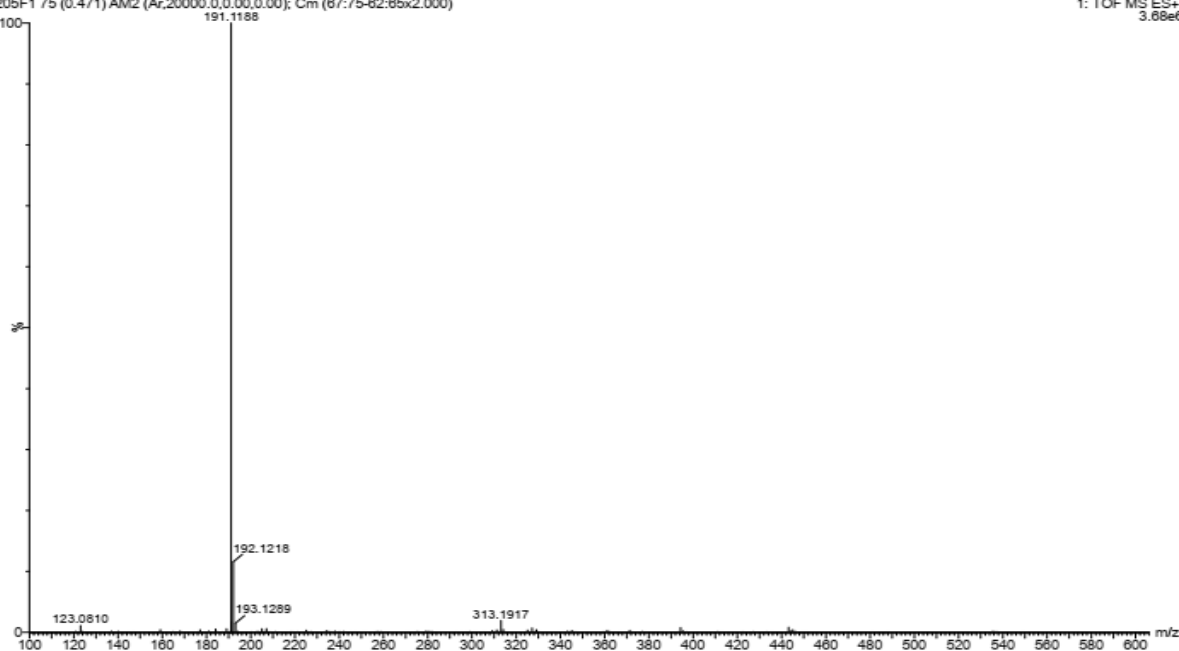
205F1 75 (0.471) AM2 (Ar,20000.0,0.00,0.00); Cm (67:75-62:65x2.000)

Xevo G2 QTof #YCA210

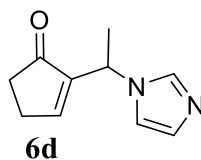
07-Jul-2022 09:20:01

1: TOF MS ES+

3.68e6



**Figure S37. ESI-HRMS spectra of 6c**



## Elemental Composition Report

Page 1

### Single Mass Analysis

Tolerance = 3.0 PPM / DBE: min = -5.0, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

196 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-80 H: 0-100 N: 0-10 O: 0-10

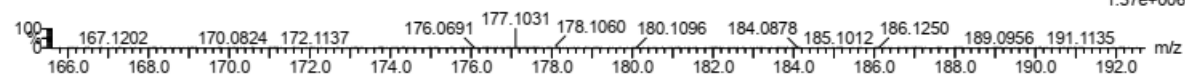
Cone voltage =30V

Xevo G2 QTof #YCA210

05-Jul-2022 15:33:15

208F1 74 (0.465) AM2 (Ar,20000.0,0.00,0.00); Cm (70:74-54:64x2.000)

1: TOF MS ES+  
1.57e+006



Minimum: -5.0  
Maximum: 3.0 3.0 80.0

| Mass     | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf (%) | Formula      |
|----------|------------|-----|-----|-----|-------|------|----------|--------------|
| 177.1031 | 177.1028   | 0.3 | 1.7 | 5.5 | 382.8 | n/a  | n/a      | C10 H13 N2 O |

Cone voltage =30V

208F1 74 (0.465) AM2 (Ar,20000.0,0.00,0.00); Cm (70:74-54:64x2.000)

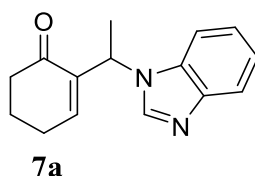
Xevo G2 QTof #YCA210

05-Jul-2022 15:33:15

1: TOF MS ES+  
1.57e6



Figure S38. ESI-HRMS spectra of **6d**



## Elemental Composition Report

Page 1

### Single Mass Analysis

Tolerance = 3.0 PPM / DBE: min = -5.0, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

333 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-80 H: 0-100 N: 0-10 O: 0-10

Cone voltage =30V

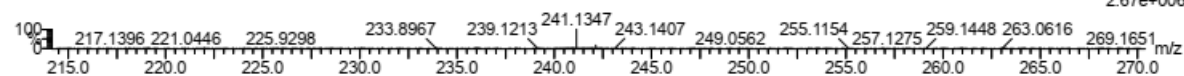
Xevo G2 QTof #YCA210

07-Jul-2022 09:45:00

250F1 68 (0.432) AM2 (Ar,20000.0,0.00,0.00); Cm (63:68-52:62x2.000)

1: TOF MS ES+

2.67e+006



Minimum: -5.0  
Maximum: 3.0 3.0 80.0

| Mass     | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf (%) | Formula      |
|----------|------------|-----|-----|-----|-------|------|----------|--------------|
| 241.1347 | 241.1341   | 0.6 | 2.5 | 8.5 | 537.5 | n/a  | n/a      | C15 H17 N2 O |

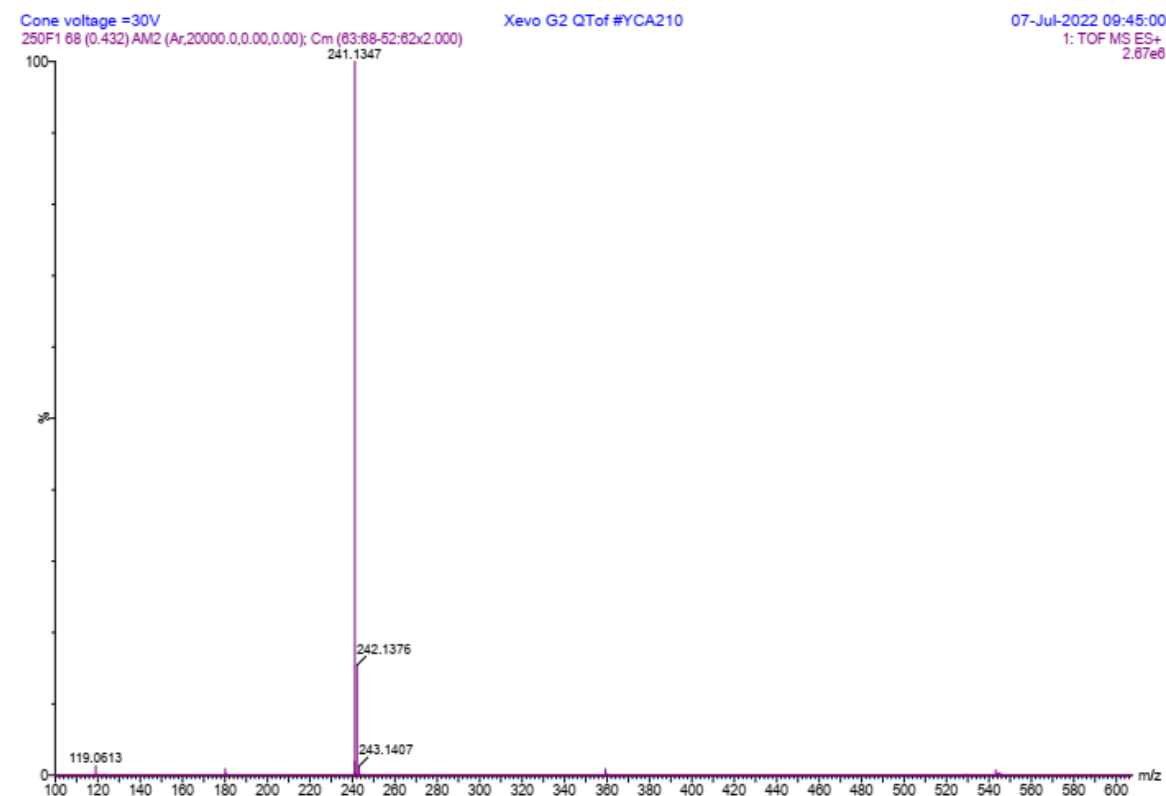
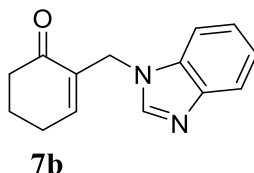


Figure S39. ESI-HRMS spectra of **7a**



## Elemental Composition Report

Page 1

### Single Mass Analysis

Tolerance = 3.0 PPM / DBE: min = -5.0, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

307 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-80 H: 0-100 N: 0-10 O: 0-10

Cone voltage = 30V

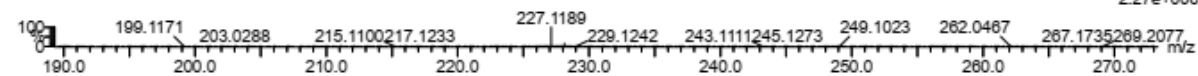
Xevo G2 QTof #YCA210

07-Jul-2022 09:24:00

246F1 68 (0.432) AM2 (Ar,20000.0,0.00,0.00); Cm (64:68-59:62x2.000)

1: TOF MS ES+

2.27e+008



Minimum:

Maximum: 3.0 3.0 -5.0

| Mass     | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf (%) | Formula      |
|----------|------------|-----|-----|-----|-------|------|----------|--------------|
| 227.1189 | 227.1184   | 0.5 | 2.2 | 8.5 | 530.7 | n/a  | n/a      | C14 H15 N2 O |

Cone voltage = 30V

Xevo G2 QTof #YCA210

07-Jul-2022 09:24:00

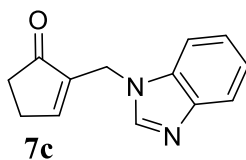
246F1 68 (0.432) AM2 (Ar,20000.0,0.00,0.00); Cm (64:68-59:62x2.000)

1: TOF MS ES+

2.27e6



Figure S40. ESI-HRMS spectra of 7b



**Elemental Composition Report**

**Single Mass Analysis**

Tolerance = 3.0 PPM / DBE: min = -5.0, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

277 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-80 H: 0-100 N: 0-10 O: 0-10

Cone voltage =30V

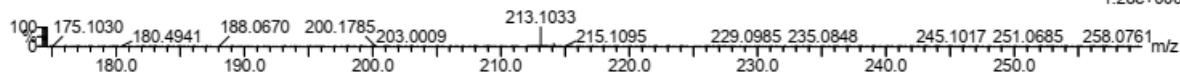
Xevo G2 QTof #YCA210

07-Jul-2022 09:28:03

247F1 68 (0.432) AM2 (Ar,20000.0,0.00,0.00); Cm (65:68-60:65x2.000)

1: TOF MS ES+

1.28e+006



Minimum: -5.0  
Maximum: 3.0 3.0 80.0

| Mass     | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf (%) | Formula      |
|----------|------------|-----|-----|-----|-------|------|----------|--------------|
| 213.1033 | 213.1028   | 0.5 | 2.3 | 8.5 | 414.9 | n/a  | n/a      | C13 H13 N2 O |

Cone voltage =30V

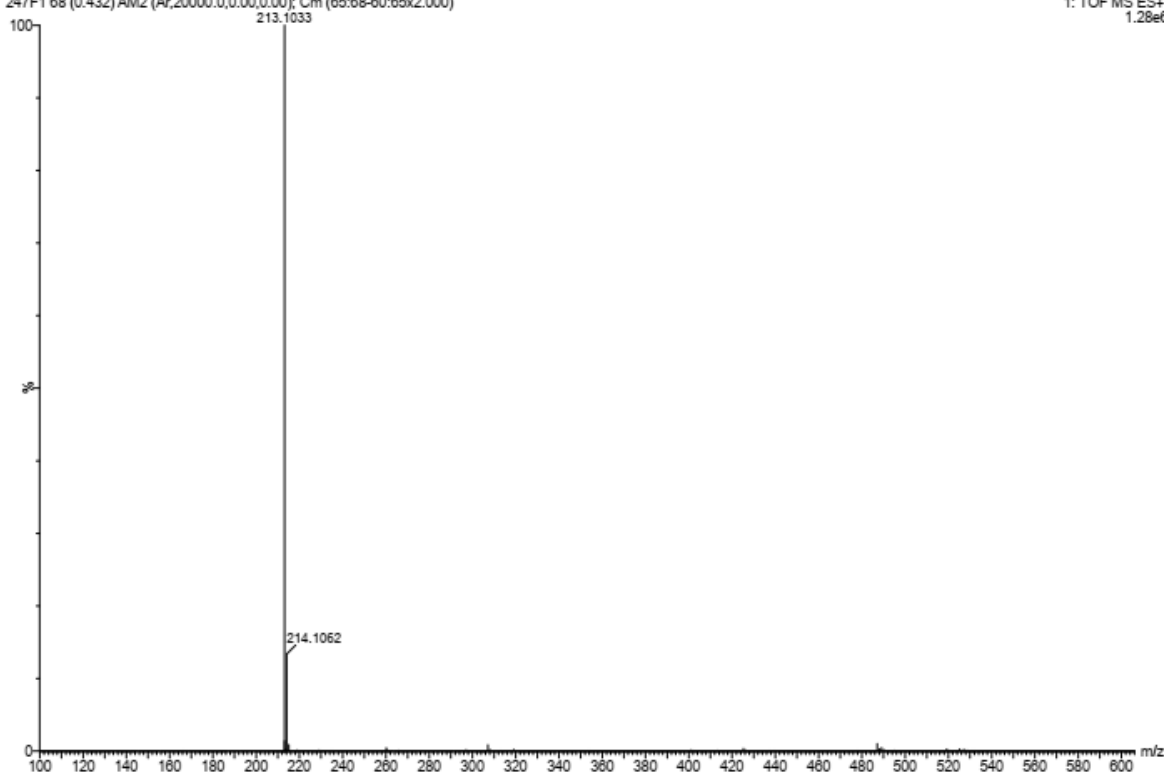
Xevo G2 QTof #YCA210

07-Jul-2022 09:28:03

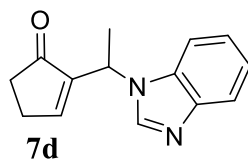
247F1 68 (0.432) AM2 (Ar,20000.0,0.00,0.00); Cm (65:68-60:65x2.000)

1: TOF MS ES+

1.28e6



**Figure S41. ESI-HRMS spectra of 7c**



## Elemental Composition Report

Page 1

### Single Mass Analysis

Tolerance = 3.0 PPM / DBE: min = -5.0, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

307 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-80 H: 0-100 N: 0-10 O: 0-10

Cone voltage =30V

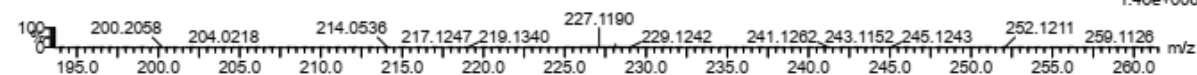
Xevo G2 QTof #YCA210

07-Jul-2022 09:40:59

249F2 68 (0.432) AM2 (Ar,20000.0,0.00,0.00); Cm (63:68-58:63x2.000)

1: TOF MS ES+

1.46e+006



Minimum: -5.0

Maximum: 3.0 3.0 80.0

| Mass     | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf (%) | Formula      |
|----------|------------|-----|-----|-----|-------|------|----------|--------------|
| 227.1190 | 227.1184   | 0.6 | 2.6 | 8.5 | 502.4 | n/a  | n/a      | C14 H15 N2 O |

Cone voltage =30V

Xevo G2 QTof #YCA210

07-Jul-2022 09:40:59

249F2 68 (0.432) AM2 (Ar,20000.0,0.00,0.00); Cm (63:68-58:63x2.000)

1: TOF MS ES+

1.46e6

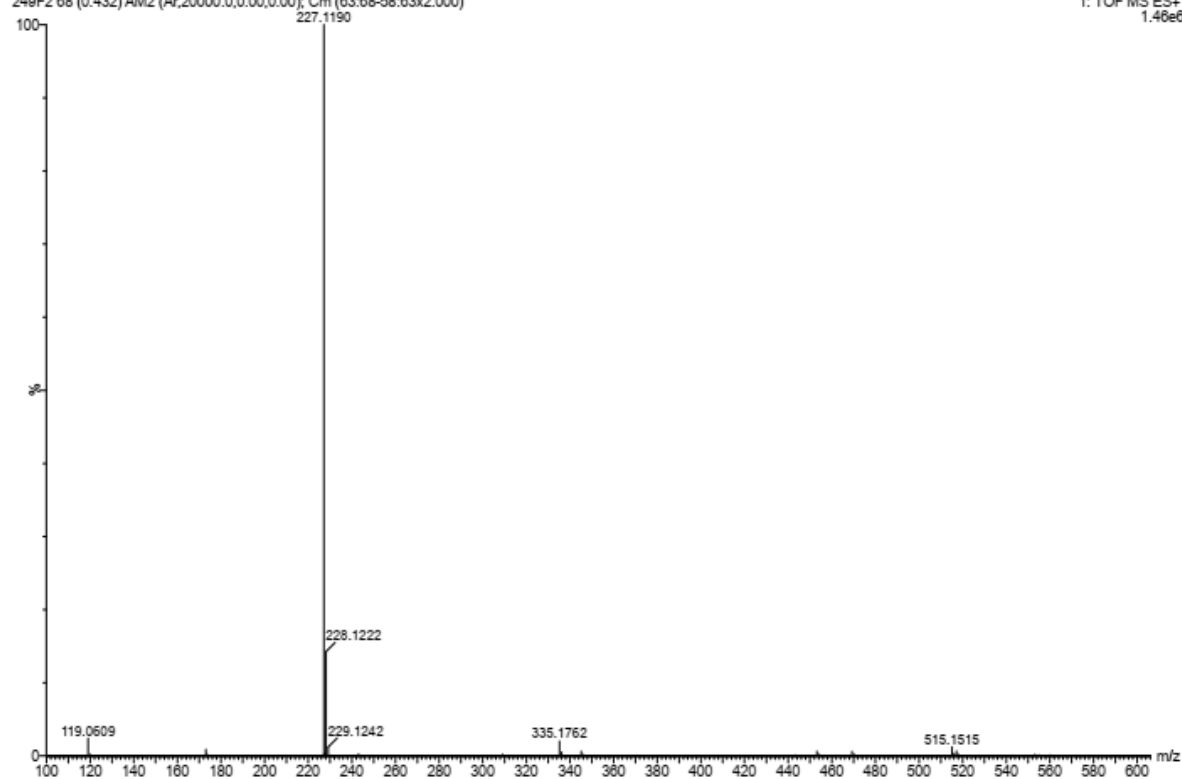
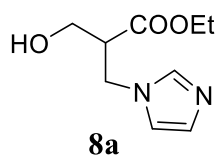


Figure S42. ESI-HRMS spectra of **7d**



## Elemental Composition Report

Page 1

### Single Mass Analysis

Tolerance = 3.0 PPM / DBE: min = -5.0, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

249 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-80 H: 0-100 N: 0-10 O: 0-10

Cone voltage = 30V

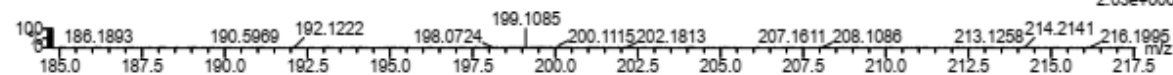
Xevo G2 QTof #YCA210

05-Jul-2022 15:38:31

252.76 (0.476) AM2 (Ar, 20000.0, 0.00, 0.00); Cm (72:76-56:85x2.000)

1: TOF MS ES+

2.03e+006



Minimum: -5.0  
Maximum: 3.0 3.0 80.0

| Mass     | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf (%) | Formula      |
|----------|------------|-----|-----|-----|-------|------|----------|--------------|
| 199.1085 | 199.1083   | 0.2 | 1.0 | 3.5 | 466.3 | n/a  | n/a      | C9 H15 N2 O3 |

Cone voltage = 30V

Xevo G2 QTof #YCA210

05-Jul-2022 15:38:31

252.76 (0.476) AM2 (Ar, 20000.0, 0.00, 0.00); Cm (72:76-56:85x2.000)

1: TOF MS ES+

2.03e6

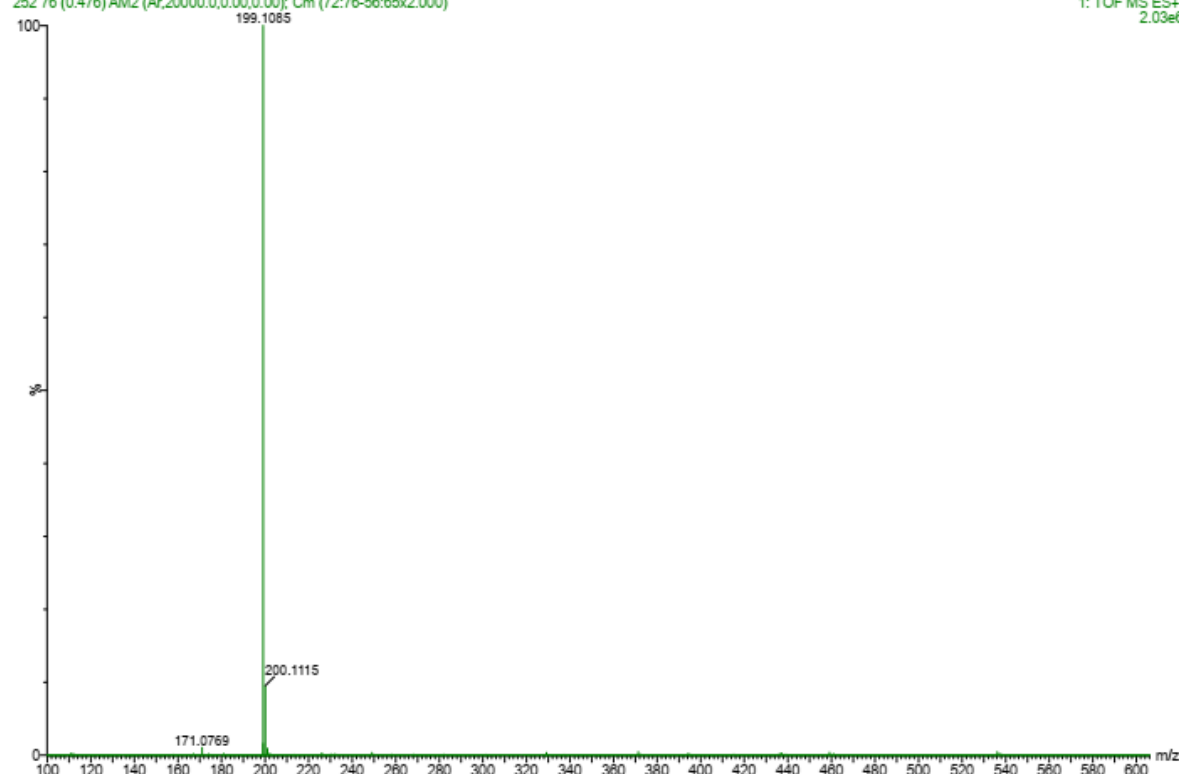
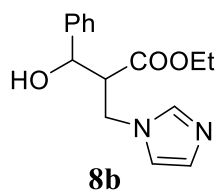


Figure S43. ESI-HRMS spectra of **8a**



**Elemental Composition Report**

**Single Mass Analysis**

Tolerance = 3.0 PPM / DBE: min = -5.0, max = 80.0

Element prediction: Off

Number of isotopic peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

406 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-80 H: 0-100 N: 0-10 O: 0-10

Cone voltage =30V

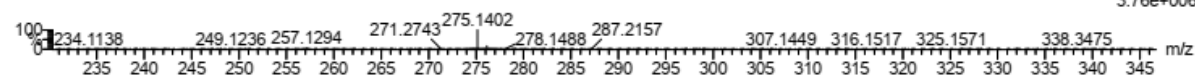
Xevo G2 QTof #YCA210

07-Jul-2022 09:57:08

255F0 70 (0.443) AM2 (Ar,20000.0,0.00,0.00); Cm (63:70-61:64x2.000)

1: TOF MS ES+

3.76e+006



Minimum: -5.0  
Maximum: 3.0 3.0 80.0

| Mass     | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf (%) | Formula       |
|----------|------------|-----|-----|-----|-------|------|----------|---------------|
| 275.1402 | 275.1396   | 0.6 | 2.2 | 7.5 | 599.2 | n/a  | n/a      | C15 H19 N2 O3 |

Cone voltage =30V

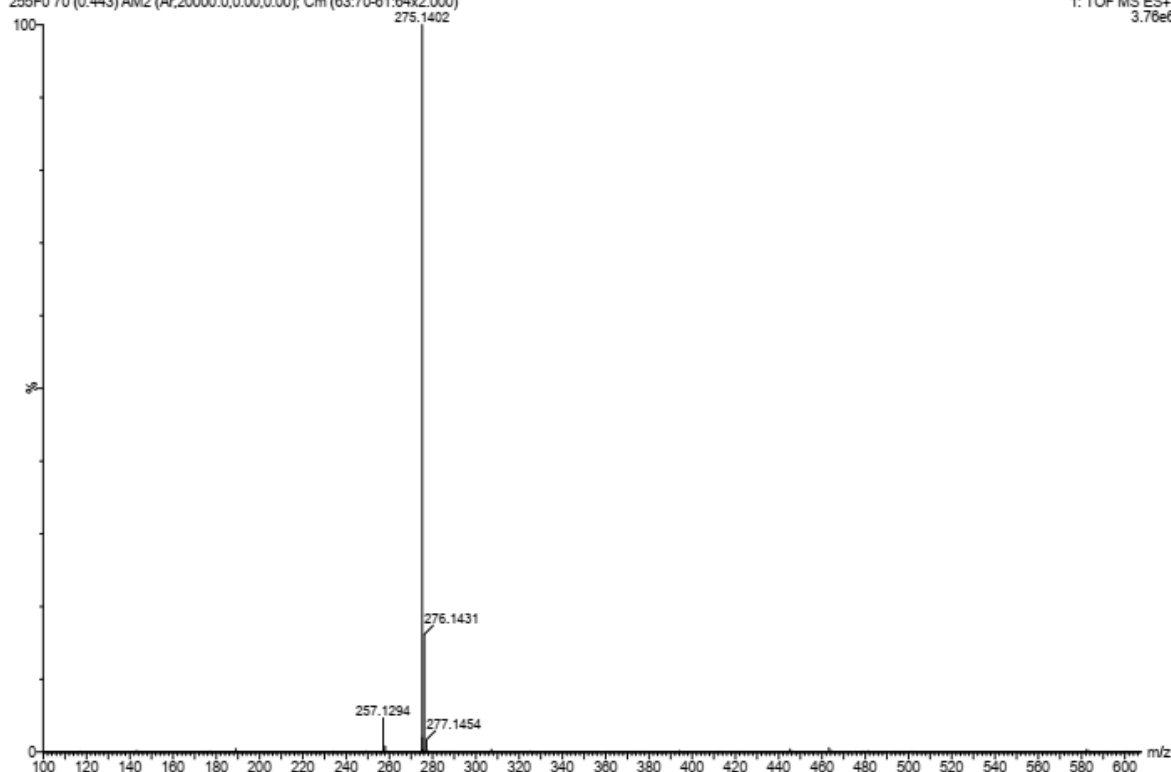
255F0 70 (0.443) AM2 (Ar,20000.0,0.00,0.00); Cm (63:70-61:64x2.000)

Xevo G2 QTof #YCA210

07-Jul-2022 09:57:08

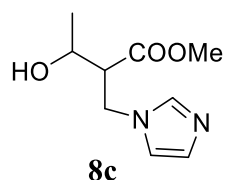
1: TOF MS ES+

3.76e6



**Figure S44. ESI-HRMS spectra of 8b**





## Elemental Composition Report

Page 1

### Single Mass Analysis

Tolerance = 3.0 PPM / DBE: min = -5.0, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

249 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-80 H: 0-100 N: 0-10 O: 0-10

Cone voltage =30V

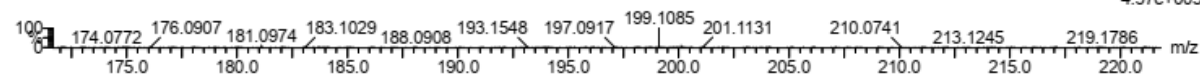
Xevo G2 QTof #YCA210

07-Jul-2022 10:01:13

256F2 72 (0.454) AM2 (Ar,20000.0,0.00,0.00); Cm (68:72-58:62x2.000)

1: TOF MS ES+

4.37e+005



Minimum: -5.0  
Maximum: 3.0 3.0 80.0

| Mass     | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf (%) | Formula      |
|----------|------------|-----|-----|-----|-------|------|----------|--------------|
| 199.1085 | 199.1083   | 0.2 | 1.0 | 3.5 | 293.4 | n/a  | n/a      | C9 H15 N2 O3 |

Cone voltage =30V

Xevo G2 QTof #YCA210

07-Jul-2022 10:01:13

256F2 72 (0.454) AM2 (Ar,20000.0,0.00,0.00); Cm (68:72-58:62x2.000)

1: TOF MS ES+

4.37e5

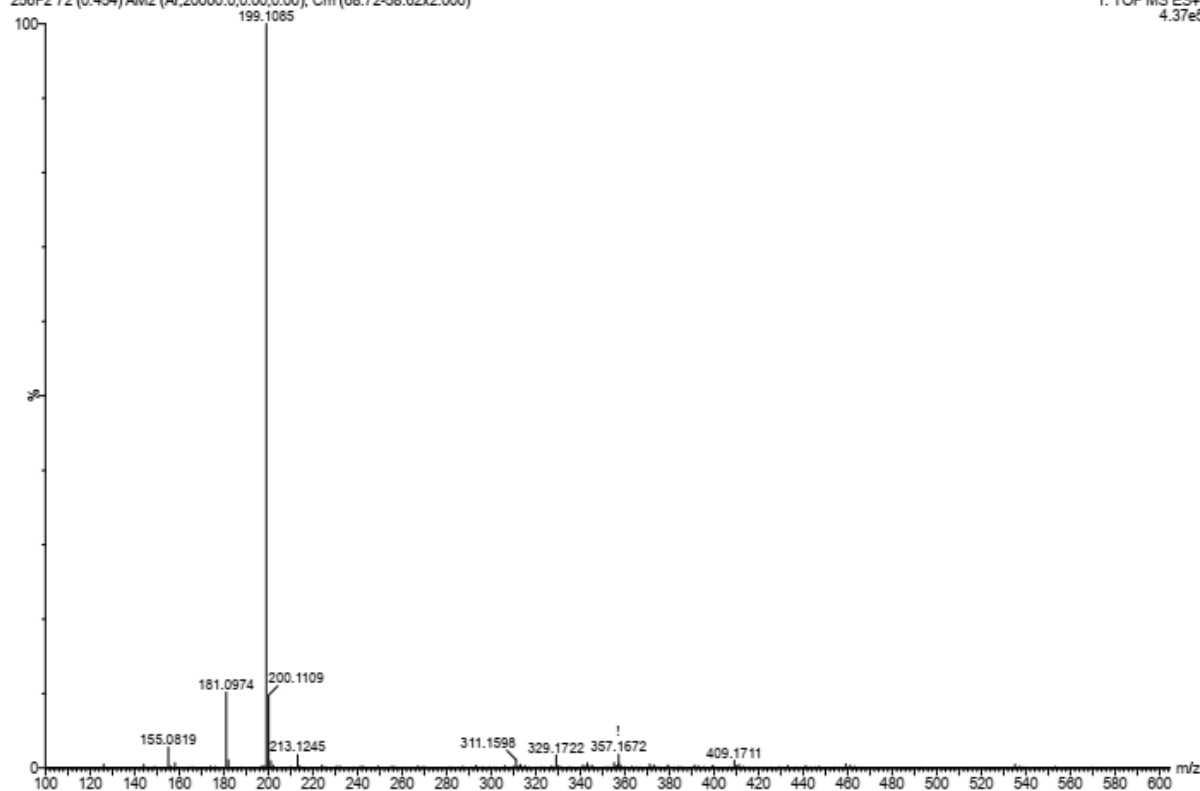
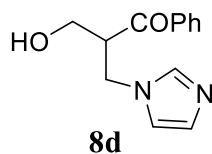


Figure S45. ESI-HRMS spectra of **8c**



**Elemental Composition Report**

**Single Mass Analysis**

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 80.0  
 Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions  
 111 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-100 H: 0-100 N: 0-5 O: 0-5

DCI-CH4

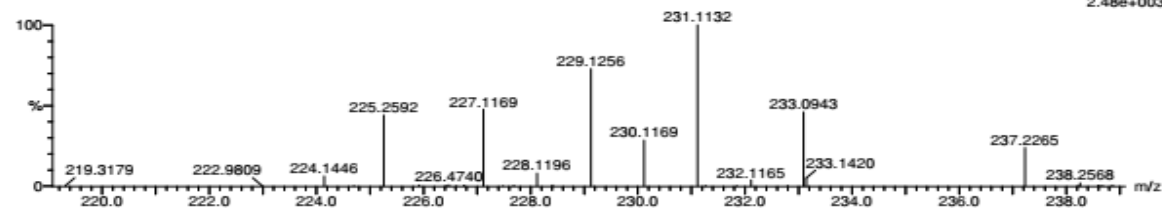
20220708-BH14- 22 (0.367) Cm (16:29-129:141x5.000)

GCT Premier CAB109

08-Jul-202210:40:52

TOF MS Cl+

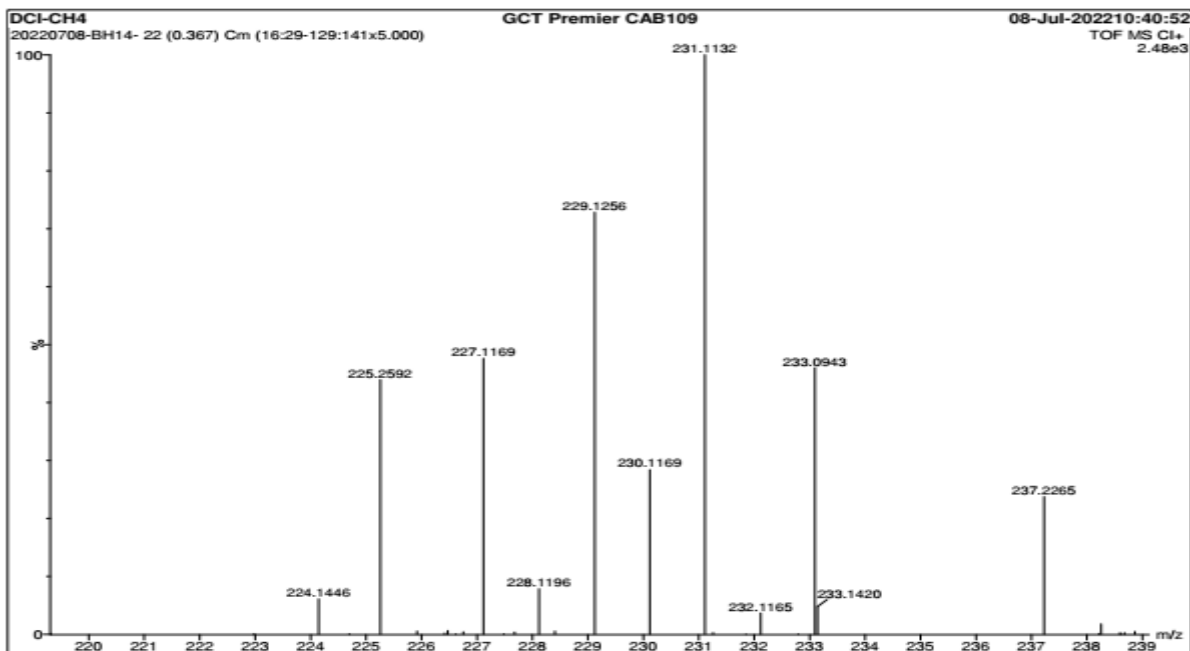
2.48e+003



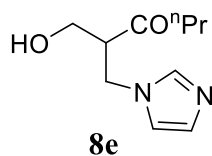
Minimum:

Maximum: 1.5 5.0 -1.5 80.0

| Mass     | Calc. Mass | mDa  | PPM  | DBE | i-FIT | Formula       |
|----------|------------|------|------|-----|-------|---------------|
| 231.1132 | 231.1134   | -0.2 | -0.9 | 7.5 | 327.2 | C13 H15 N2 O2 |



**Figure S46. ESI-HRMS spectra of 8d**



**Elemental Composition Report**

**Single Mass Analysis**

Tolerance = 3.0 PPM / DBE: min = -5.0, max = 80.0  
 Element prediction: Off  
 Number of isotopic peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions  
 243 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-80 H: 0-100 N: 0-10 O: 0-10

Cone voltage =15V

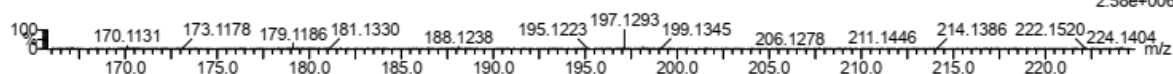
Xevo G2 QTof #YCA210

07-Jul-2022 10:13:19

BH19 83 (0.529) AM2 (Ar,20000.0,0.00,0.00); Cm (83:86-42:54x2.000)

2: TOF MS ES+

2.58e+006



Minimum: -5.0  
 Maximum: 3.0 3.0 80.0

| Mass     | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf (%) | Formula       |
|----------|------------|-----|-----|-----|-------|------|----------|---------------|
| 197.1293 | 197.1290   | 0.3 | 1.5 | 3.5 | 588.4 | n/a  | n/a      | C10 H17 N2 O2 |

Cone voltage =15V

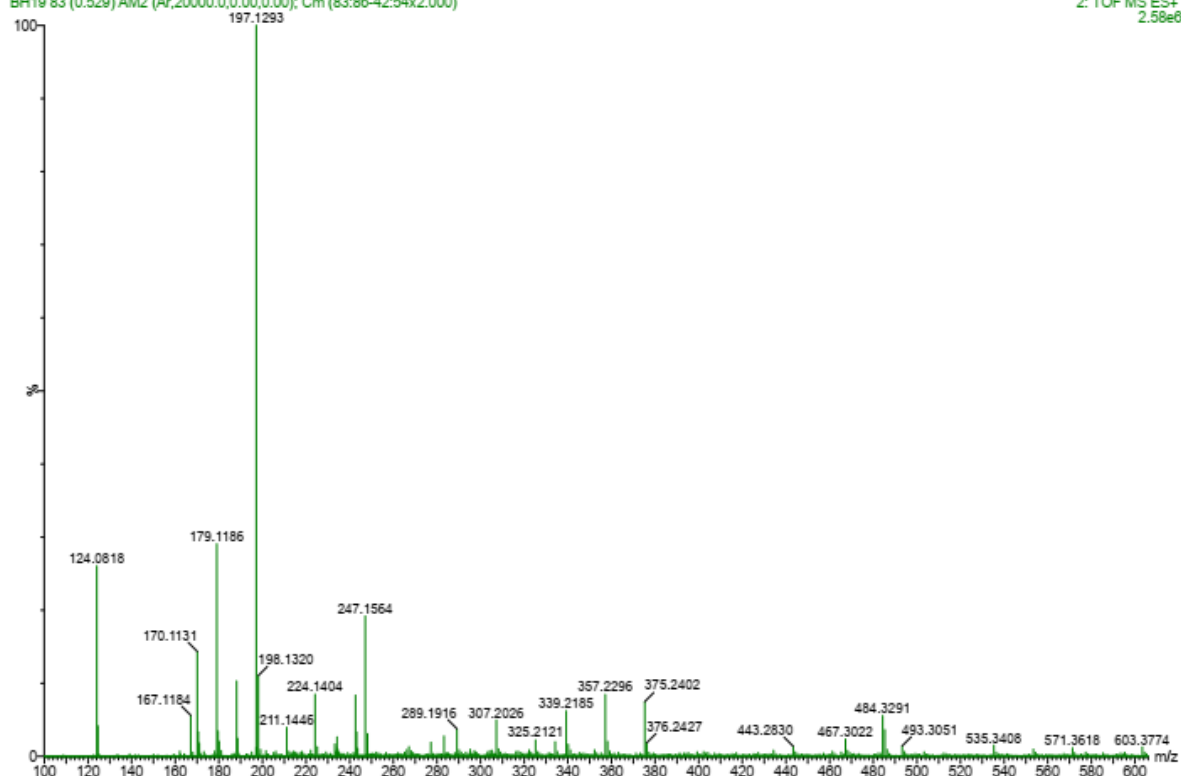
Xevo G2 QTof #YCA210

07-Jul-2022 10:13:19

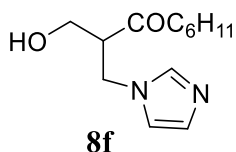
BH19 83 (0.529) AM2 (Ar,20000.0,0.00,0.00); Cm (83:86-42:54x2.000)

2: TOF MS ES+

2.58e6



**Figure S47. ESI-HRMS spectra of 8e**



## Elemental Composition Report

Page 1

### Single Mass Analysis

Tolerance = 3.0 PPM / DBE: min = -5.0, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

320 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-80 H: 0-100 N: 0-10 O: 0-10

Cone voltage =15V

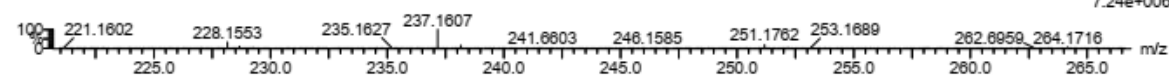
Xevo G2 QTof #YCA210

05-Jul-2022 15:42:36

BH16 83 (0.528) AM2 (Ar,20000.0,0.00,0.00); Cm (81:94-61:67x2.000)

2: TOF MS ES+

7.24e+006



Minimum: -5.0  
Maximum: 3.0 3.0 80.0

| Mass     | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf(%) | Formula       |
|----------|------------|-----|-----|-----|-------|------|---------|---------------|
| 237.1607 | 237.1603   | 0.4 | 1.7 | 4.5 | 687.8 | n/a  | n/a     | C13 H21 N2 O2 |

Cone voltage =15V

Xevo G2 QTof #YCA210

05-Jul-2022 15:42:36

BH16 83 (0.528) AM2 (Ar,20000.0,0.00,0.00); Cm (81:94-61:67x2.000)

2: TOF MS ES+

7.24e6

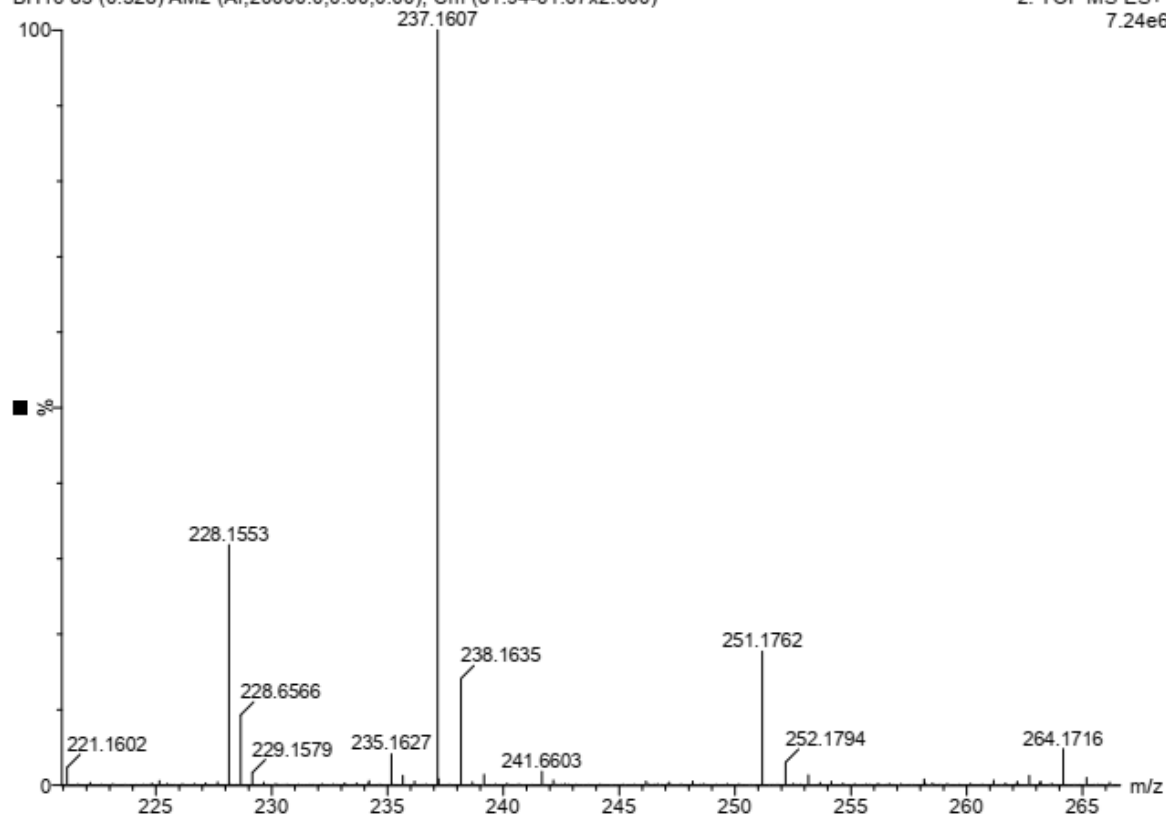


Figure S48. ESI-HRMS spectra of **8f**