

## SUPPLEMENTARY DATA

### Synthesis and Cytotoxic Activity of Methoxylated Chalcones in Breast Cancer MCF-7 and Prostate Cancer DU-145 Cell Lines

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## SPECTRAL DATA OF CHALCONES

### Chalcone (1)

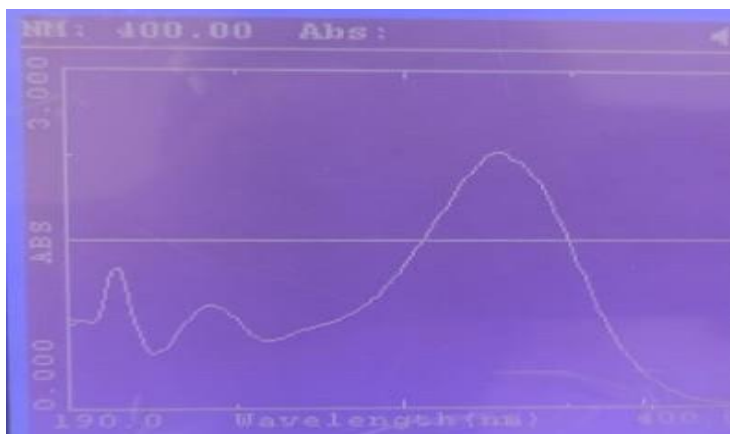


Figure 1a. Spectrum UV of compound (1)

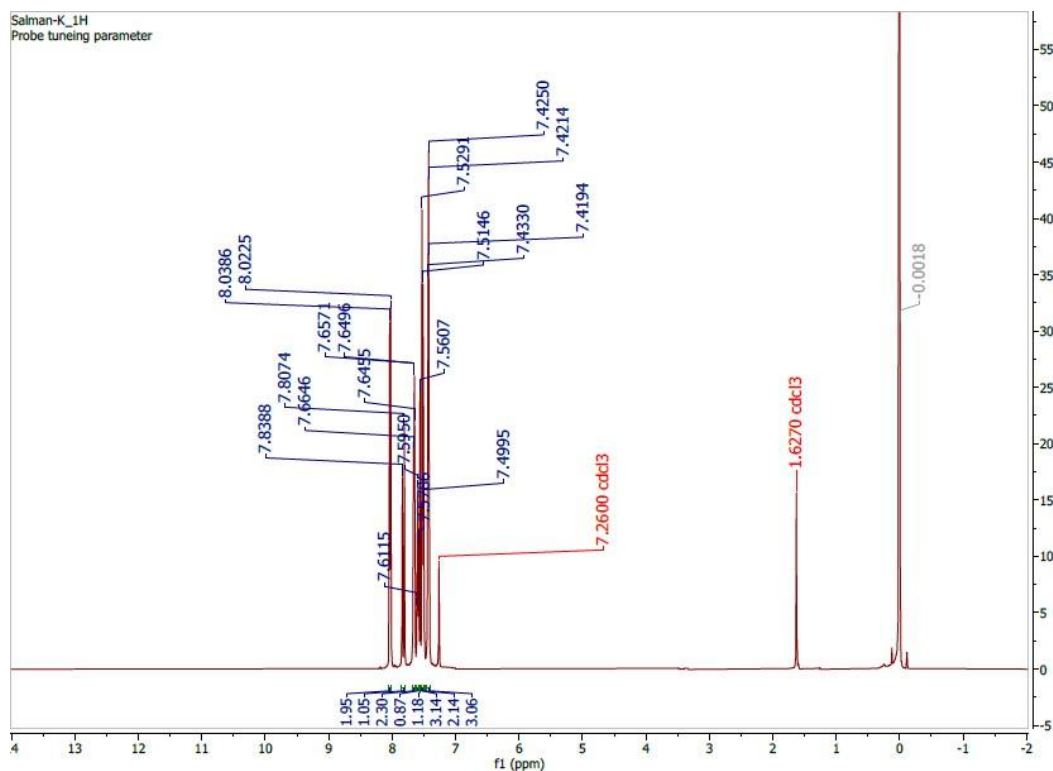


Figure 1b. Spectrum <sup>1</sup>H-NMR of compound (1)

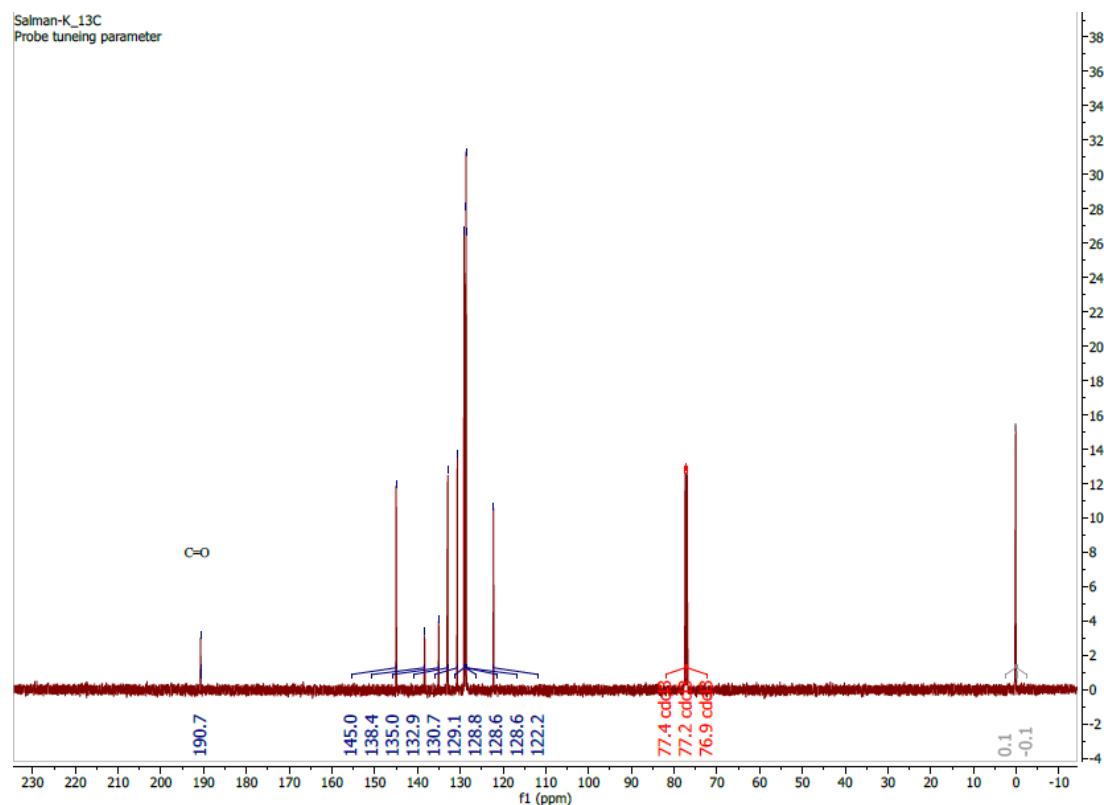


Figure 1c. Spectrum  $^{13}\text{C}$ -NMR of compound (1)

# Elemental Composition Report

Page 1

## Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

251 formula(e) evaluated with 5 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-500 H: 0-1000 N: 0-200 O: 0-200

K 34 (0.595) Cm (32-34)

TOF MS ES+

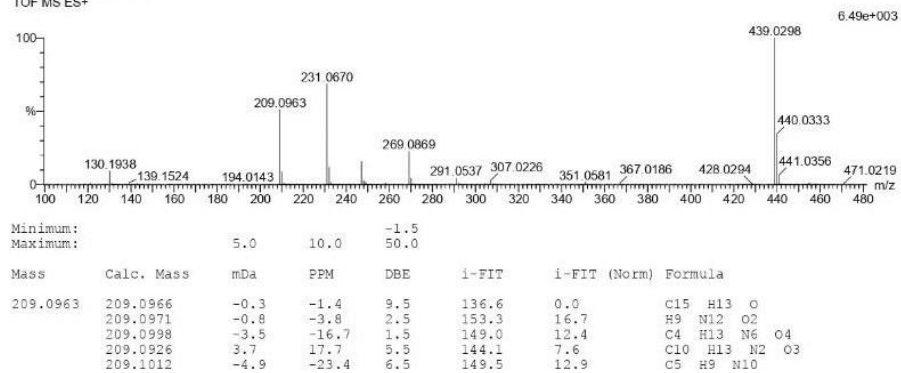


Figure 2b. Spectrum  $^1\text{H}$ -NMR of compound (2)

## 4-Bromochalcone (2)

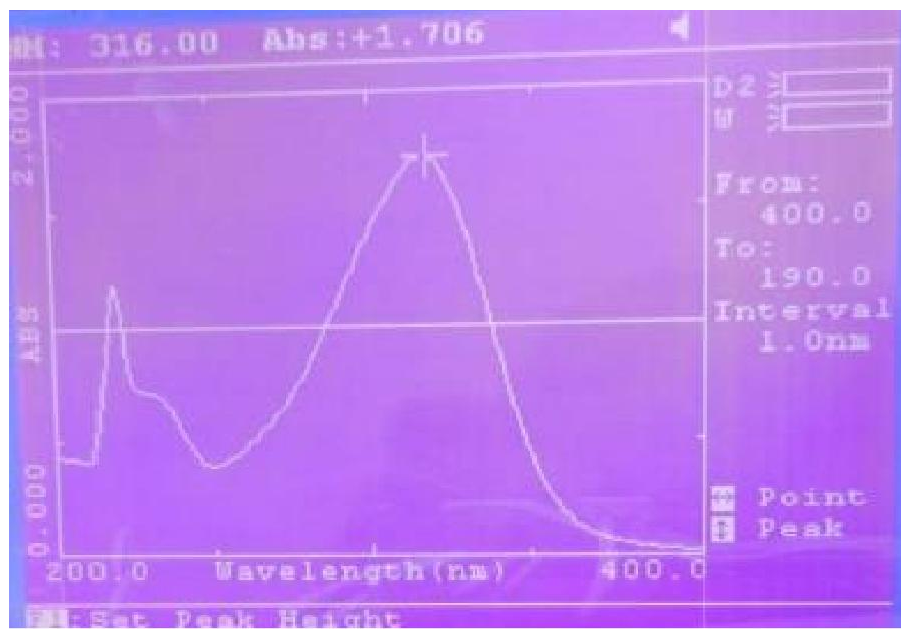


Figure 2a. Spectrum UV of compound (2)

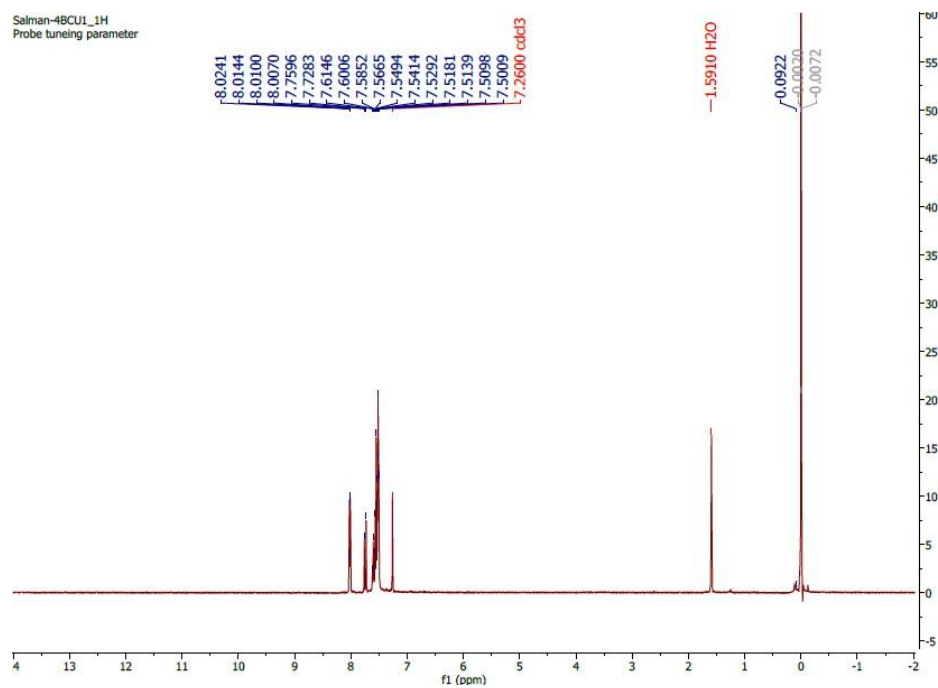
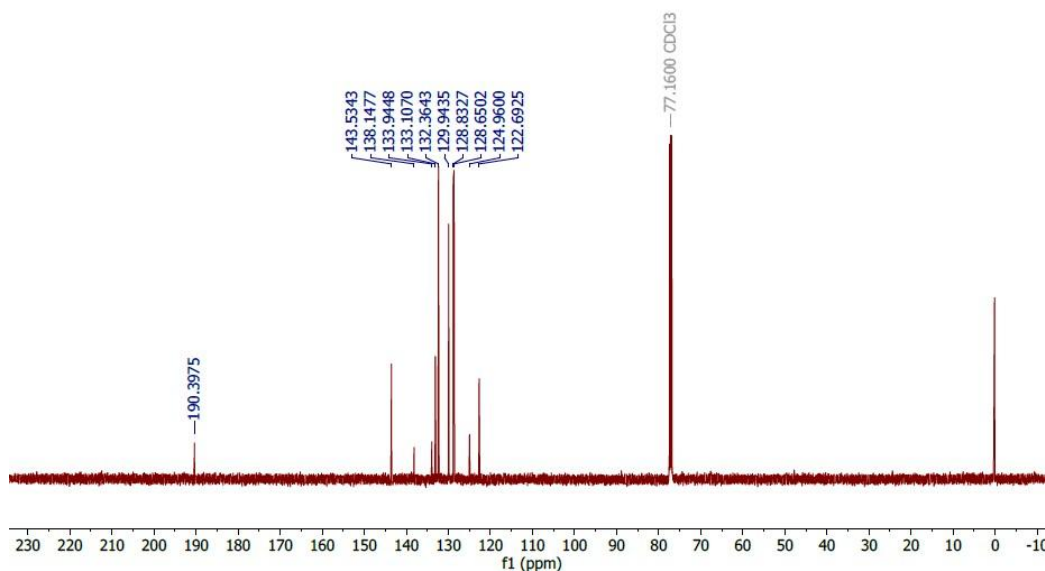


Figure 1d. Spectrum HRESI-TOF-MS of compound (1)

Figure 2c. Spectrum  $^{13}\text{C}$ -NMR of compound (2)

## Elemental Composition Report

Page 1

## Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

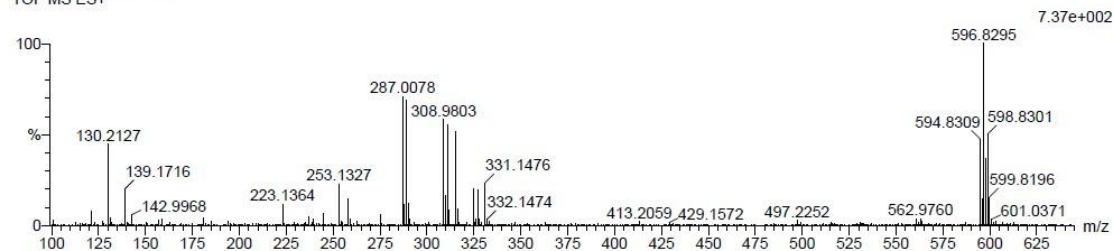
102 formula(e) evaluated with 3 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-500 H: 0-1000 O: 0-200 Br: 0-8

4 BC 2 (0.051) Cm (2:6)

TOF MS ES+



Minimum:

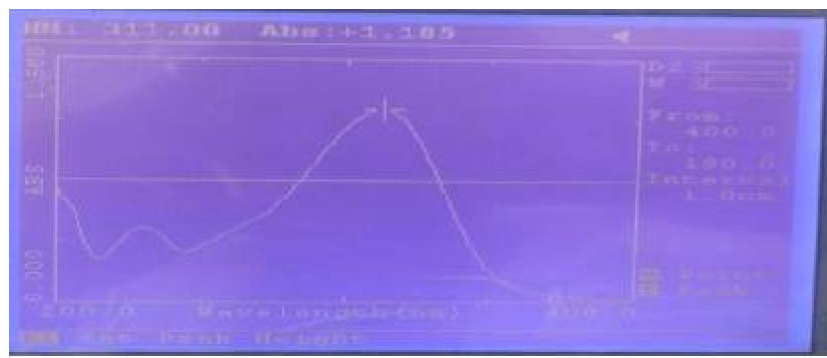
Maximum:

5.0 10.0 -1.5  
-2.0 -7.0 -1.5  
3.9 13.6 7.5

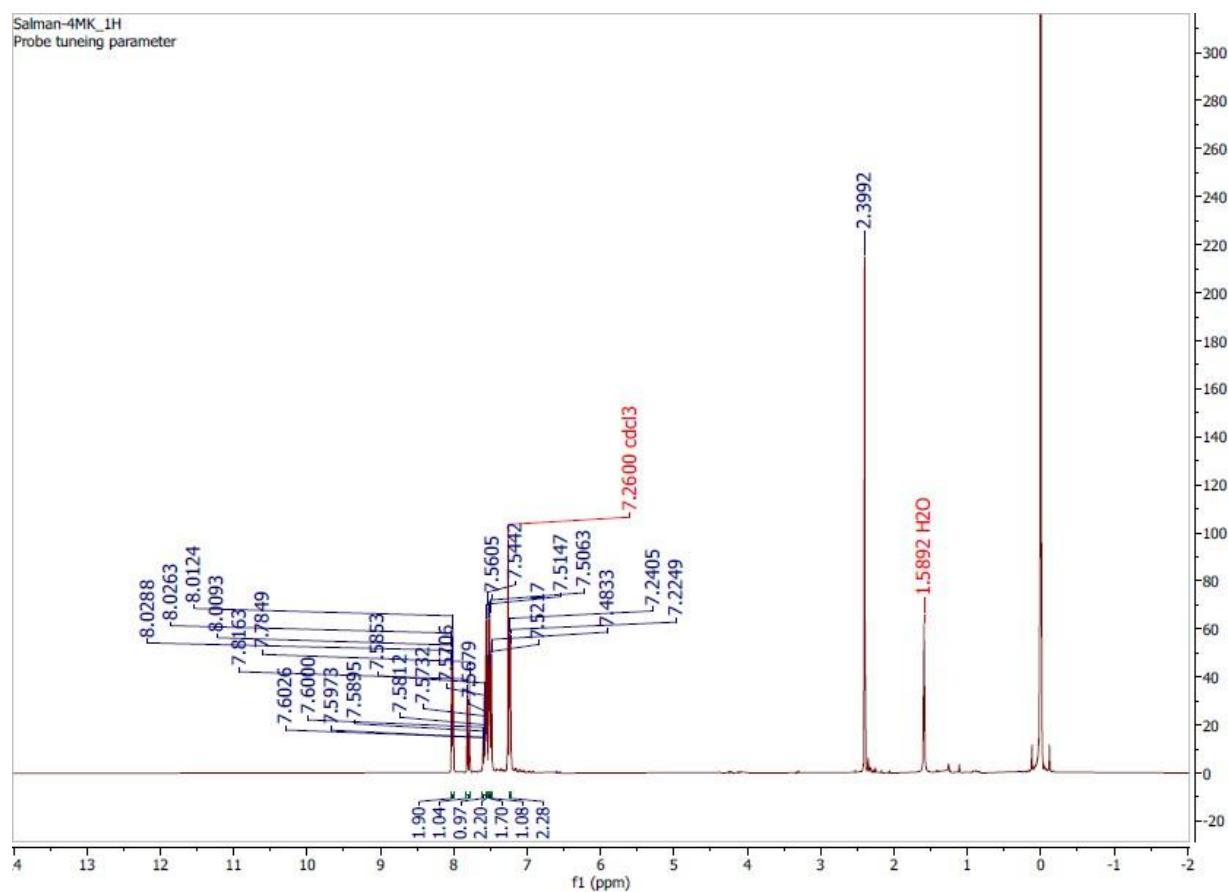
| Mass     | Calc. Mass | mDa  | PPM  | DBE  | i-FIT | i-FIT (Norm) | Formula      |
|----------|------------|------|------|------|-------|--------------|--------------|
| 287.0078 | 287.0072   | 0.6  | 2.1  | 9.5  | 55.3  | 0.0          | C15 H12 O Br |
|          | 287.0098   | -2.0 | -7.0 | -1.5 | 70.1  | 14.7         | C3 H11 O15   |
|          | 287.0039   | 3.9  | 13.6 | 7.5  | 69.7  | 14.4         | C10 H7 O10   |

Figure 2b. Spectrum  $^1\text{H}$ -NMR of compound (2)

### 4-Methylchalcone (3)

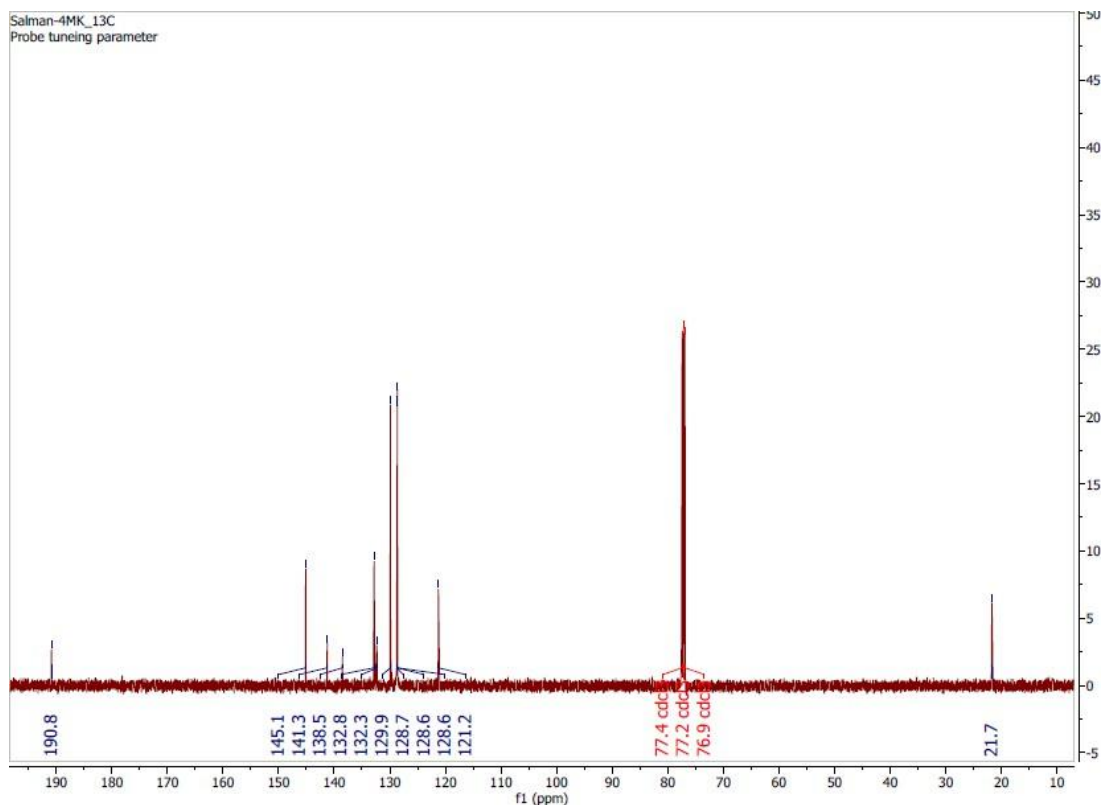


**Figure 3a.** Spectrum UV of compound (3)



**Figure 3b.** Spectrum <sup>1</sup>H-NMR of compound (3)

**Figure 2d.** Spectrum HRESI-TOF-MS of compound (2)



**Figure 3c.** Spectrum  $^{13}\text{C}$ -NMR of compound (3)

#### Elemental Composition Report

Page 1

#### Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

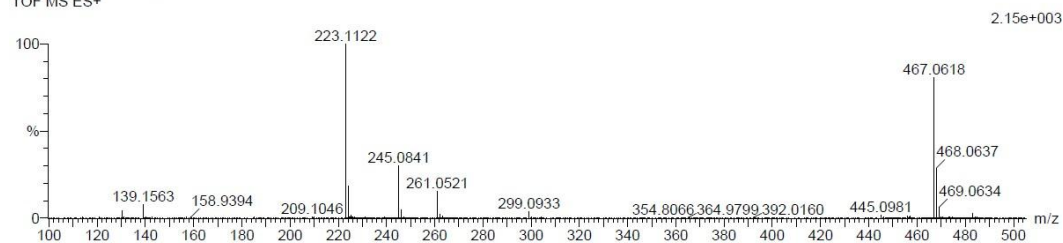
294 formula(e) evaluated with 5 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-500 H: 0-1000 N: 0-200 O: 0-200

4 MTC 9 (0.170) Cm (8.9)

TOF MS ES+



Minimum:

Maximum:

5.0 10.0 -1.5 50.0

| Mass     | Calc. Mass | mDa  | PPM   | DBE | i-FIT | i-FIT (Norm) | Formula       |
|----------|------------|------|-------|-----|-------|--------------|---------------|
| 223.1122 | 223.1123   | -0.1 | -0.4  | 9.5 | 102.8 | 0.0          | C16 H15 O     |
|          | 223.1128   | -0.6 | -2.7  | 2.5 | 115.1 | 12.3         | C H11 N12 O2  |
|          | 223.1155   | -3.3 | -14.8 | 1.5 | 112.2 | 9.4          | C5 H15 N6 O4  |
|          | 223.1083   | 3.9  | 17.5  | 5.5 | 108.6 | 5.8          | C11 H15 N2 O3 |
|          | 223.1168   | -4.6 | -20.6 | 6.5 | 112.4 | 9.6          | C6 H11 N10    |

**Figure 4b.** Spectrum  $^1\text{H}$ -NMR of compound (4)

#### 4-Methoxychalcone (4)



Figure 4a. Spectrum UV of compound (4)

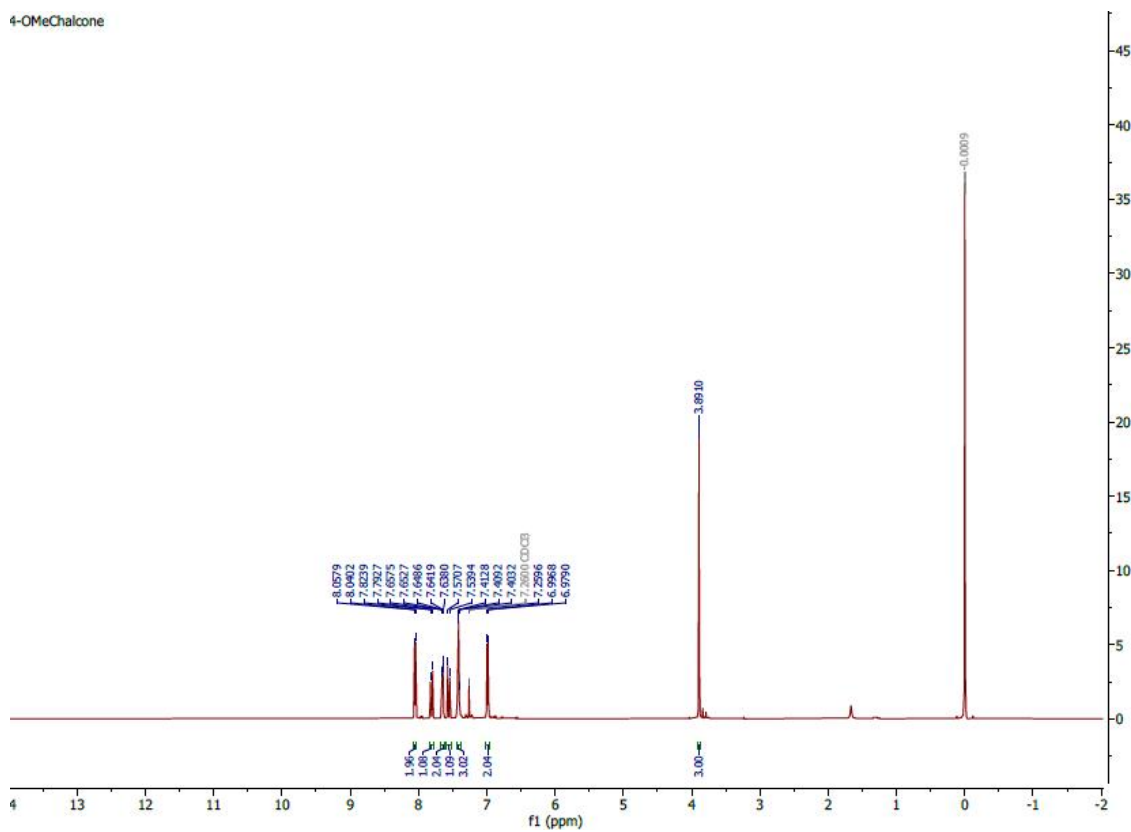
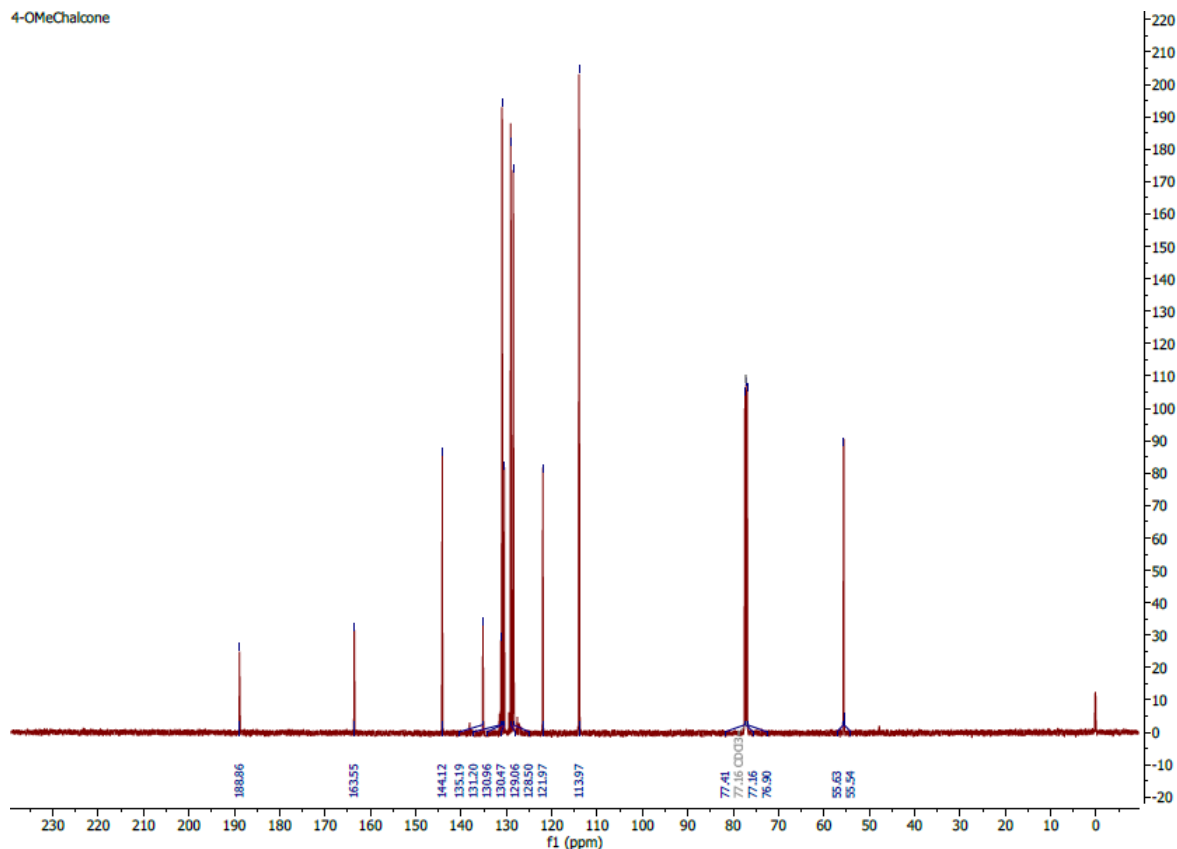


Figure 3d. Spectrum HRESI-TOF-MS of compound (3)

Figure 4c. Spectrum  $^{13}\text{C}$ -NMR of compound (4)

## Elemental Composition Report

Page 1

## Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

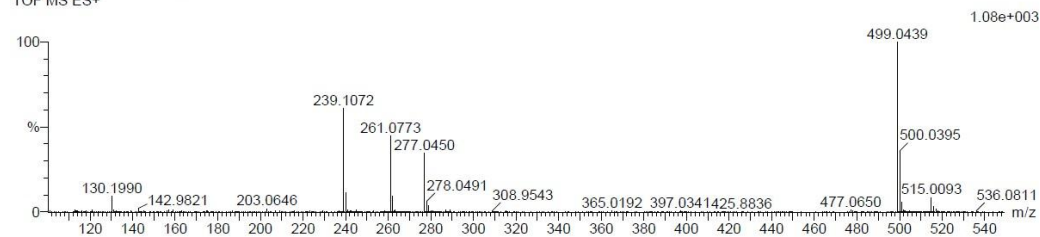
39 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-500 H: 0-1000 O: 0-200

4 MC, 1.7 (0.136) Cm (7.8)

TOF MS ES+



Minimum:

Maximum:

5.0

10.0

-1.5

50.0

Mass

Calc. Mass

mDa

PPM

DBE

i-FIT

i-FIT (Norm)

Formula

239.1072

239.1072

0.0

0.0

9.5

50.4

0.0

C16 H15 O2

Figure 5b. Spectrum  $^1\text{H}$ -NMR of compound (5)

### 4'-Methoxychalcone (5)

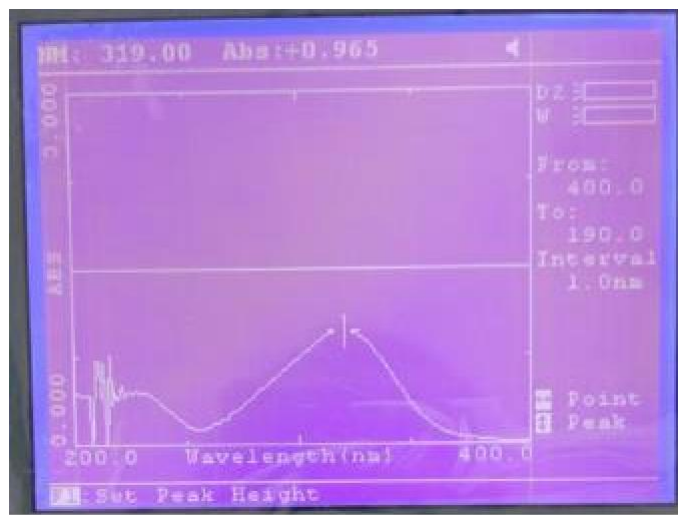


Figure 5a. Spectrum UV of compound (5)

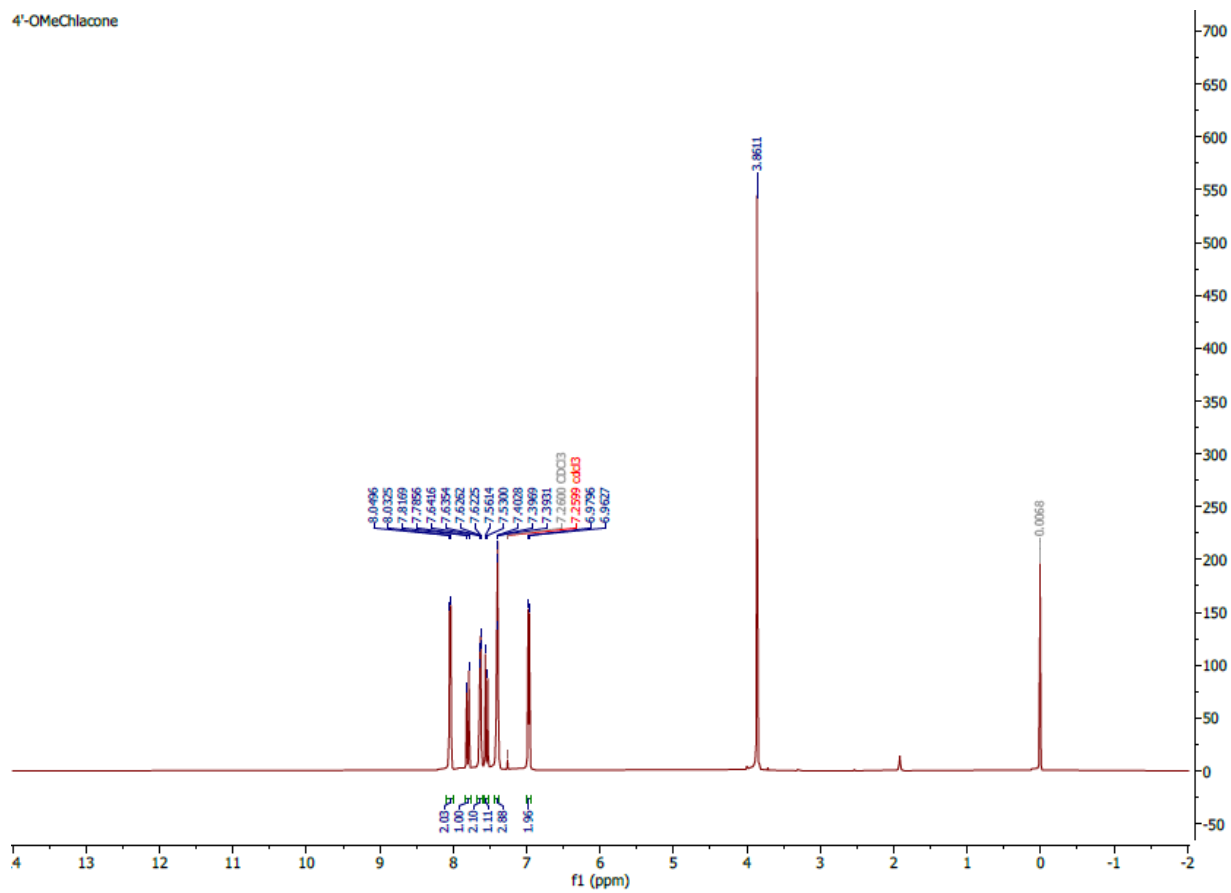


Figure 4d. Spectrum HRESI-TOF-MS of compound (4)

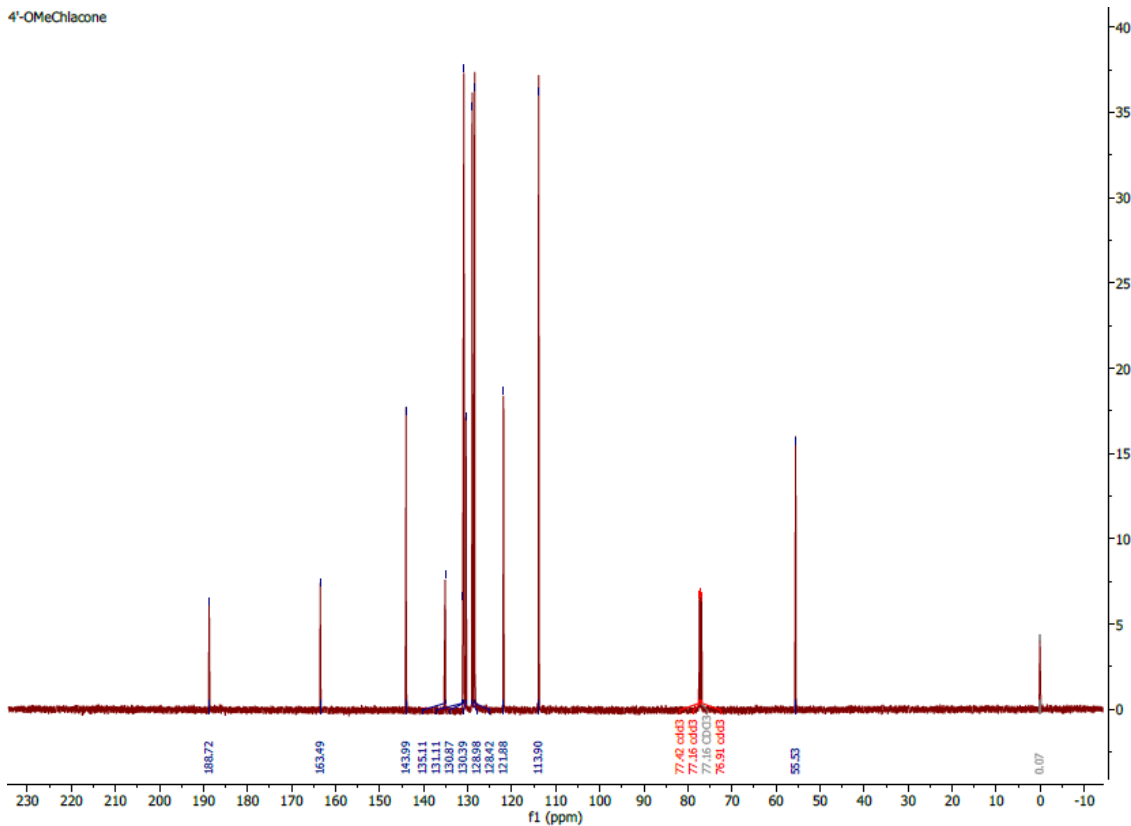


Figure 5c. Spectrum  $^{13}\text{C}$ -NMR of compound (5)

## Elemental Composition Report

Page 1

### Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

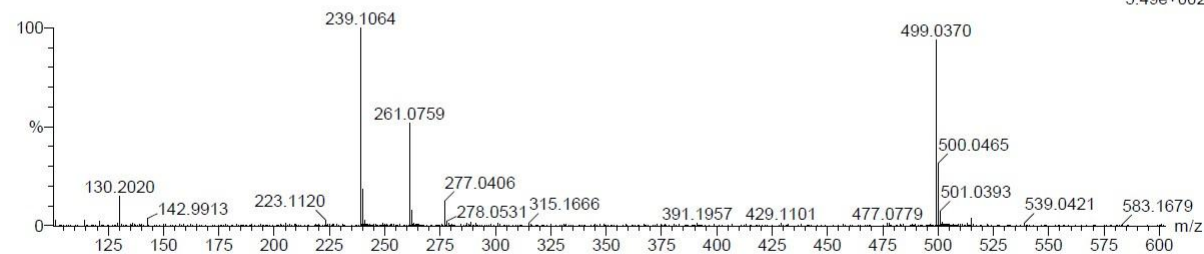
39 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-500 H: 0-1000 O: 0-200

4 MC 7 (0.136) Cm (6:7)

TOF MS ES+

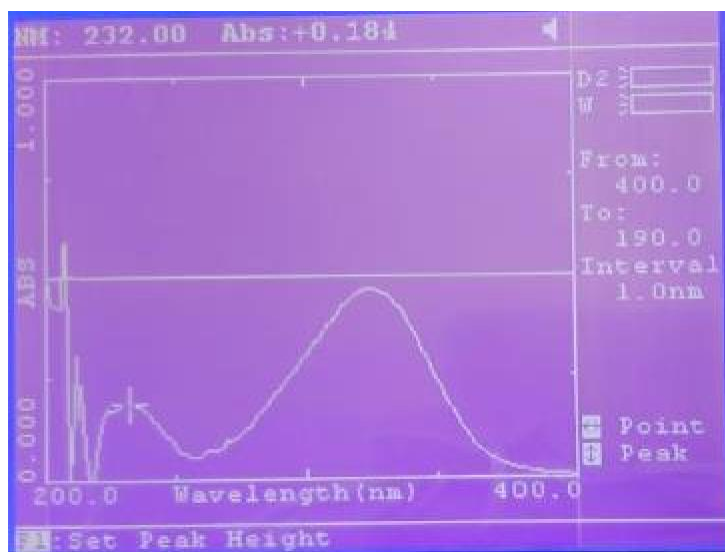


Minimum: -1.5  
Maximum: 5.0 10.0 50.0

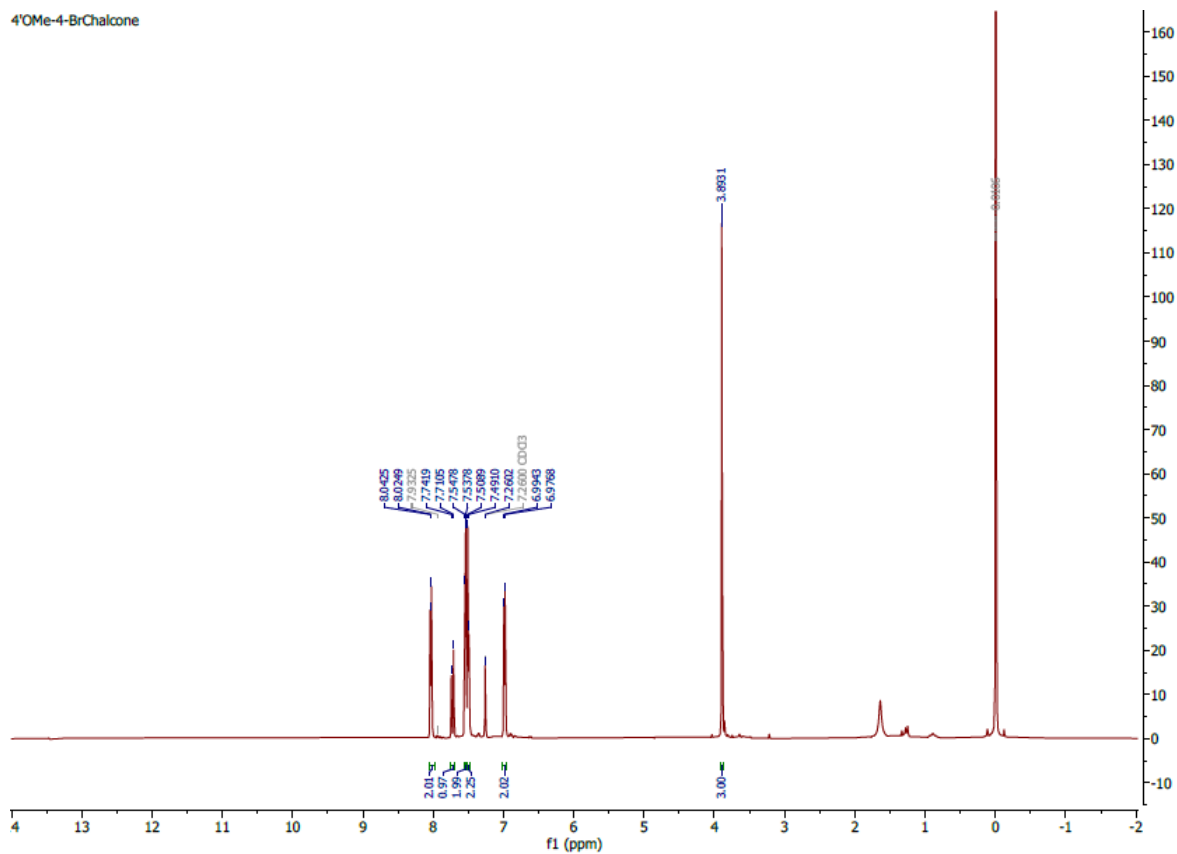
| Mass     | Calc. Mass | mDa  | PPM  | DBE | i-FIT | i-FIT (Norm) | Formula    |
|----------|------------|------|------|-----|-------|--------------|------------|
| 239.1064 | 239.1072   | -0.8 | -3.3 | 9.5 | 40.6  | 0.0          | C16 H15 O2 |

Figure 6b. Spectrum  $^1\text{H}$ -NMR of compound (6)

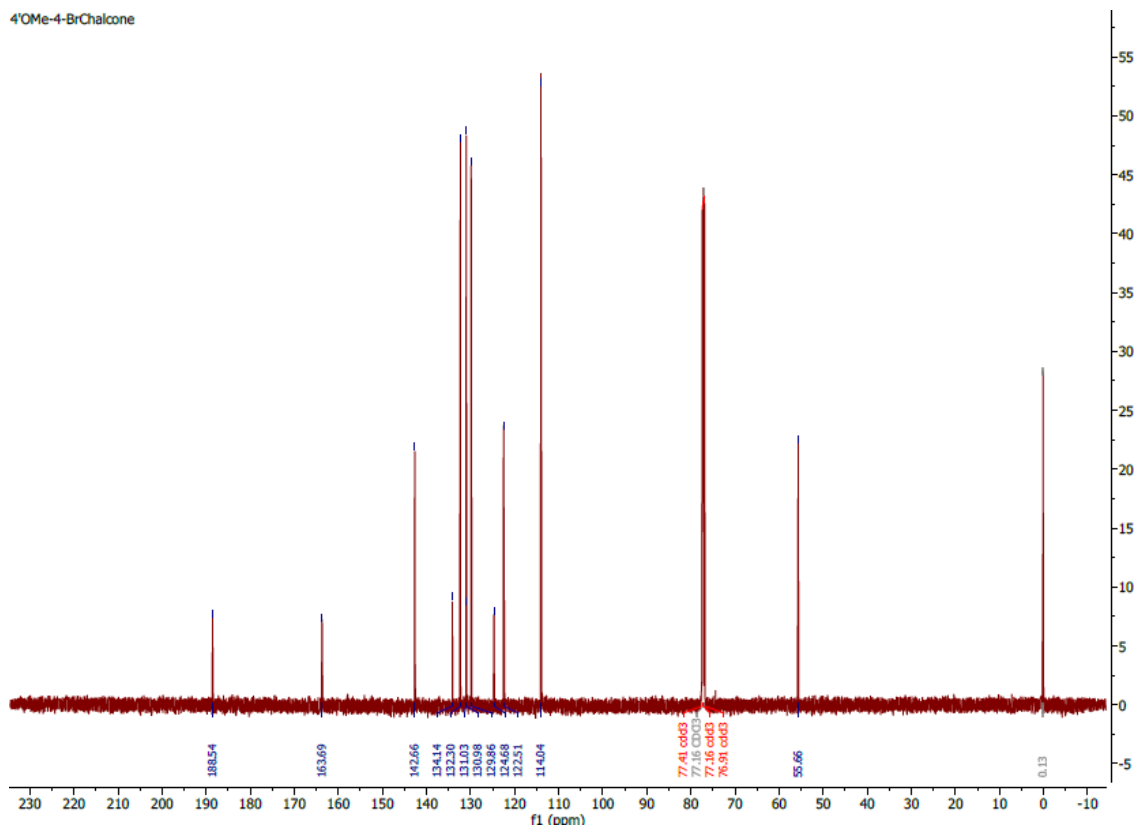
### **4-Bromo-4'-Methoxychalcone (6)**



**Figure 6a.** Spectrum UV of compound (6)



**Figure 5d.** Spectrum HRESI-TOF-MS of compound (**5**)



#### Elemental Composition Report

Page 1

#### Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

121 formula(e) evaluated with 3 results within limits (up to 50 closest results for each mass)

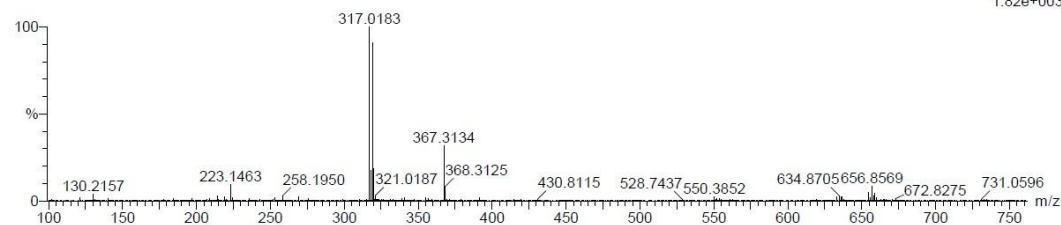
Elements Used:

C: 0-500 H: 0-1000 O: 0-200 Br: 0-8

4 B 4MC 2 (0.051) Cm (2)

TOF MS ES+

1.82e+003



Minimum:

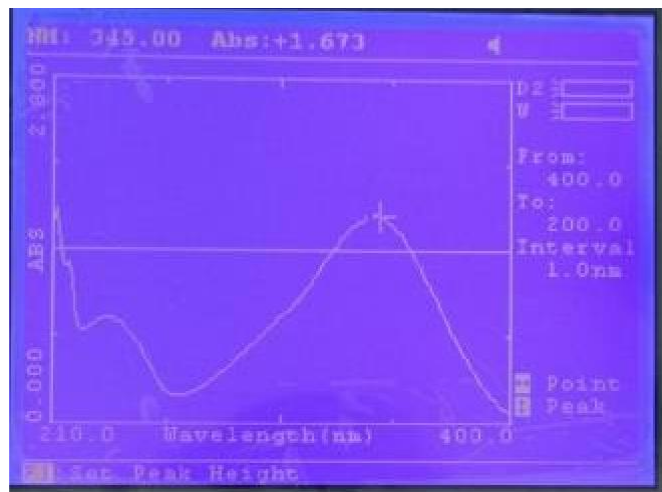
Maximum:

Mass Calc. Mass mDa PPM DBE i-FIT i-FIT (Norm) Formula

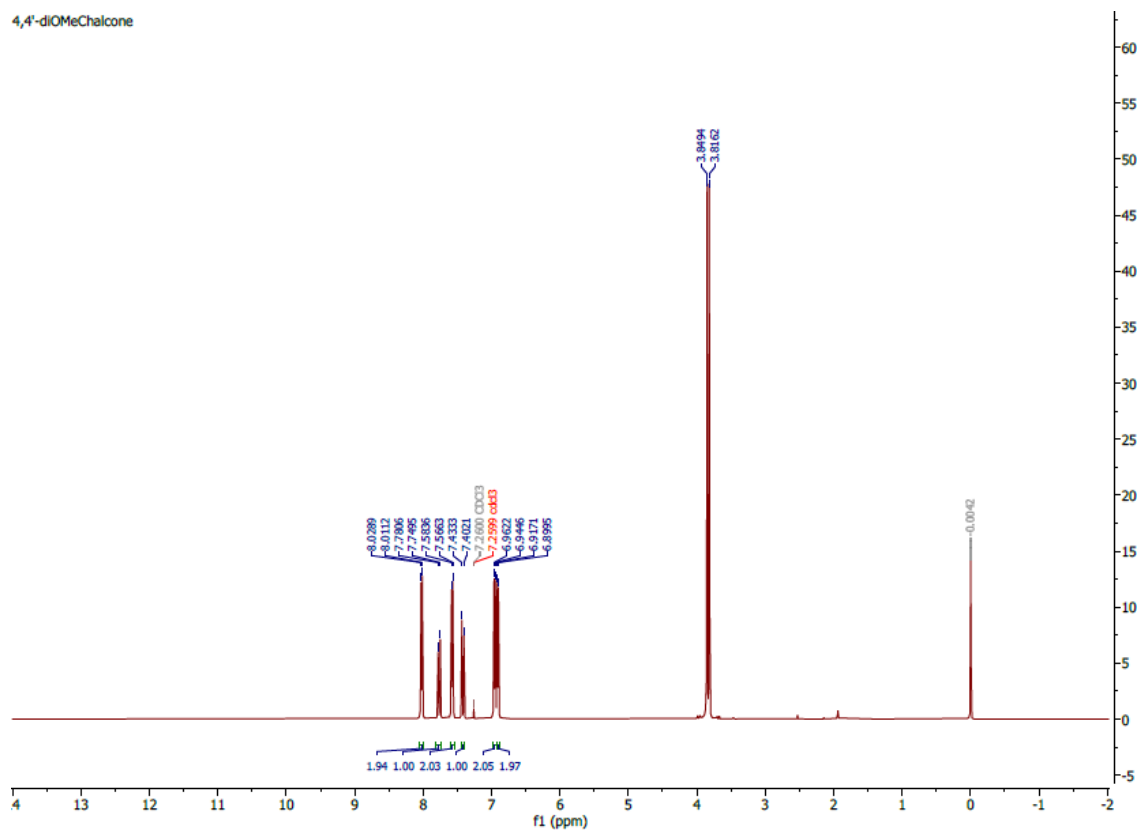
|          |          |      |      |      |      |      |               |
|----------|----------|------|------|------|------|------|---------------|
| 317.0183 | 317.0177 | 0.6  | 1.9  | 9.5  | 54.5 | 0.0  | C16 H14 O2 Br |
|          | 317.0204 | -2.1 | -6.6 | -1.5 | 73.3 | 18.8 | C4 H13 O16    |
|          | 317.0145 | 3.8  | 12.0 | 7.5  | 73.3 | 18.8 | C11 H9 O11    |

Figure 7b. Spectrum  $^1\text{H}$ -NMR of compound (7)

### 4,4'-Dimethoxychalcone (7)



**Figure 7a.** Spectrum UV of compound (7)



**Figure 6d.** Spectrum HRESI-TOF-MS of compound (6)

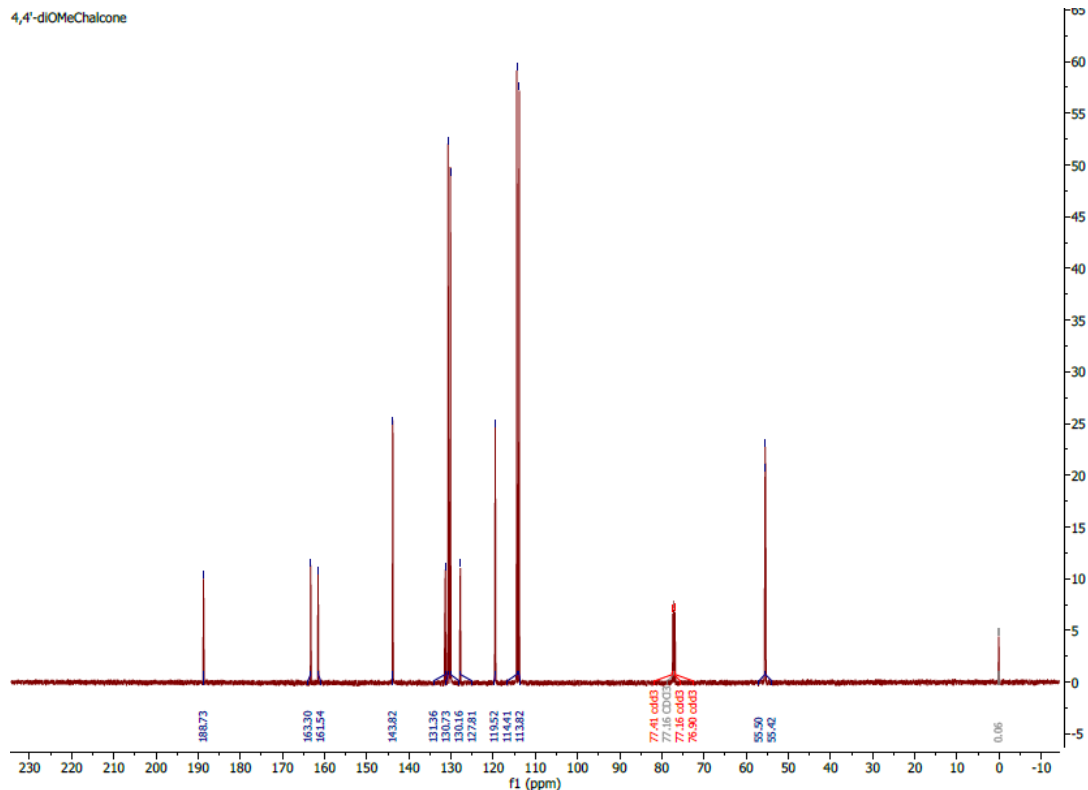


Figure 7c. Spectrum <sup>13</sup>C-NMR of compound (7)

#### Elemental Composition Report

Page 1

##### Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

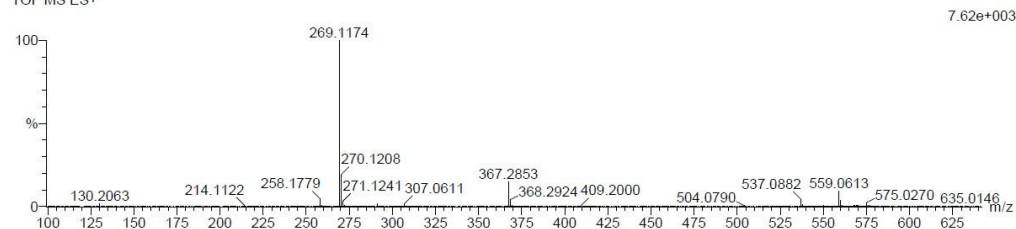
461 formula(e) evaluated with 7 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-500 H: 0-1000 N: 0-200 O: 0-200

4.4 DMC 33 (0.578) Cm (32.33)

TOF MS ES+



Minimum:

Maximum:

5.0

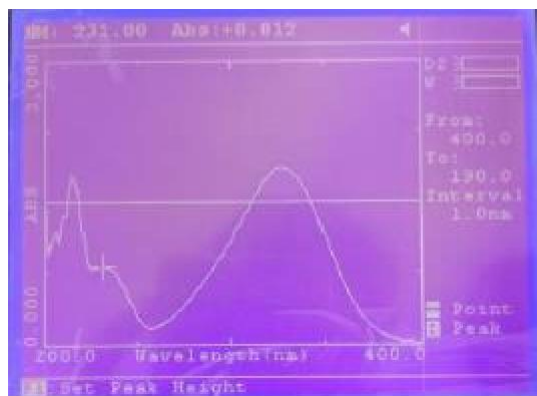
10.0

-1.5

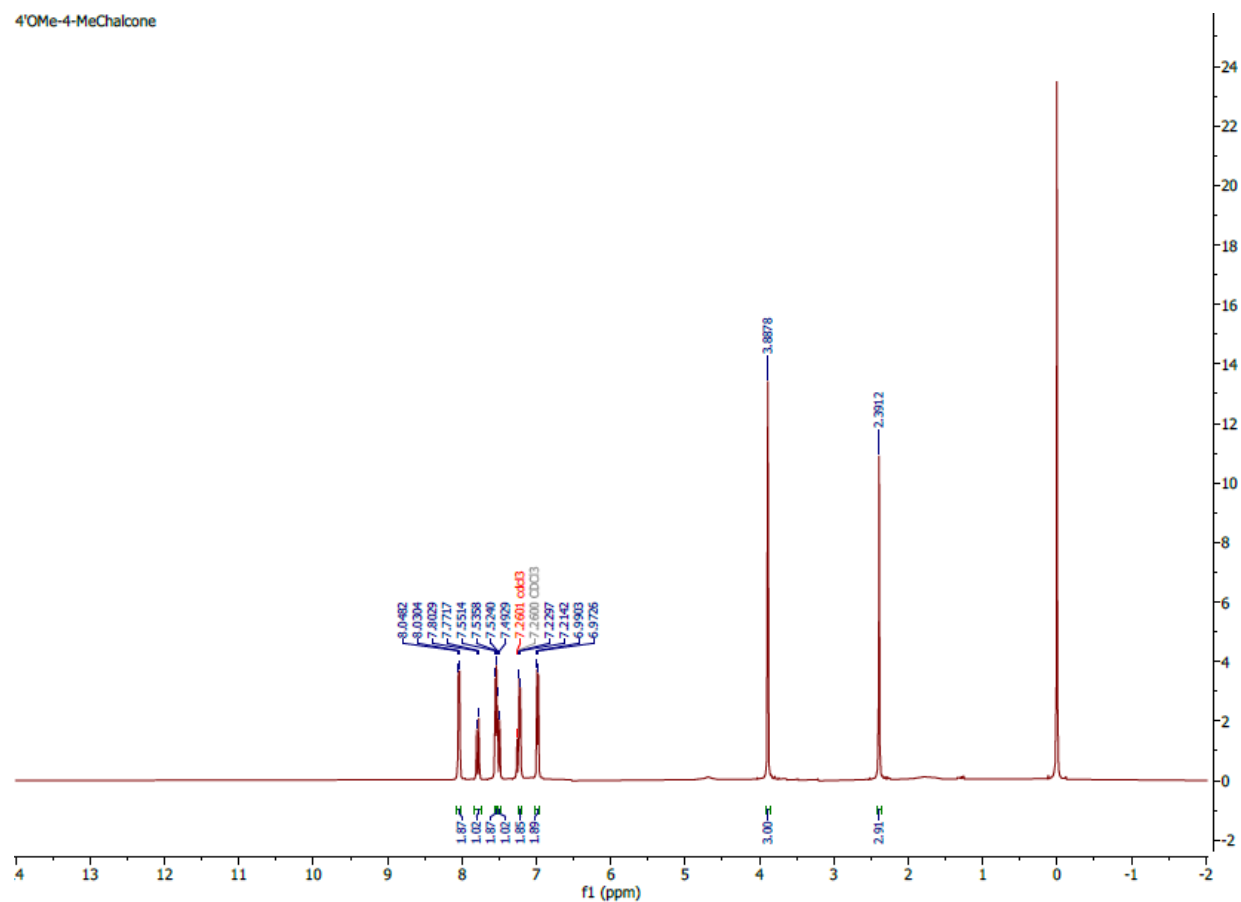
50.0

| Mass     | Calc. Mass | mDa  | PPM   | DBE  | i-FIT | i-FIT (Norm) | Formula       |
|----------|------------|------|-------|------|-------|--------------|---------------|
| 269.1174 | 269.1178   | -0.4 | -1.5  | 9.5  | 137.4 | 0.0          | C17 H17 O3    |
|          | 269.1183   | -0.9 | -3.3  | 2.5  | 152.7 | 15.3         | C2 H13 N12 O4 |
|          | 269.1196   | -2.2 | -8.2  | 7.5  | 153.2 | 15.8         | C3 H9 N16     |
|          | 269.1151   | 2.3  | 8.5   | 10.5 | 143.7 | 6.4          | C13 H13 N6 O  |
|          | 269.1210   | -3.6 | -13.4 | 1.5  | 149.1 | 11.7         | C6 H17 N6 O6  |
|          | 269.1137   | 3.7  | 13.7  | 5.5  | 144.9 | 7.5          | C12 H17 N2 O5 |
|          | 269.1223   | -4.9 | -18.2 | 6.5  | 149.6 | 12.2         | C7 H13 N10 O2 |

### **4-Methyl-4'-Methoxychalcone (8)**



**Figure 8a.** Spectrum UV of compound (8)



**Figure 7d.** Spectrum HRESI-TOF-MS of compound (7)

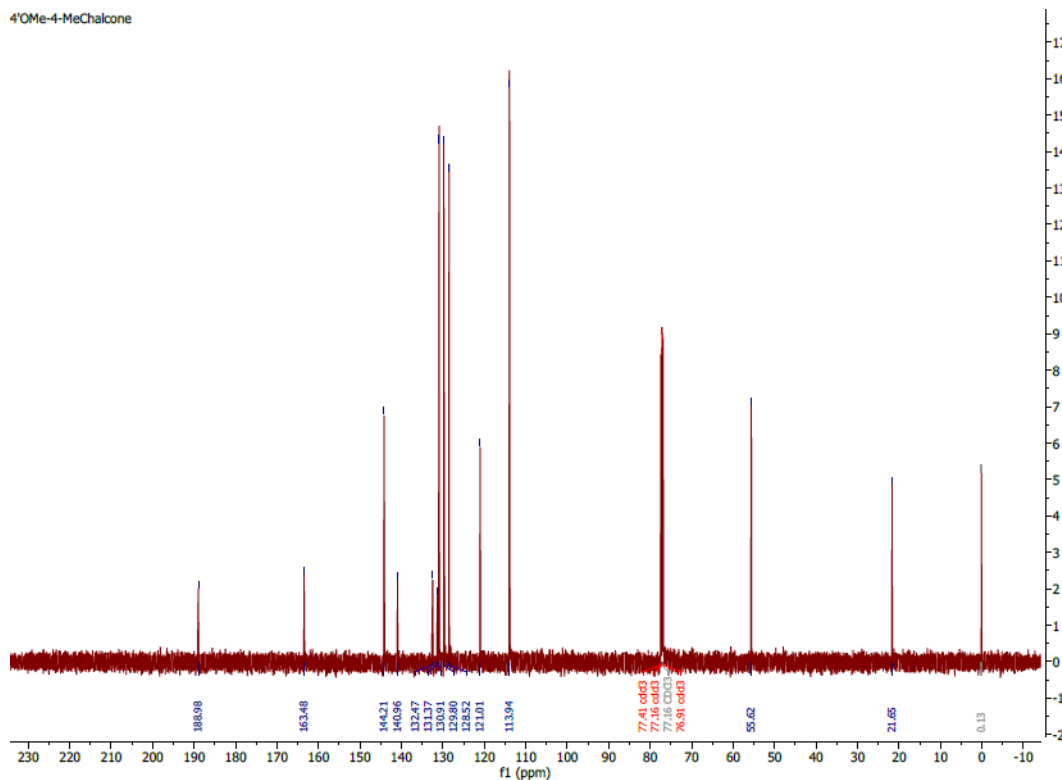


Figure 8c. Spectrum  $^{13}\text{C}$ -NMR of compound (8)

## Elemental Composition Report

Page 1

### Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

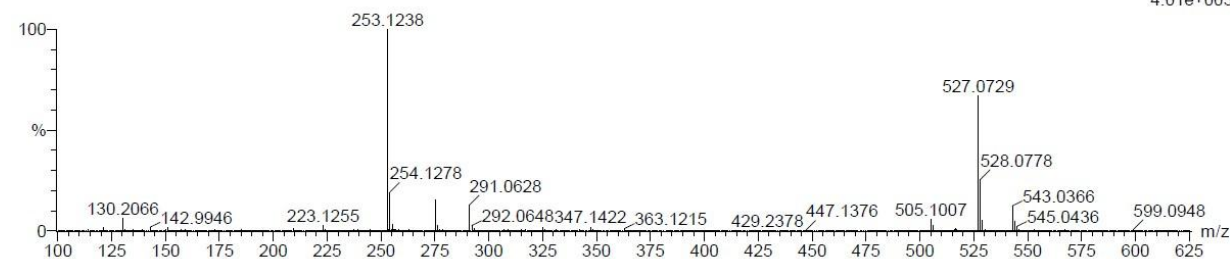
40 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-500 H: 0-1000 O: 0-200

4 B 4MC 10 (0.187) Cm (10:11)

TOF MS ES+



Minimum:

Maximum: 5.0 10.0 -1.5

Mass Calc. Mass mDa PPM DBE i-FIT i-FIT (Norm) Formula

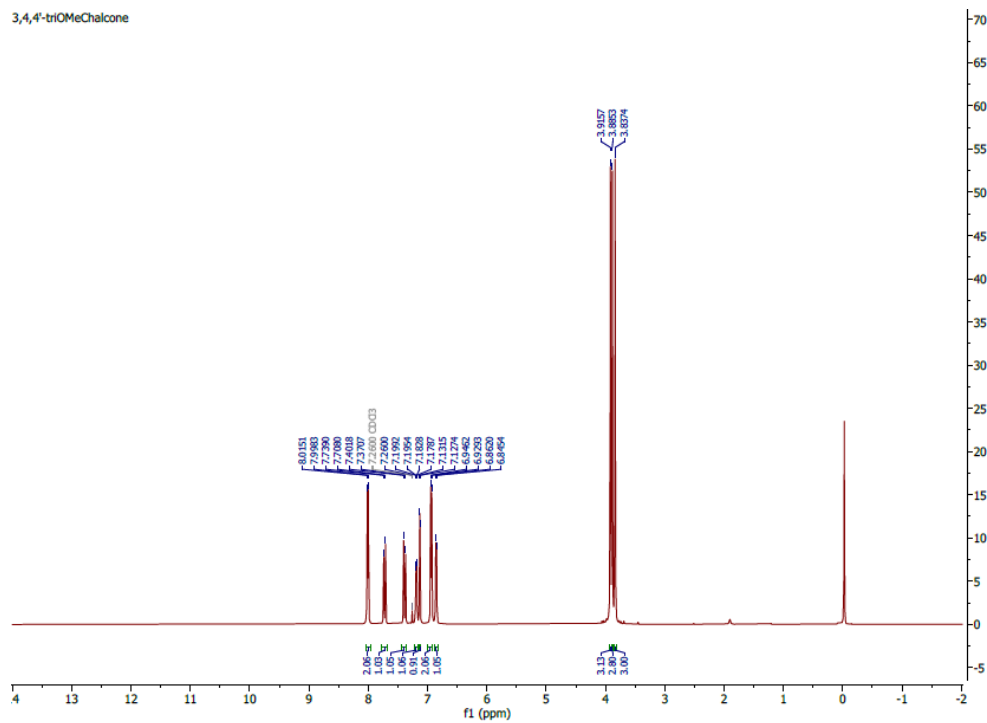
| Mass     | Calc. Mass | mDa  | PPM   | DBE | i-FIT | i-FIT (Norm) | Formula    |
|----------|------------|------|-------|-----|-------|--------------|------------|
| 253.1238 | 253.1229   | 0.9  | 3.6   | 9.5 | 104.3 | 0.0          | C17 H17 O2 |
|          | 253.1287   | -4.9 | -19.4 | 0.5 | 112.1 | 7.8          | C10 H21 O7 |

Figure 9b. Spectrum  $^1\text{H}$ -NMR of compound (9)

### 3,4,4'-Trimethoxychalcone (9)



**Figure 9a.** Spectrum UV of compound (9)



**Figure 8d.** Spectrum HRESI-TOF-MS of compound (8)

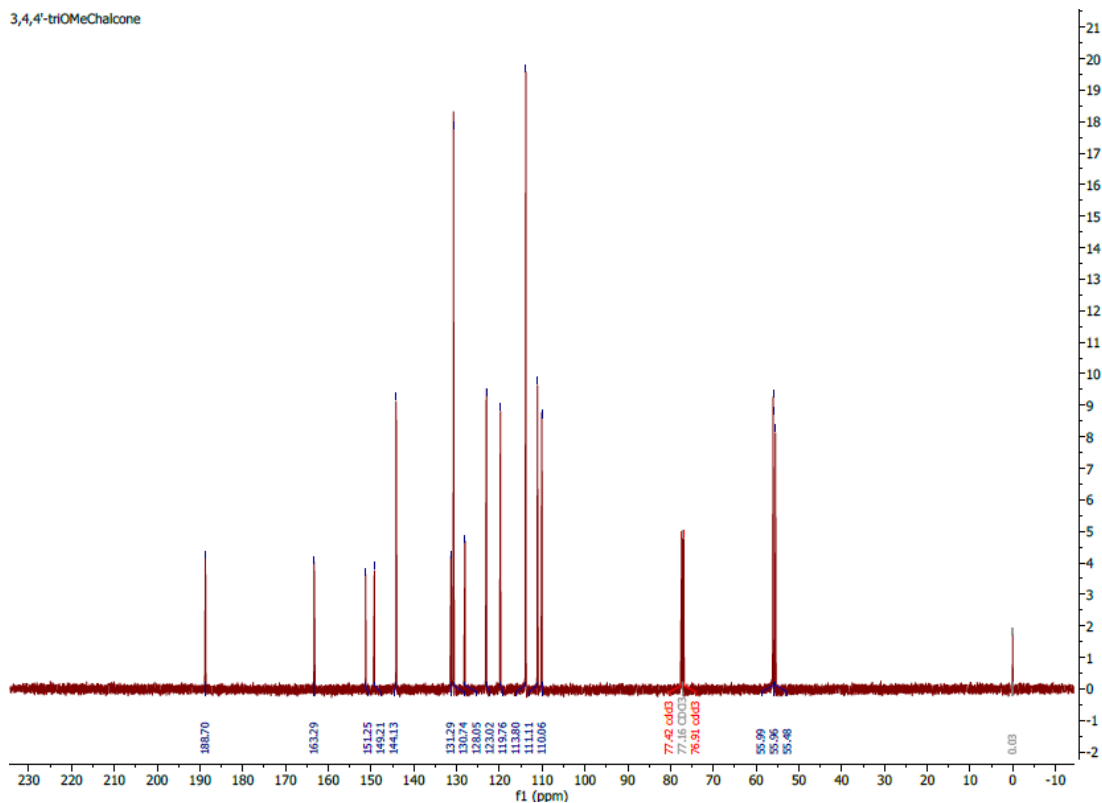


Figure 9c. Spectrum  $^{13}\text{C}$ -NMR of compound (9)

#### Elemental Composition Report

Page 1

#### Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

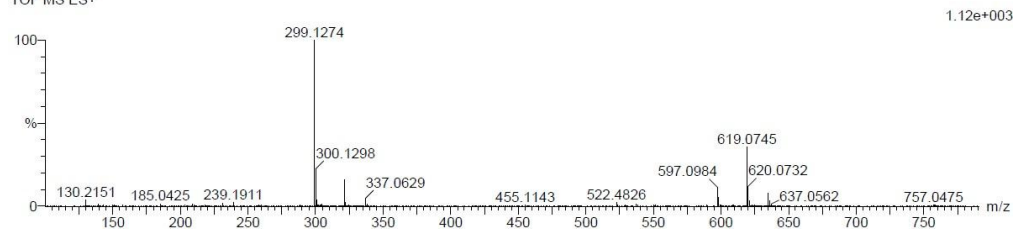
600 formula(e) evaluated with 8 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-500 H: 0-1000 N: 0-200 O: 0-200

3.4.4 TMC 7 (0.136) Cm (7)

TOF MS ES+



| Minimum: |            |      |       | -1.5 |       |              |               |
|----------|------------|------|-------|------|-------|--------------|---------------|
| Maximum: | 5.0        | 10.0 |       | 50.0 |       |              |               |
| Mass     | Calc. Mass | mDa  | PPM   | DBE  | i-FIT | i-FIT (Norm) | Formula       |
| 299.1274 | 299.1283   | -0.9 | -3.0  | 9.5  | 48.7  | 0.4          | C18 H19 O4    |
|          | 299.1288   | -1.4 | -4.7  | 2.5  | 56.6  | 8.3          | C3 H15 N12 O5 |
|          | 299.1256   | 1.8  | 6.0   | 10.5 | 51.1  | 2.8          | C14 H15 N6 O2 |
|          | 299.1297   | -2.3 | -7.7  | 14.5 | 49.5  | 1.2          | C19 H15 N4    |
|          | 299.1302   | -2.8 | -9.4  | 7.5  | 57.3  | 9.0          | C4 H11 N16 O  |
|          | 299.1243   | 3.1  | 10.4  | 5.5  | 53.0  | 4.7          | C13 H19 N2 O6 |
|          | 299.1315   | -4.1 | -13.7 | 1.5  | 56.2  | 7.9          | C7 H19 N6 O7  |
|          | 299.1230   | 4.4  | 14.7  | 11.5 | 55.6  | 7.3          | C10 H11 N12   |

Figure 9b. Spectrum  $^1\text{H}$ -NMR of compound (9)