An Efficient Synthesis of 2-Substituted Quinazolin-4(3H)-ones Catalyzed by Iron(III) Chloride

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Section A: General Information

All reagents were used as received from commercial sources without further purification or prepared as described in the literature. Reactions were stirred using Teflon-coated magnetic stirring bars. TLC plates were visualized by ultraviolet light or by treatment with a spray of Pancaldi reagent \((\text{NH}_4)_6\text{MoO}_4, \text{Ce(SO}_4)_2, \text{H}_2\text{SO}_4, \text{H}_2\text{O}\). Chromatographic purification of products was carried out by flash column chromatography on silica gel (60-120mesh). Melting points were determined using an electro thermal melting point apparatus and are uncorrected. NMR spectra were measured in CDCl$_3$, acetone, DMSO-d$_6$ (all with TMS as internal standard) on a Varian Gemini 400 MHz FT NMR spectrometer magnetic resonance spectrometer. Chemical shifts (\(\delta\)) are reported in ppm, and coupling constants (\(J\)) are in Hz. The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t= triplet, q = quartet, m = multiplet. Mass spectra were recorded on an HP-5989A quadrupole mass spectrometer.
Section B: Experimental Procedures

General procedure for synthesis of 2-aryl Quinazolinones (8a−8m)

To a solution of isatoic anhydride (1 mmol.) in 1, 4-dioxane (10 vol.) was added amidoxime (1.1 mmol.) followed by FeCl₃ (10 mol %). The reaction mixture was stirred at 80 °C for 2-9 h (TLC monitored). After completion of reaction, diluted with EtOAc (10 vol.) and washed with water (2 x 5 vol.). The organic layer was dried over anhydrous Na₂SO₄, filtered, and concentrated under reduced pressure to give the crude product. Column chromatographic purification of crude on silica gel (30% EtOAc in hexanes) afforded the product (8a-m) in 79-93% yield.

General procedure for Synthesis of Amidoximes (7a–m).

50 % Aq. Hydroxylamine (1.05 mmole) was added to a solution of nitrile (10, 1.0 mmole) in ethanol (10 vol) at room temperature. Reflux the reaction mass for 1 hr (TLC monitored). After completion of reaction, cooled to room temperature and concentrated under reduced pressure to get the corresponding amidoxime (7a-m) as a white to yellow colored solid which was used directly in the next step without further purification.
Section C: Analytical data of 2-Substituted-4(3H)-Quinazolinones (8a-m)

1. 2-Phenylquinazolin-4(3H)-one (8a):

White solid; Yield: 84.6 %; Mp: 236-238°C; \(^1\)HNMR (DMSO-\(d_6\), 400 MHz): \(\delta\) 7.53-7.58 (m, 4H, ArH), 7.74 (d, \(J = 7.6\) Hz, 1H, ArH), 7.82-7.86 (m, 1H, ArH), 8.15-8.19 (m, 3H, ArH), 12.54 (s, br, 1H, NH); \(^{13}\)C NMR (DMSO-\(d_6\),100 MHz): \(\delta\) 120.9, 125.8, 126.9, 127.4, 127.7, 128.1, 128.6, 131.4, 132.7, 134.6, 152.3, 162.2; MS: \(m/z = 223.1\) [M +H]; HRMS(ESI):calcd.for C\(_{14}\)H\(_{11}\)N\(_2\)O [M + H]: 223.0871; found: 223.0882.

2. 2-(4-Bromophenyl)quinazolin-4(3H)-one (8b):

White solid; Yield: 80.4%; Mp: 295-296°C; \(^1\)HNMR (DMSO-\(d_6\), 400 MHz): \(\delta\) 7.52-7.56 (m, 1H, ArH), 7.74-7.78 (m, 2H, ArH), 7.83-7.87 (m, 1H, ArH), 8.12-8.17 (m, 3H, ArH), 12.60 (s, br, 1H, NH); \(^{13}\)CNMR (DMSO-\(d_6\), 100 MHz): \(\delta\) 121.0, 125.2,125.8, 127.5, 129.8, 131.6, 131.9, 134.6, 148.5, 151.4, 162.1; MS: \(m/z = 301.0\) [M +H]; HRMS(ESI):calcd.for C\(_{14}\)H\(_{10}\)N\(_2\)OBr(M+H): 300.9976; found: 300.9977.

3. 2-(p-Tolyl)quinazolin-4(3H)-one(8c):

White solid; Yield: 83.2%; Mp: 239-240°C; \(^1\)HNMR (DMSO-\(d_6\), 400 MHz): \(\delta\) 2.39 (s, 3H, CH\(_3\)), 7.36 (d, \(J = 7.8\) Hz, 2H, ArH), 7.51 (t, \(J = 7.8\) Hz, 1H, ArH), 7.72 (d, \(J = 7.8\) Hz, 1H, ArH),
7.81-7.85 (m, 1H, ArH), 8.10 (d, J = 7.8 Hz, 2H, ArH), 8.15 (d, J = 7.3 Hz, 1H, ArH), 12.46 (s, br, 1H, NH); $^{13}$CNMR (DMSO-$d_6$, 100MHz): δ 21.0, 120.9, 125.8, 126.4, 127.4, 127.6, 129.2, 129.9, 134.5, 141.4, 148.8, 152.2, 162.2; MS: $m/z$ = 237.1[M +H]; HRMS(ESI): calcd. for C$_{15}$H$_{13}$N$_2$O(M+H): 237.1028; found: 237.1031.

4. **2-(4-Hydroxyphenyl)quinazolin-4(3H)-one (8d):**

![8d]

White solid; Yield: 80.0%; Mp: 261-263°C; $^1$HNMR (DMSO-$d_6$, 400 MHz): δ 6.89 (d, J = 8.8 Hz, 2H, ArH), 7.47 (t, J = 8.0 Hz, 1H, ArH), 7.67 (d, J = 7.6 Hz, 1H, ArH), 7.78-7.89 (m, 1H, ArH), 8.07-8.12 (m, 3H, ArH), 10.14 (s, br, 1H, OH), 12.30 (s, br, 1H, NH); $^{13}$CNMR (DMSO-$d_6$, 100MHz): δ 115.3, 123.2, 125.8, 125.9, 127.2, 129.5, 134.5, 149.0, 160.5, 184.3; MS: $m/z$ = 239.1[M +H]; HRMS(ESI): calcd. for C$_{14}$H$_{11}$N$_2$O$_2$(M+H): 239.0821; found: 239.0813.

5. **2-(4-Aminophenyl)quinazolin-4(3H)-one (8e):**

![8e]

Yellow solid; Yield: 78.2%; Mp: 250-254°C; $^1$H NMR (DMSO-$d_6$, 400 MHz): δ 5.83 (s, 2H, NH$_2$), 6.62 (d, J = 8.8 Hz, 2H, ArH), 7.40 (t, J = 6.9 Hz, 1H, ArH), 7.61 (d, J = 8.3 Hz, 1H, ArH), 7.76 (t, J = 6.8 Hz, 1H, ArH), 7.95 (d, J = 8.8 Hz, 2H, ArH), 8.08 (dd, J = 6.9, 1 Hz, 1H, ArH), 12.06 (s, br, 1H, NH); $^{13}$C NMR (DMSO-$d_6$, 100MHz): δ 113.0, 125.3, 125.8, 126.9, 129.1, 134.4, 152.2, 162.4; MS: $m/z$ = 238.1[M +H]; HRMS(ESI): calcd. for C$_{14}$H$_{12}$N$_3$O[M+H]: 238.0980; found: 238.0969.
6. **2-(4-Methoxyphenyl)quinazolin-4\(\text{3}H\)\)-one (8f):**

![Image](image1)

White Solid; Yield: 90.1%; Mp: 245.5-247.2°C; \(^1\)HNMR (CDCl\(_3\), 400 MHz): \(δ\) 3.91 (s, 3H, OCH\(_3\)), 7.06 (dd, \(J = 6.8, 2.0\) Hz, 2H, ArH), 7.45-7.49 (m, 1H, ArH), 7.76-7.81 (m, 2H, ArH), 8.06 (dd, \(J = 6.8, 2.0\) Hz, 2H, ArH), 8.30 (d, \(J = 7.8\) Hz, 1H, ArH), 10.04 (s, br, 1H, NH); \(^1\)^13^C\)NMR (CDCl\(_3\) + DMSO-\(d_6\), 100MHz): \(δ\) 54.1, 112.6, 119.7, 123.9, 124.6, 124.7, 126.1, 128.2, 132.9, 148.1, 150.8, 160.8, 161.7; MS: \(m/z = 253.1\)[M +H]; HRMS(ESI): calcd for C\(_{15}\)H\(_{13}\)N\(_2\)O\(_2\)[M + H]: 253.0977; found: 253.0966.

7. **2-(4-(Methylthio)phenyl)quinazolin-4\(\text{3}H\)\)-one (8g):**

![Image](image2)

White solid; Yield: 93.2%; Mp: 237-239°C; \(^1\)HNMR (DMSO-\(d_6\), 400 MHz): \(δ\) 2.55 (s, 3H, SCH\(_3\)), 7.40 (d, \(J = 8.4\) Hz, 2H, ArH), 7.50 (t, \(J = 7.2\) Hz, 1H, ArH), 7.72 (d, \(J = 7.6\) Hz, 1H, ArH), 7.83 (t, \(J = 7.6\) Hz, 1H, ArH), 8.13-8.16 (m, 3H, ArH), 12.48 (s, br, 1H,NH); \(^1\)^13^C\)NMR (DMSO-\(d_6\), 400 MHz): \(δ\) 14.1, 120.8, 125.1, 125.8, 126.4, 127.4, 128.0, 128.6, 134.6, 143.0, 148.7, 151.78, 162.2; MS: \(m/z = 269.0\)[M +H]; HRMS(ESI): calcd for C\(_{15}\)H\(_{13}\)N\(_2\)OS(M+H): 269.07486; found: 269.07446.

8. **2-(4-Nitrophenyl)quinazolin-4\(\text{3}H\)\)-one (8h):**

![Image](image3)
Yellow solid; Yield: 84.0%; Mp: >300 °C; ¹H NMR (DMSO- d₆, 400 MHz): δ 7.59 (t, J = 8.0 Hz, 1H, ArH), 7.80 (d, J = 8.0 Hz, 1H, ArH), 7.86-7.91 (m, 1H, ArH), 8.19 (d, J = 7.2 Hz, 1H, ArH), 8.37-8.43 (m, 4H, ArH), 12.91 (s, br, 1H, NH); ¹³C NMR (DMSO- d₆, 100 MHz): δ 121.2, 123.6, 125.9, 127.3, 127.8, 129.3, 134.8, 138.5, 148.3, 148.9, 150.7, 162.0; MS: m/z = 268.1[M +H]; HRMS(ESI): calcd.for C₁₄H₁₀N₃O₃(M+H): 268.0722; found: 268.0718;

9. 2-(Pyridin-2-yl)quinazolin-4(3H)-one(8i):

Brown solid; Yield: 79.2%; Mp: 168-170°C; ¹H NMR (DMSO- d₆, 400 MHz): δ 7.58 (t, J = 7.6 Hz, 1H, ArH), 7.65-7.68 (m, 1H, ArH), 7.81 (d, J = 8.0 Hz, 1H, ArH), 7.89 (t, J = 7.6 Hz, 1H, ArH), 8.06-8.09 (m, 1H, ArH), 8.19 (d, J = 7.6 Hz, 1H, ArH), 8.47 (d, J = 8.0 Hz, 1H, ArH), 8.76 (d, J = 5.2 Hz, 1H, ArH), 11.83 (s, br, NH); ¹³C NMR (DMSO- d₆, 100 MHz): δ 122.0, 122.1, 126.1, 126.5, 127.2, 127.7, 134.7, 137.9, 148.6, 148.9, 149.9, 160.7; MS: m/z = 224.1[M +H]; HRMS(ESI): calcd.for C₁₃H₁₀N₃O (M+H):224.0824; found: 224.0826.

10. 2-(5-Fluoropyridin-2-yl)quinazolin-4(3H)-one(8j):

Brown solid; Yield: 80.2%; Mp: 180-183 °C; ¹H NMR (CDCl₃, 400 MHz): δ 7.51-7.56 (m, 1H, ArH), 7.61-7.65 (m, 1H, ArH), 7.77-7.80 (m, 2H, ArH), 8.35 (d, J = 7.4 Hz, 1H, ArH), 8.51 (d, J = 2.9 Hz, 1H, ArH), 8.63 (dd, J = 8.8, 4.8 Hz, 1H, ArH), 10.76 (s, 1H, br, NH); ¹³C NMR (CDCl₃, 100 MHz): δ 122.2, 123.7(d, J = 5.4 Hz ), 124.4(d, J = 18.4 Hz), 126.7, 127.4, 127.9, 134.6, 137.2 (d, J = 25.2 Hz), 144.7, 147.9, 148.9, 161.1 (d, J = 260.0Hz), 161.3; MS: m/z = 242.1[M +H]; HRMS(ESI): calcd.for C₁₃H₉N₃OF (M+H):242.0730; found:242.0722.
11. 2-(Cyclopropylmethyl)quinazolin-4(3\text{H})-one (8k):

![8k]

White solid; Yield: 91.0 \%; Mp: 210-213°C; $^1$HNMR (CDCl$_3$, 400 MHz): $\delta$ 0.38-0.42 (m, 2H, CH$_2$), 0.70-0.73 (m, 2H, CH$_2$), 1.14-1.21 (m, 1H, CH), 2.70 (d, $J = 7.6$Hz, 2H, CH$_2$), 7.26-7.49 (m, 1H, ArH), 7.68 (d, $J = 7.6$ Hz, 1H, ArH), 7.74-7.79 (m, 1H, ArH), 8.28 (dd, $J = 6.8$, 1.2 Hz, 1H, ArH), 10.20 (s, br 1H, NH); $^{13}$CNMR (DMSO-$d_6$, 100 MHz): $\delta$ 4.2, 9.2, 39.2, 120.8, 125.7, 126.0, 126.8, 134.3, 149.0, 157.2, 161.8; MS: $m/z = 201.1 \ [M +H]$; HRMS(ESI):calcd for C$_{12}$H$_{13}$N$_2$O(M+H): 201.1028; found: 201.1037.

12. 2-(tert-Butyl)quinazolin-4(3\text{H})-one (8l):

![8l]

White solid; Yield: 89.0\%; Mp: 205-208°C; $^1$HNMR (DMSO-$d_6$, 400 MHz): $\delta$ 1.35 (s, 9H, 3xCH$_3$), 7.44-7.48 (m, 1H, ArH), 7.61 (d, $J = 8.4$ Hz, 1H, ArH), 7.75-7.79 (m, 1H, ArH), 8.08 (dd, $J = 6.4$, 1.6 Hz, 1H, ArH), 11.79 (s, br, 1H, NH); $^{13}$C NMR (DMSO-$d_6$, 100 MHz): $\delta$ 27.7, 27.8, 37.2, 120.6, 125.6, 126.2, 127.3, 134.3, 148.3, 162.3, 162.6; MS: $m/z = 203.1 \ [M +H]$; HRMS(ESI):calcd for C$_{12}$H$_{15}$N$_2$O(M+H): 203.1184; found: 203.1185.

13. 2-(4-Nitrobenzyl)quinazolin-4(3\text{H})-one (8m):

![8m]

Light brown solid; Yield: 89.0\%; Mp: >300 °C; $^1$H NMR (DMSO-$d_6$, 400 MHz): $\delta$ 4.11 (s, 2H, PhCH$_2$), 7.48 (t, $J = 7.4$Hz, 1H, ArH), 7.58 (d, $J = 8.4$Hz, 1H, ArH), 7.65 (d, $J = 8.4$ Hz, 2H, ArH), 7.75-7.79 (m, 1H, ArH), 8.08 (d, $J = 6.9$Hz, 1H, ArH), 8.20 (d, $J = 8.8$ Hz, 2H, ArH),
12.49 (s, br, 1H, NH); $^{13}$C NMR (DMSO-$d_6$ 100 MHz): $\delta$ 40.7, 123.6, 125.7, 126.4, 126.9, 128.3, 128.6, 130.4, 134.4, 144.4, 154.9, 161.7; MS: $m/z = 282.0$ [M +H]; HRMS(ESI): calcd. for C$_{15}$H$_{12}$N$_3$O$_3$(M+H): 282.0879; found: 282.0877.
Section D: $^1$H, $^{13}$C, Mass and HRMS spectra:
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Sample Type: Sample
Instrument Name: Instrument 1
Acq Method: ESI.m
DA Method: Default.m
Position:
User Name:
IRM Calibration Status: Success
Comment:

User Spectra

Fragmenter Voltage: 100
Collision Energy: 0
Ionization Mode: ESI

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Counts (%) vs. Mass-to-Charge (m/z)

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Elemental Composition Report

Single Mass Analysis
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Element prediction: Off
Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ion
67 formula(e) evaluated with 1 results within limits (up to 5 best isotope matches for each mass)
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C: 0-30 H: 0-30 N: 0-4 O: 0-4

1: TIC MS ES+

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Comment: 

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Elemental Composition Report

Single Mass Analysis
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Monoisotopic Mass, Even Electron Ions
115 formula(e) evaluated with 1 results within limits (up to 6 best isotopic matches for each mass)

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Elemental Composition Report

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Element prediction: Off
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Monosotopic Mass, even Electron ions
67 formula(e) evaluated with 1 results within limits (up to 5 best isotopic matches for each mass)
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1: TOF MS ES+

| Mass  | Calc. Mass | %Da | ppm  | DSE  | |FIT | Formula |
|-------|------------|-----|------|------|-----|-------|
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Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -5.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron ions
67 formula(s) evaluated with 1 results within limits (up to 5 best isotopic matches for each mass)
Elements Used:
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**Mass Analysis Report**

![Chemical Structure](image)

**User Spectra**

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  - 0.40
  - 0.60
  - 0.80
  - 1.00

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Page 1 of 1
Printed at: 2:01 PM on 3/4/2013
Elemental Composition Report

Single Mass Analysis
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Element prediction: Off
Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions
67 formula(s) evaluated with 1 results within limits (up to 6 best isotopic matches for each mass)
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i: TOFMS ES+

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9.46e+003

Minimum:
Maximum:
Mass  Calc. Mass mDa  PPM  DBE  i-FIT  Formula
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**Acq Method:** SSLm

**DA Method:** Default

**Position:** Val 70

**User Name:**

**IRM Calibration Status:** Success

**Comment:**

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Counts (%) vs. Mass-to-Charge (m/z)

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Page 1 of 1

Printed at: 11:58 AM on 2/7/2013
Elemental Composition Report

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Element prediction: Off
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Monoisotopic Mass, Even Electron Ions
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Elements Used:
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1302110074 (0.254) C11 H13 N O

253.0959

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Mass Analysis Report

User Spectra

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x10^2

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120.00

468.10

Counts (%) vs. Mass-to-Charge (m/z)

--- End Of Report ---
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DEE: min = -50.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron ions
92 formula(s) evaluated with 1 results within limits (up to 8 best isotopic matches for each mass)
Elements Used:
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<th>Mass</th>
<th>Calc. Mass</th>
<th>m/z</th>
<th>PPM</th>
<th>DEE</th>
<th>i-FIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>268.0722</td>
<td>268.0722</td>
<td></td>
<td>-0.4</td>
<td>-1.5</td>
<td>11.5</td>
<td>C14 N10 N3 O3</td>
</tr>
</tbody>
</table>

Page 1
Mass Analysis Report

User Spectra

- Scan (0.29 min) 130219016.d Subtract (1)

+100 0 66

Counts (%) vs. Mass-to-Charge (m/z)

--- End Of Report ---

Page 1 of 1

Printed at: 3:25 PM on: 2/19/2013
Elemental Composition Report

Single Mass Analysis
Tolerance = ±0.0 PPM / DBE: min = -6.0, max = 90.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions
67 formula(e) evaluated with 1 results within limits (up to 5 best isotopic matches for each mass)
Elements Used:
C: 0-30  H: 0-30  N: 0-4  O: 0-4
1-TOF MS-ES+

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>RDA</th>
<th>PPM</th>
<th>DBE</th>
<th>i-FIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>224.0826</td>
<td>224.0824</td>
<td>0.2</td>
<td>0.9</td>
<td>10.5</td>
<td>10.9</td>
<td>C13 H10 N3 O</td>
</tr>
</tbody>
</table>
Mass Analysis Report

User Spectra

Fragmentor Voltage | Collision Energy | Ionization Mode
---|---|---
100 | 0 | EsI

+ Scan (0.29 min) 1302222023.d Subtract (1)

242.10

Counts (%) vs. Mass-to-Charge (m/z)

--- End Of Report ---
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -5.0, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron ion
55 formula(e) evaluated with 1 results within limits (up to 5 best isotopic matches for each mass)
Elements Used:
C: 0-15  H: 0-15  N: 0-4  O: 0-4  F: 0-2

1: TROP 0-0

Minimum: 5.0  5.0  5.0
Maximum: 85.0  85.0  85.0

Mass  Calcd Mass  mDa  ppm  DBE  i-FIT  Formula
242.0722  242.0730  -0.8  -3.3  10.5  0.7  C13 H9 N3 O F
Elemental Composition Report

**Single Mass Analysis**
Tolerance = 5.0 PPM / DBE: min = -5.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ion
Of formula(s) evaluated with 1 results within limits (up to 10 best isotopic matches for each mass)
Elements Used:
C: 0-25 H: 0-25 N: 0-4 O: 0-4
Instrument: 1-TOF MS ES+

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>ppm</th>
<th>DBE</th>
<th>i-FIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>201.1037</td>
<td>201.1038</td>
<td>0.9</td>
<td>4.8</td>
<td>7.5</td>
<td>4.7</td>
<td>C12 H13 N2 O</td>
</tr>
</tbody>
</table>

10430021: 14 (0.44%) Cm (14:16) 4.42e+003
Mass Analysis Report

User Spectra

Fragmentor Voltage | Collision Energy | Ionization Mode
--- | --- | ---
100 | 0 | ESI

+ Scan (0.28 min) 130506016.d Subtract (1)

203.10

Counts (%) vs. Mass-to-Charge (m/z)

--- End Of Report ---
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -50.0, max = 60.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Odd and Even Electron Ions
67 formula(s) evaluated with 1 results within limits (up to 6 best isotopic matches for each mass)
Elements Used:
C: 0.20  H: 0.30  N: 0.4  O: 0.4
1: TOF MS ES+

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>i-FIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>203.1185</td>
<td>203.1184</td>
<td>0.1</td>
<td>0.5</td>
<td>6.5</td>
<td>3.2</td>
<td>C112 H15 N2 O</td>
</tr>
</tbody>
</table>
Mass Analysis Report

Fragmentor Voltage | Collision Energy | Ionization Mode
130 | 0 | ESI

+ Scan (0.28 min) 130403016.d Subtract (1)

282.00
234.00
320.00
342.10

--- End Of Report ---
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -6.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions
67 formula(s) evaluated with 1 results within limits (up to 5 best isotope matches for each mass)
Elements Used:
C: 0.30  H: 0.30  N: 0.4  O: 0.4
1-TOF MS ES+

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>i-FIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>282.0977</td>
<td>282.0979</td>
<td>-0.2</td>
<td>-0.7</td>
<td>11.5</td>
<td>22.8</td>
<td>C15 H12 N3 O3</td>
</tr>
</tbody>
</table>