# Supporting Information

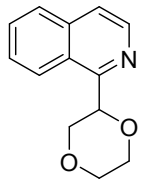
## Cross-dehydrogenative coupling of $\alpha$-C($sp^3$)-H of ethers/alkanes with C($sp^2$)-H of heteroarenes under metal-free condition

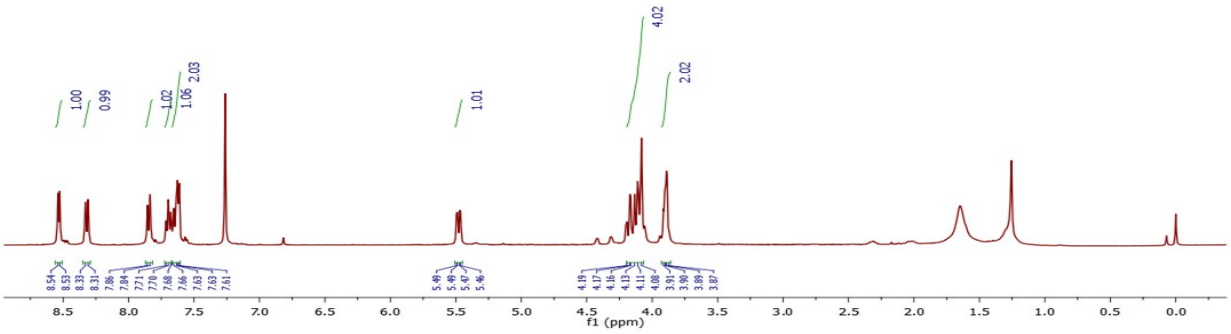
Srinivas Ambala,[1,2] Thanusha Thatikonda,[1,2] Shweta Sharma,[1] Gurunadham Munagala,[1,2] Kushalava Reddy Yempalla,[1,2] Ram A. Vishwakarma[1,2] and Parvinder Pal Singh[1,2]*

[1]Medicinal Chemistry Division, CSIR-Indian Institute of Integrative Medicine, Canal Road, Jammu-180001, India; [2]Academy of Scientific and Innovative Research, Canal Road, Jammu-180001, India

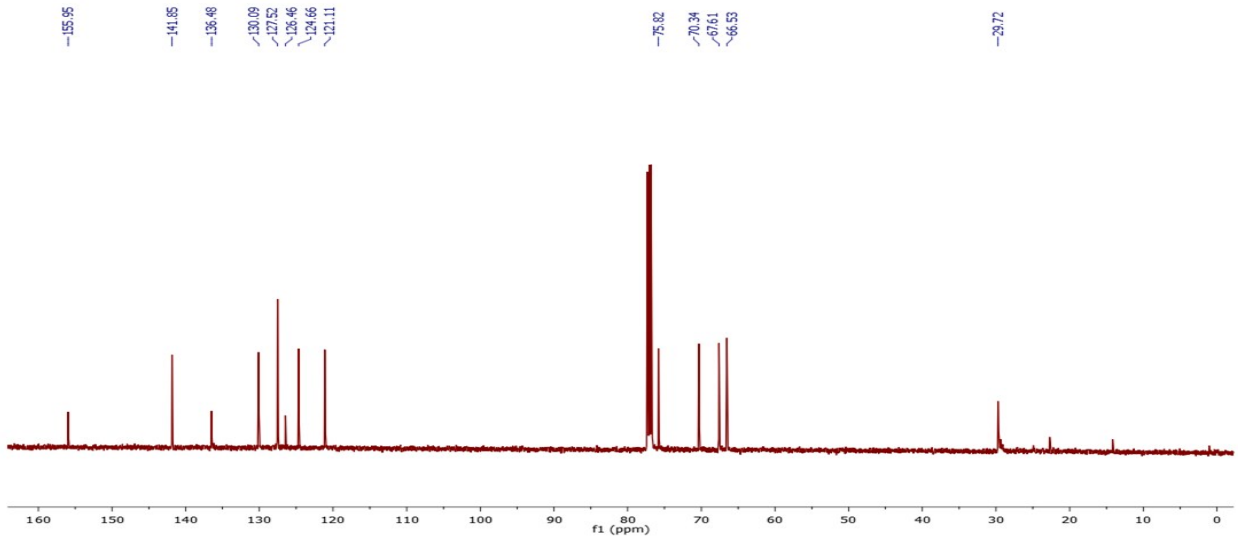
## Spectras ($^{1}$H NMR, $^{13}$C NMR, DEPT and HRMS) of synthesized products

### $^{1}$H NMR of 1-(1,4-dioxan-2-yl)*iso*-quinoline (3aa)

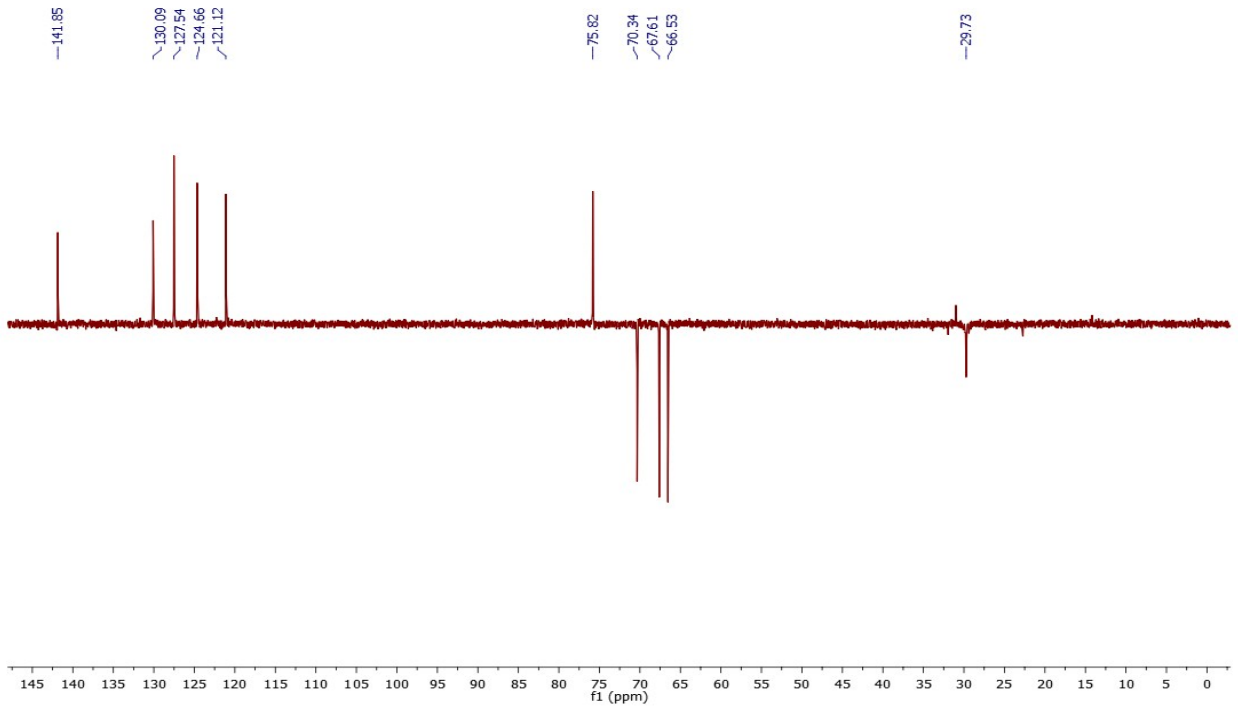


**$^{13}$C NMR of 1-(1,4-dioxan-2-yl)*iso*-quinoline (3aa)**



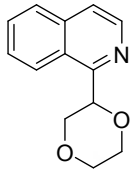

**DEPT of 1-(1,4-dioxan-2-yl)*iso*-quinoline (3aa)**



**HRMS of 1-(1,4-dioxan-2-yl)*iso*-quinoline (3aa)**

## Qualitative Compound Report

| | | | |
|---|---|---|---|
| **Data File** | E-91.d | **Sample Name** | E-91 |
| **Sample Type** | Sample | **Position** | Vial 11 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | vishal_12-01-13.m | **Acquired Time** | 07-02-2015 PM 12:17:16 |
| **IRM Calibration Status** | Success | **DA Method** | daily_report.m |
| **Comment** | | | |



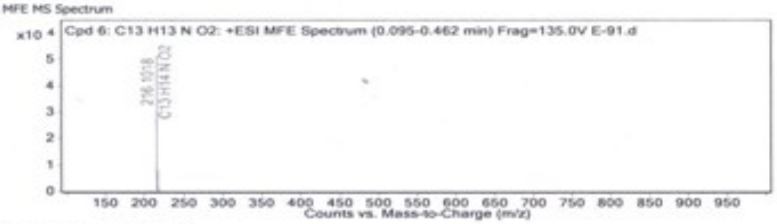
| | |
|---|---|
| **Sample Group** | **Info.** |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) |

**Compound Table**

| Compound Label | RT | Mass | Formula | MFG Formula | MFG Diff (ppm) | DB Formula |
|---|---|---|---|---|---|---|
| Cpd 6: C13 H13 N O2 | 0.275 | 215.0946 | C13 H13 N O2 | C13 H13 N O2 | 0.14 | C13 H13 N O2 |

| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 6: C13 H13 N O2 | 216.1018 | 0.275 | Find by Molecular Feature | 215.0946 |

MFE MS Spectrum




**MS Spectrum Peak List**

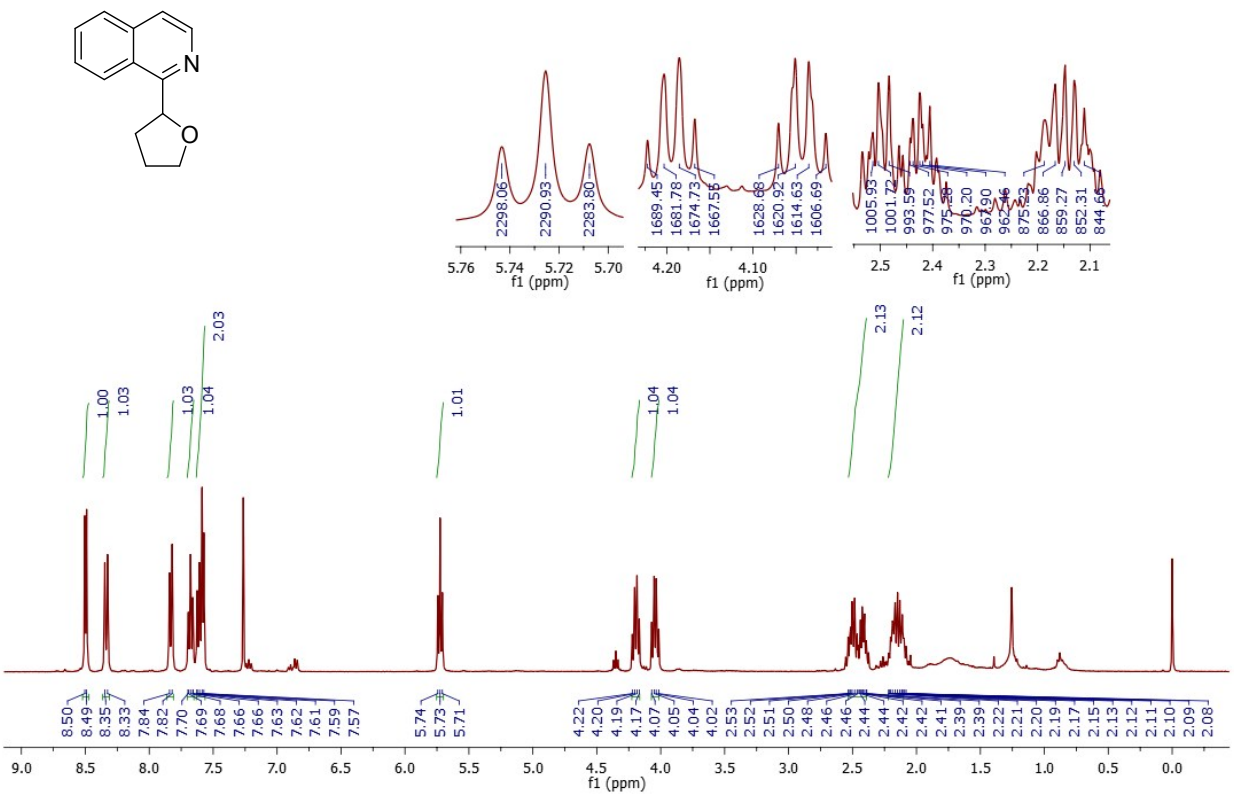
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 216.1018 | 1 | 51559.12 | C13 H14 N O2 | (M+H)+ |
| 217.1056 | 1 | 8053.13 | C13 H14 N O2 | (M+H)+ |
| 218.1078 | 1 | 1032.47 | C13 H14 N O2 | (M+H)+ |

**Predicted Isotope Match Table**

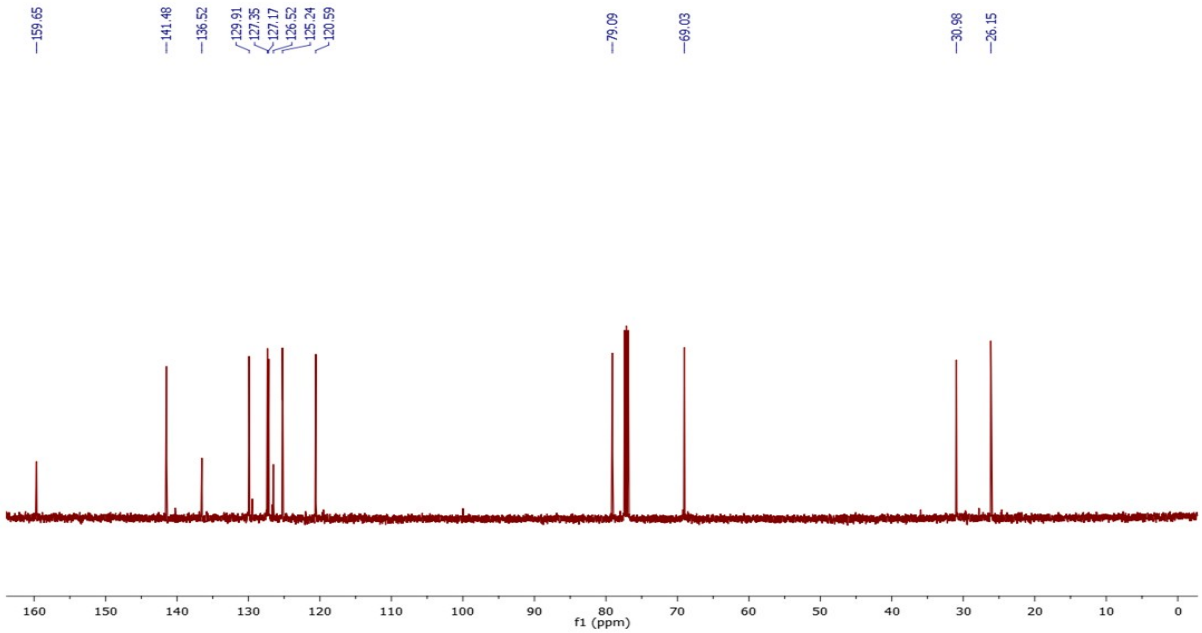
| Isotope | *m/z* | Calc m/z | Diff (ppm) | Abund % | Calc Abund % | Abund Sum % | Calc Abund Sum % |
|---|---|---|---|---|---|---|---|
| 1 | 216.1018 | 216.1019 | 0.48 | 100 | 100 | 85.02 | 86.15 |
| 2 | 217.1056 | 217.1051 | -1.98 | 15.62 | 14.66 | 13.28 | 12.63 |
| 3 | 218.1078 | 218.1077 | -0.29 | 2 | 1.41 | 1.7 | 1.21 |

--- End Of Report ---

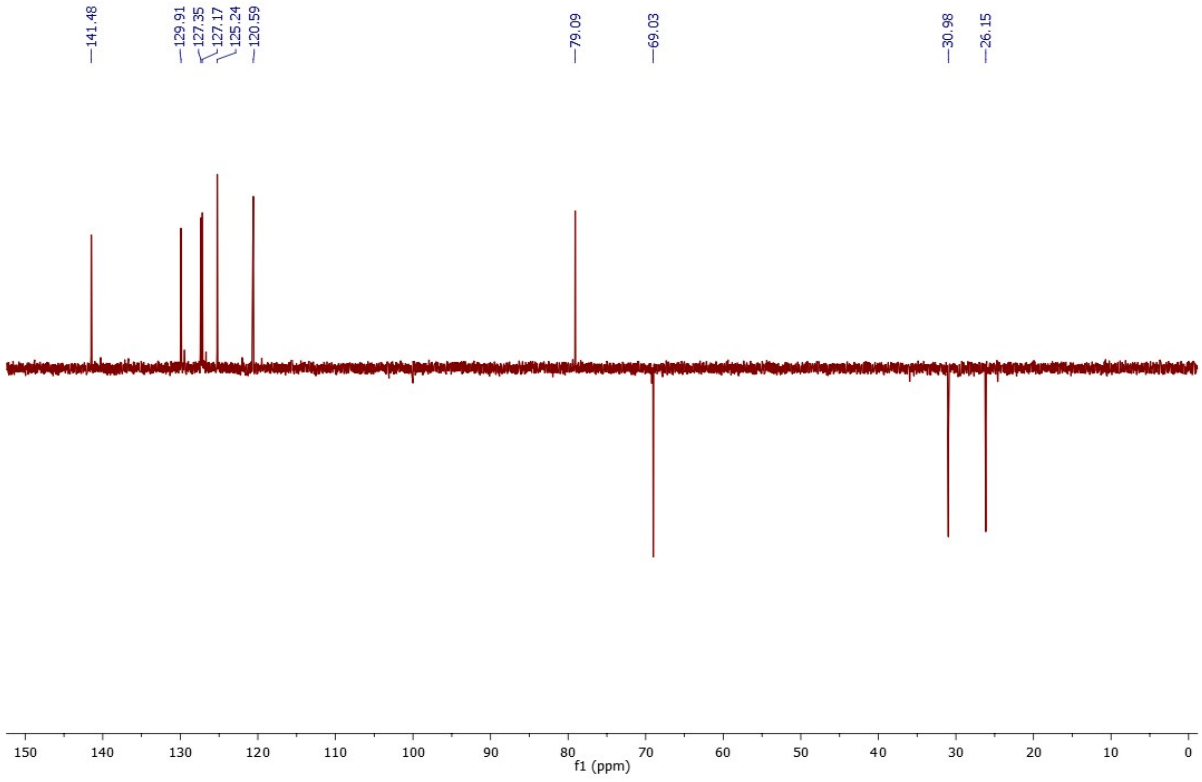
**$^{1}$H NMR of 1-(tetrahydrofuran-2-yl)*iso*-quinoline (3ab)**



**$^{13}$C NMR of 1-(tetrahydrofuran-2-yl)*iso*-quinoline (3ab)**




**DEPT of 1-(tetrahydrofuran-2-yl)*iso*-quinoline (3ab)**

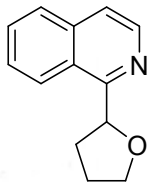


**HRMS of 1-(tetrahydrofuran-2-yl)*iso*-quinoline (3ab)**

## Qualitative Compound Report

| | | | |
|---|---|---|---|
| **Data File** | F-12.1d1.d | **Sample Name** | F-12 |
| **Sample Type** | Sample | **Position** | Vial 3 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | vishal_12-01-13.m | **Acquired Time** | 11-02-2015 PM 3:11:01 |
| **IRM Calibration Status** | Success | **DA Method** | daily_report.m |
| **Comment** | | | |

**Sample Group** **Info.**
**Acquisition SW** 6200 series TOF/6500 series
**Version** Q-TOF B.05.01 (B5125)

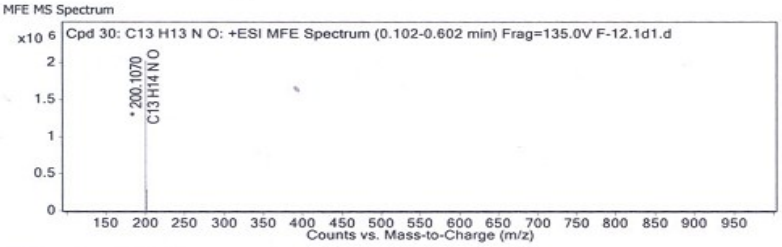



**Compound Table**

| Compound Label | RT | Mass | Formula | MFG Formula | MFG Diff (ppm) | DB Formula |
|---|---|---|---|---|---|---|
| Cpd 30: C13 H13 N O | 0.276 | 199.0998 | C13 H13 N O | C13 H13 N O | -0.38 | C13 H13 N O |

| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 30: C13 H13 N O | 200.107 | 0.276 | Find by Molecular Feature | 199.0998 |

MFE MS Spectrum




**MS Spectrum Peak List**

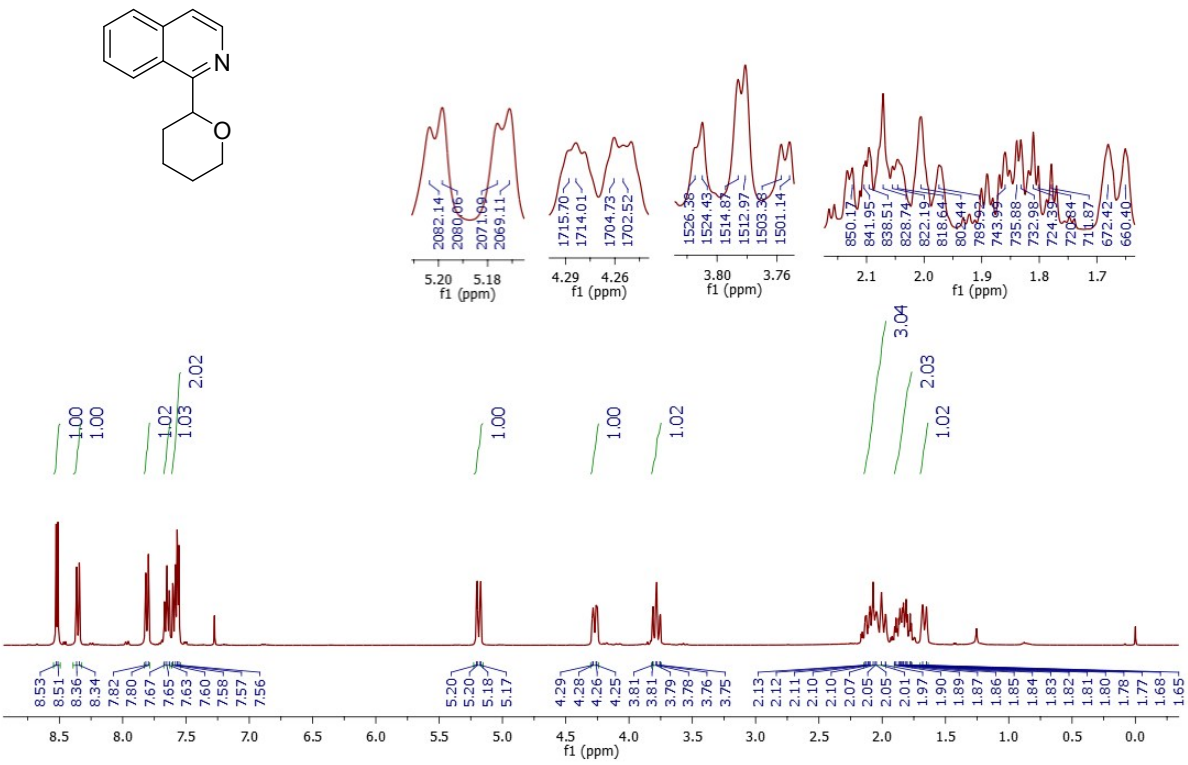
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 200.107 | 1 | 2026024.13 | C13 H14 N O | (M+H)+ |
| 201.1107 | 1 | 286573.25 | C13 H14 N O | (M+H)+ |
| 202.1134 | 1 | 21760.46 | C13 H14 N O | (M+H)+ |

**Predicted Isotope Match Table**

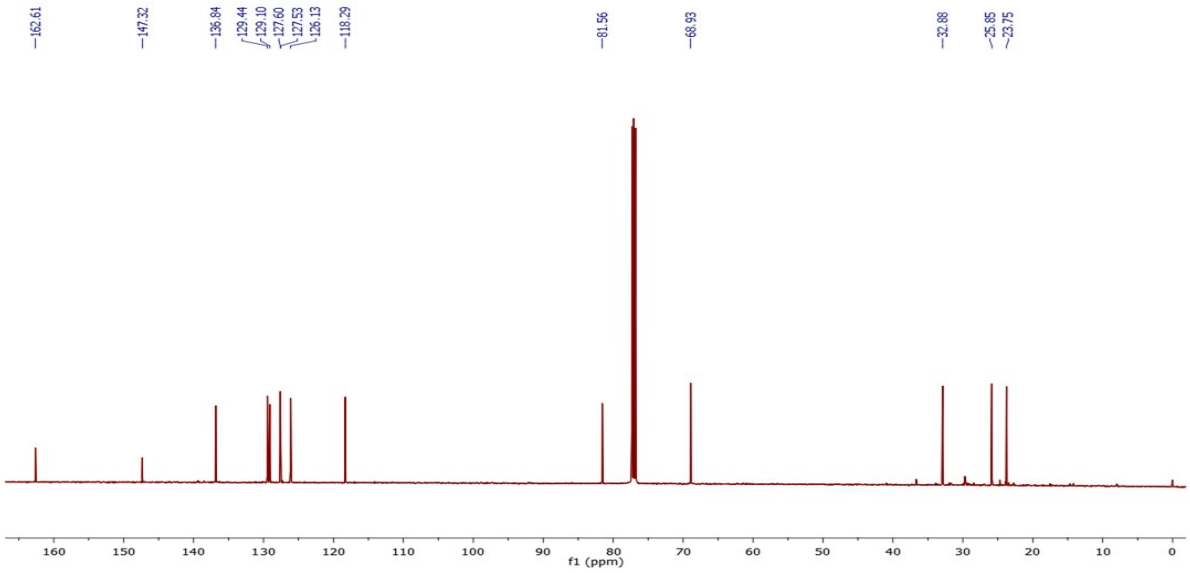
| Isotope | *m/z* | Calc m/z | Diff (ppm) | Abund % | Calc Abund % | Abund Sum % | Calc Abund Sum % |
|---|---|---|---|---|---|---|---|
| 1 | 200.107 | 200.107 | -0.1 | 100 | 100 | 86.79 | 86.34 |
| 2 | 201.1107 | 201.1102 | -2.3 | 14.14 | 14.62 | 12.28 | 12.63 |
| 3 | 202.1134 | 202.1131 | -1.42 | 1.07 | 1.2 | 0.93 | 1.03 |

--- End Of Report ---

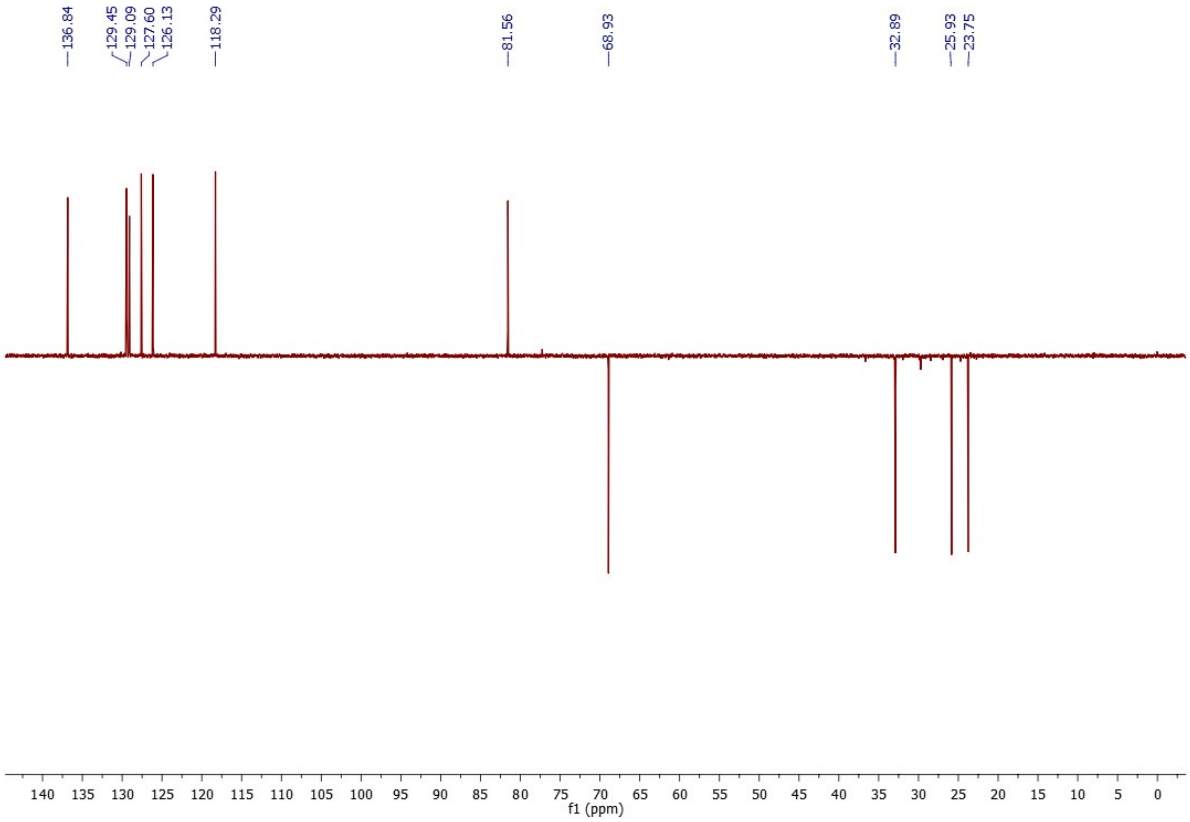
**$^{1}$H NMR of 1-(tetrahydro-2H-pyran-2-yl)*iso*-quinoline (3ac)**



**$^{13}$C NMR of (±)-1-(tetrahydro-2H-pyran-2-yl)*iso*-quinoline (3ac)**



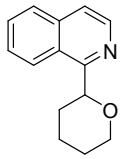

**DEPT of 1-(tetrahydro-2H-pyran-2-yl)*iso*-quinoline (3ac)**



**HRMS of 1-(tetrahydro-2H-pyran-2-yl)*iso*-quinoline (3ac)**

## Qualitative Compound Report

| | | | |
|---|---|---|---|
| **Data File** | E-102.d | **Sample Name** | E-102 |
| **Sample Type** | Sample | **Position** | Vial 6 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | vishal_12-01-13.m | **Acquired Time** | 10-02-2015 PM 12:14:39 |
| **IRM Calibration Status** | Success | **DA Method** | daily_report.m |
| **Comment** | | | |



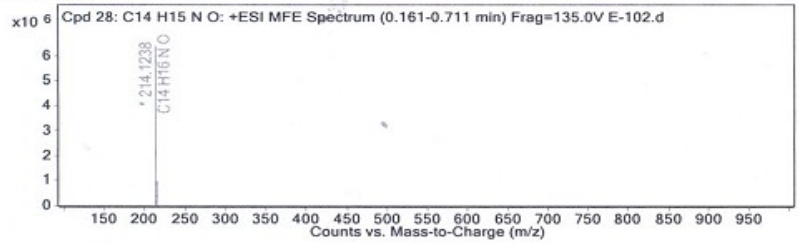

| | |
|---|---|
| **Sample Group** | **Info.** |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) |

**Compound Table**

| Compound Label | RT | Mass | Formula | MFG Formula | MFG Diff (ppm) | DB Formula |
|---|---|---|---|---|---|---|
| Cpd 28: C14 H15 N O | 0.277 | 213.1167 | C14 H15 N O | C14 H15 N O | -6.09 | C14 H15 N O |

| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 28: C14 H15 N O | 214.1238 | 0.277 | Find by Molecular Feature | 213.1167 |

MFE MS Spectrum




**MS Spectrum Peak List**

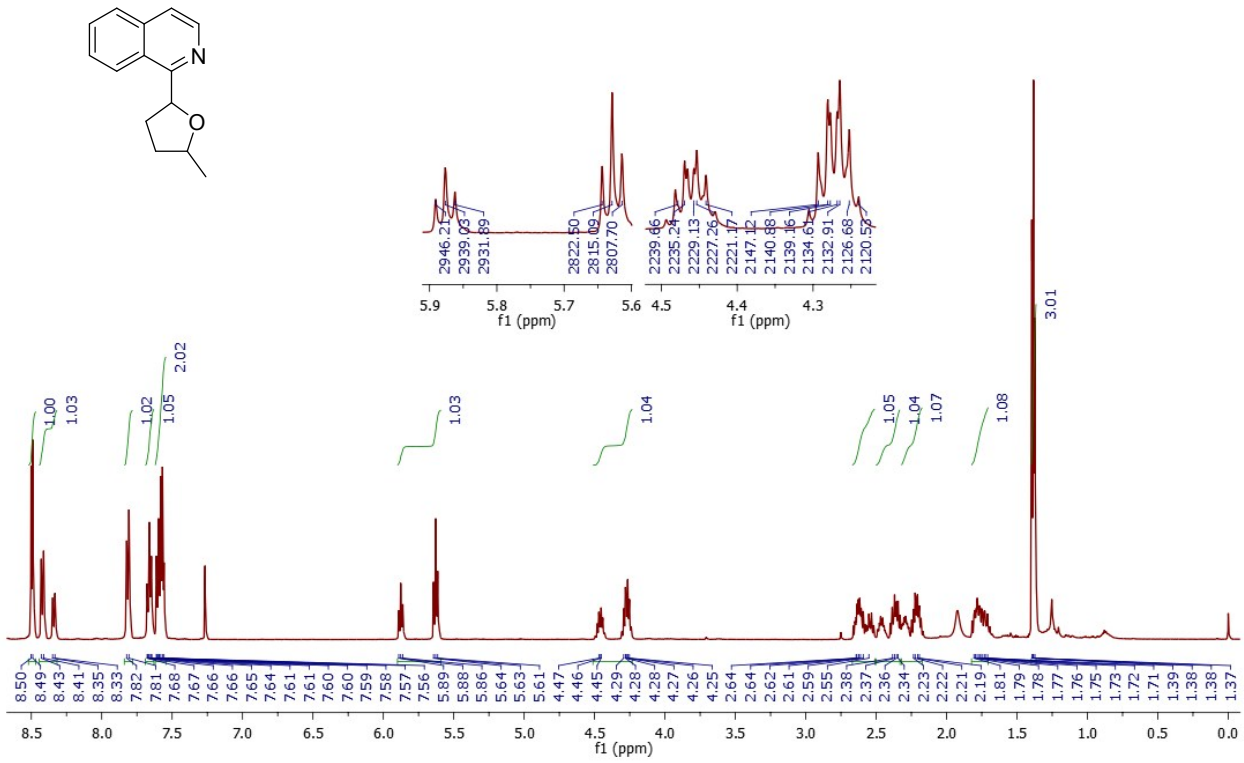
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 214.1238 | 1 | 6378150.5 | C14 H16 N O | (M+H)+ |
| 215.1282 | 1 | 957703.69 | C14 H16 N O | (M+H)+ |
| 216.1312 | 1 | 78061.56 | C14 H16 N O | (M+H)+ |
| 217.1314 | 1 | 7213.03 | C14 H16 N O | (M+H)+ |

**Predicted Isotope Match Table**

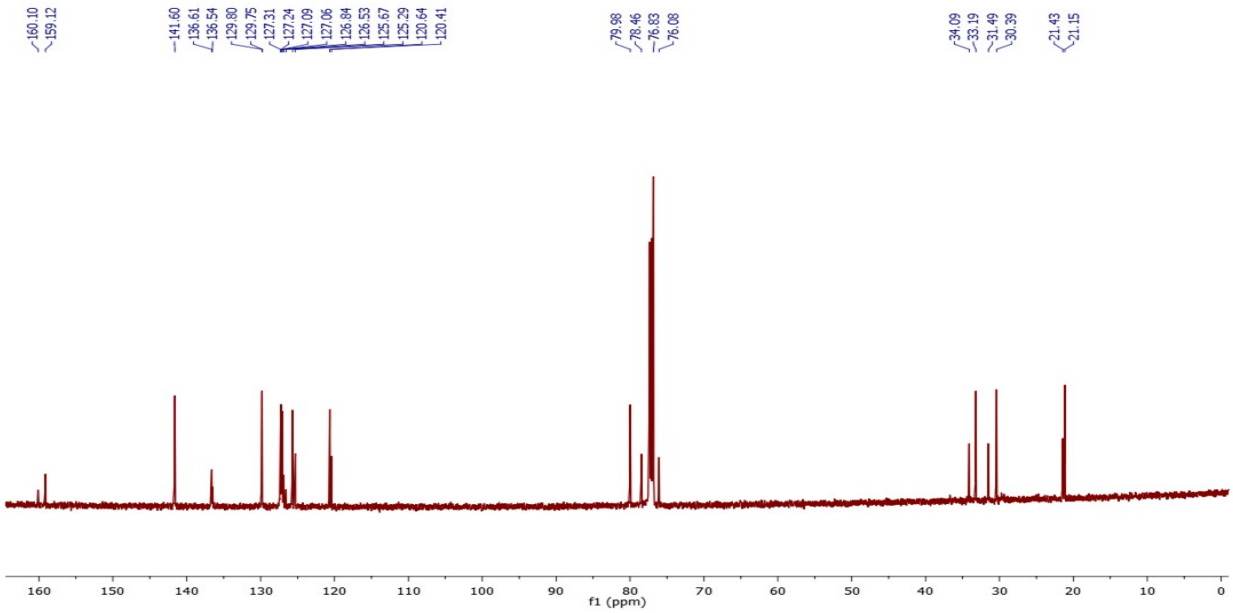
| Isotope | *m/z* | Calc m/z | Diff (ppm) | Abund % | Calc Abund % | Abund Sum % | Calc Abund Sum % |
|---|---|---|---|---|---|---|---|
| 1 | 214.1238 | 214.1226 | -5.27 | 100 | 100 | 85.95 | 85.34 |
| 2 | 215.1282 | 215.1259 | -10.9 | 15.02 | 15.73 | 12.91 | 13.42 |
| 3 | 216.1312 | 216.1288 | -11.4 | 1.22 | 1.36 | 1.05 | 1.16 |
| 4 | 217.1314 | 217.1315 | 0.35 | 0.11 | 0.08 | 0.1 | 0.07 |

--- End Of Report ---

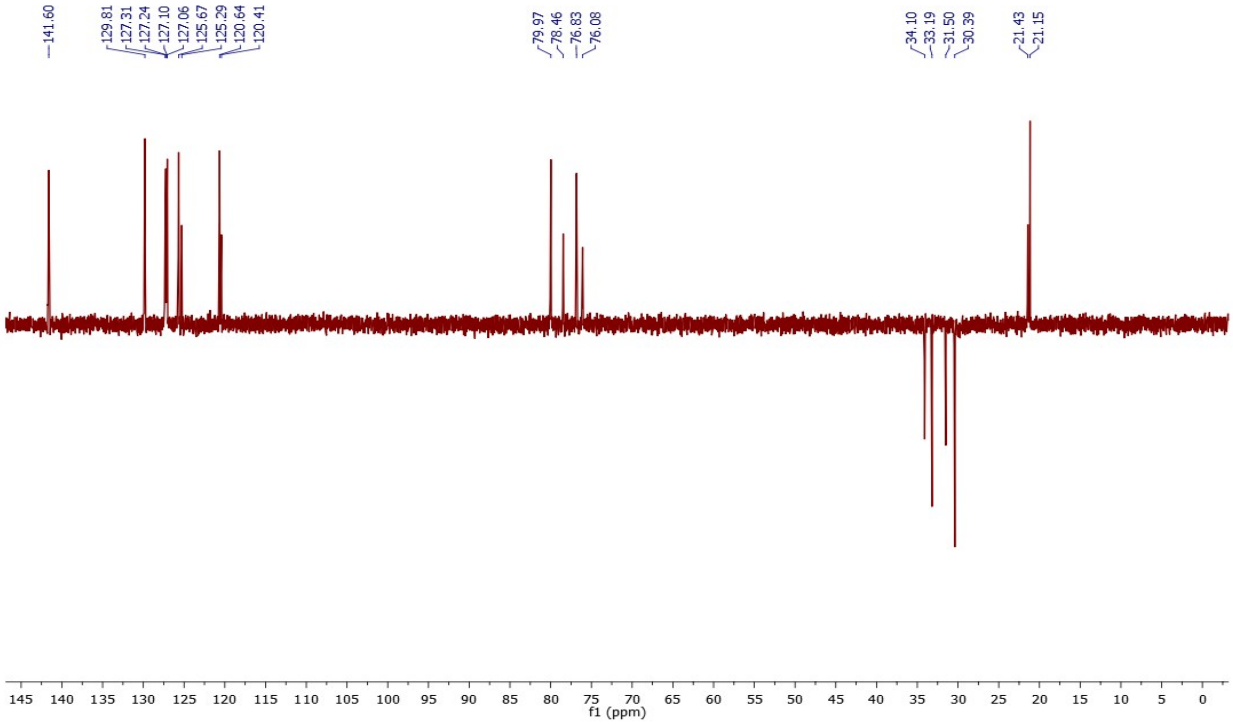
**$^{1}$H NMR of 1-(5-methyltetrahydrofuran-2-yl)*iso*-quinoline (3ad)**



**$^{13}$C NMR of 1-(5-methyltetrahydrofuran-2-yl)*iso*-quinoline (3ad)**



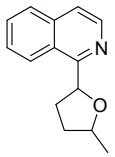

**DEPT of 1-(5-methyltetrahydrofuran-2-yl)*iso*-quinoline (3ad)**



**HRMS of 1-(5-methyltetrahydrofuran-2-yl)*iso*-quinoline (3ad)**

## Qualitative Compound Report

| | | | |
|---|---|---|---|
| **Data File** | E-97(2).d | **Sample Name** | E-97(2) |
| **Sample Type** | Sample | **Position** | Vial 12 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | vishal_12-01-13.m | **Acquired Time** | 07-02-2015 PM 12:22:55 |
| **IRM Calibration Status** | Success | **DA Method** | daily_report.m |
| **Comment** | | | |



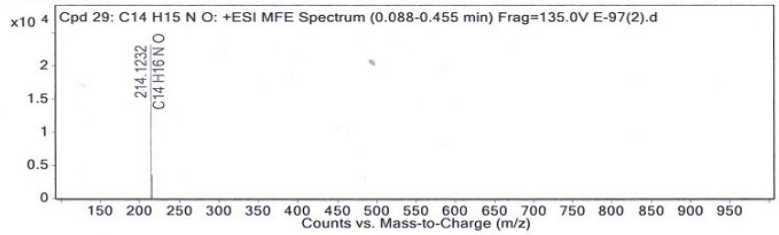

| | |
|---|---|
| **Sample Group** | **Info.** |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) |

**Compound Table**

| Compound Label | RT | Mass | Formula | MFG Formula | MFG Diff (ppm) | DB Formula |
|---|---|---|---|---|---|---|
| Cpd 29: C14 H15 N O | 0.279 | 213.1157 | C14 H15 N O | C14 H15 N O | -1.61 | C14 H15 N O |

| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 29: C14 H15 N O | 214.1232 | 0.279 | Find by Molecular Feature | 213.1157 |

MFE MS Spectrum




**MS Spectrum Peak List**

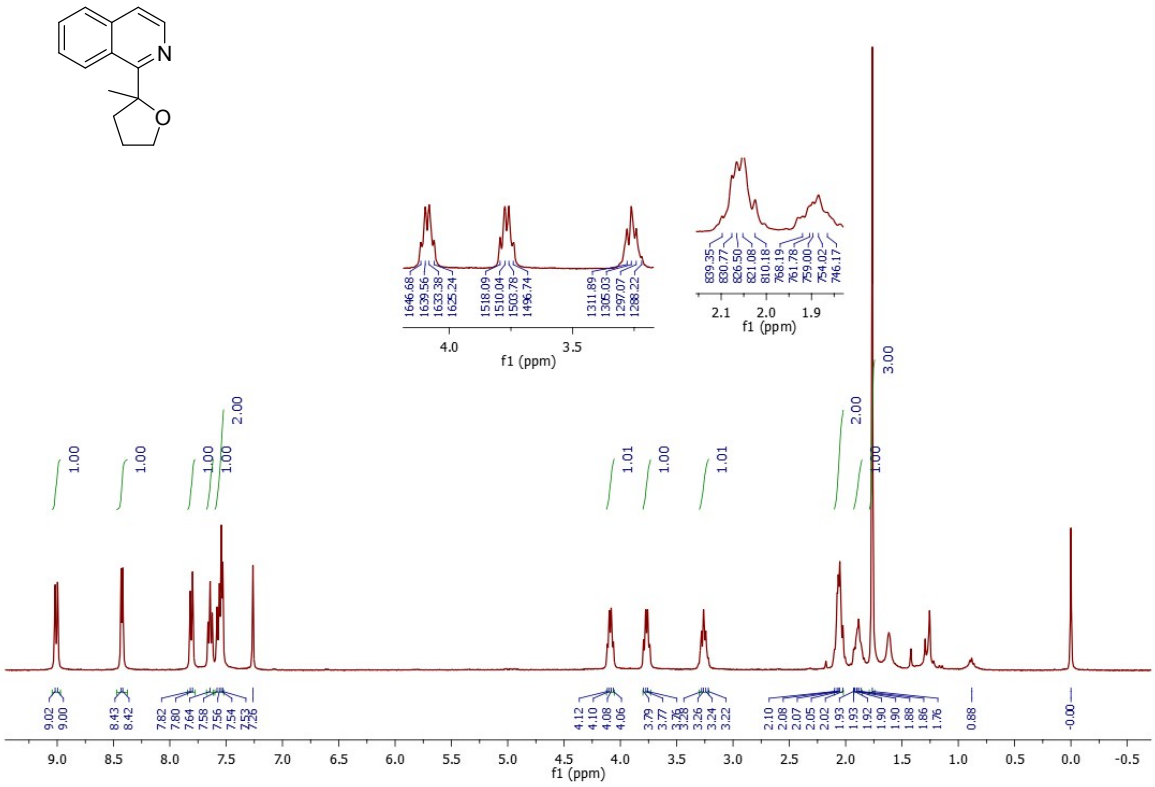
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 214.1232 | 1 | 23281.37 | C14 H16 N O | (M+H)+ |
| 215.1259 | 1 | 3570.55 | C14 H16 N O | (M+H)+ |
| 216.1257 | 1 | 1117.32 | C14 H16 N O | (M+H)+ |

**Predicted Isotope Match Table**

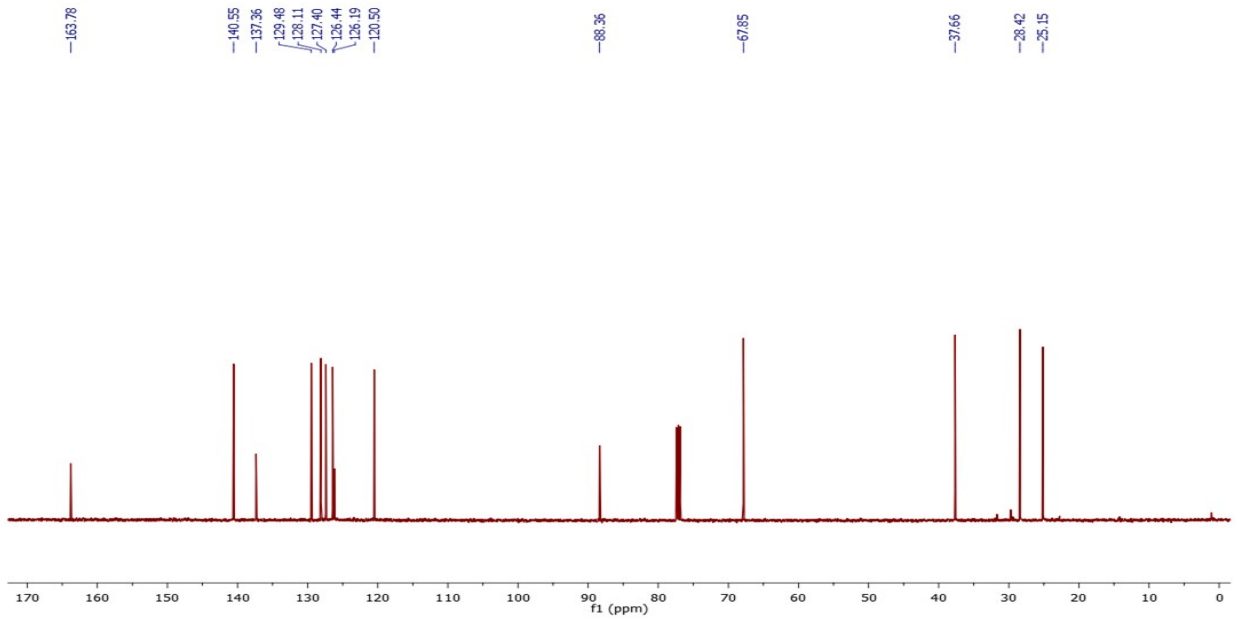
| Isotope | *m/z* | Calc m/z | Diff (ppm) | Abund % | Calc Abund % | Abund Sum % | Calc Abund Sum % |
|---|---|---|---|---|---|---|---|
| 1 | 214.1232 | 214.1226 | -2.57 | 100 | 100 | 83.24 | 85.4 |
| 2 | 215.1259 | 215.1259 | -0.29 | 15.34 | 15.73 | 12.77 | 13.43 |
| 3 | 216.1257 | 216.1288 | 14.12 | 4.8 | 1.36 | 3.99 | 1.16 |

--- End Of Report ---

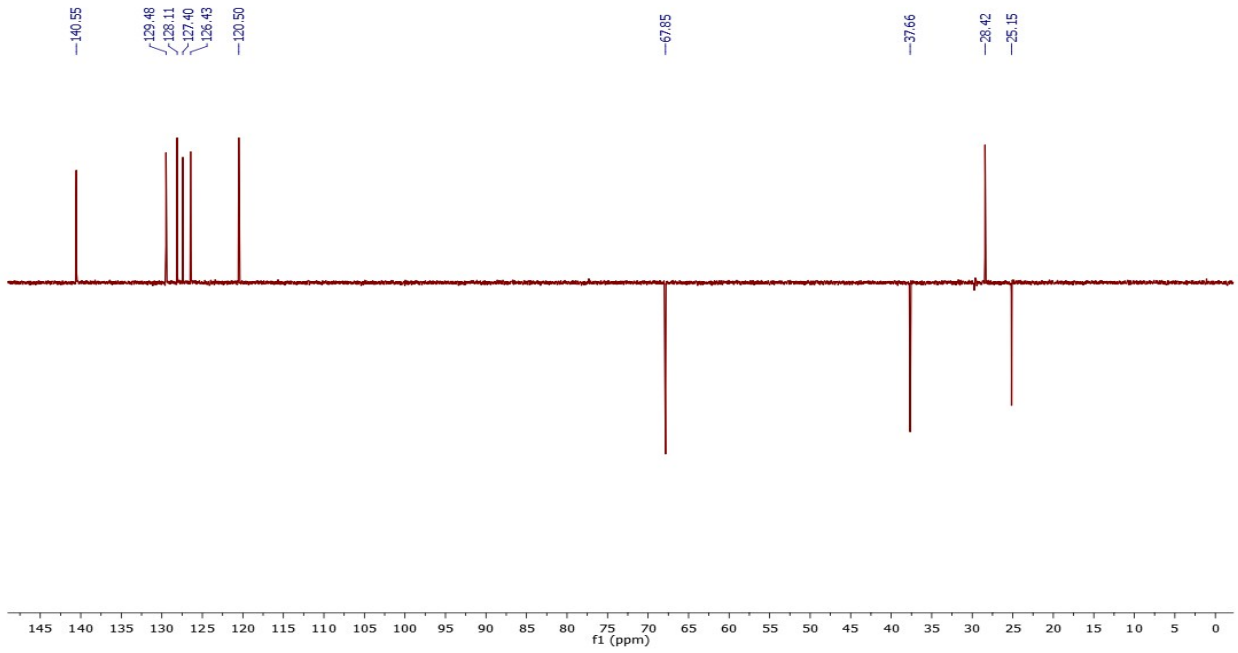
**[1]HNMR of 1-(2-methyltetrahydrofuran-2-yl)*iso*-quinoline (3ad')**



**$^{13}$C NMR of 1-(2-methyltetrahydrofuran-2-yl)*iso*-quinoline (3ad')**



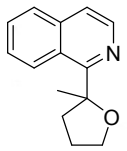

**DEPT of 1-(2-methyltetrahydrofuran-2-yl)*iso*-quinoline (3ad')**



**HRMS of 1-(2-methyltetrahydrofuran-2-yl)*iso*-quinoline (3ad')**

## Qualitative Compound Report

| | | | |
|---|---|---|---|
| **Data File** | E-97(1).d | **Sample Name** | E-97(1) |
| **Sample Type** | Sample | **Position** | Vial 9 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | vishal_12-01-13.m | **Acquired Time** | 09-02-2015 PM 12:33:25 |
| **IRM Calibration Status** | Success | **DA Method** | daily_report.m |
| **Comment** | | | |



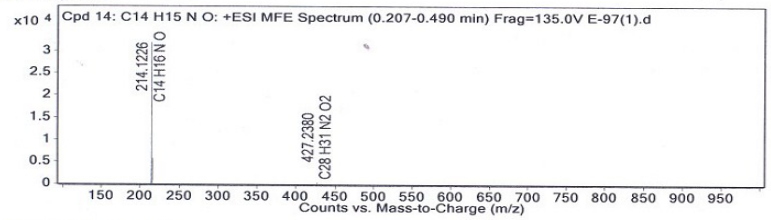

| | |
|---|---|
| **Sample Group** | **Info.** |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) |

**Compound Table**

| Compound Label | RT | Mass | Formula | MFG Formula | MFG Diff (ppm) | DB Formula |
|---|---|---|---|---|---|---|
| Cpd 14: C14 H15 N O | 0.273 | 213.1153 | C14 H15 N O | C14 H15 N O | 0.4 | C14 H15 N O |

| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 14: C14 H15 N O | 214.1226 | 0.273 | Find by Molecular Feature | 213.1153 |

MFE MS Spectrum




**MS Spectrum Peak List**

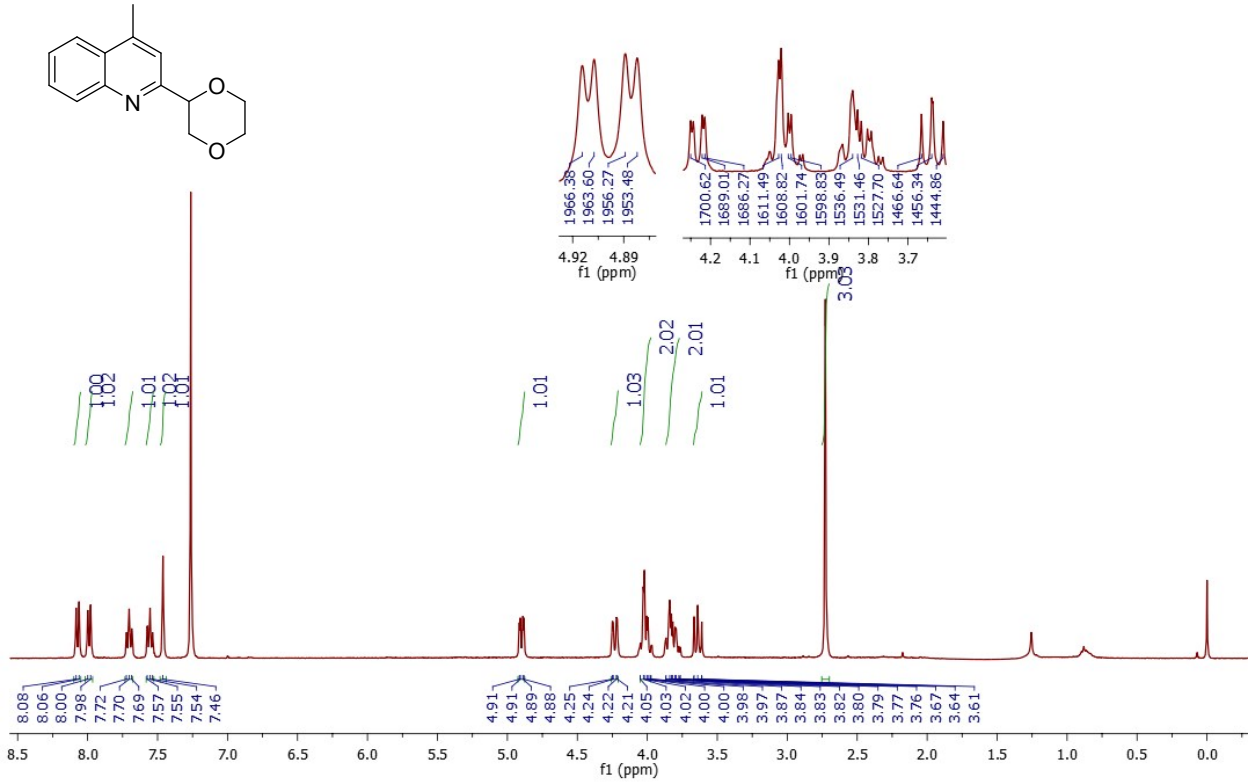
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 214.1226 | 1 | 31910.55 | C14 H16 N O | (M+H)+ |
| 215.1258 | 1 | 5780.93 | C14 H16 N O | (M+H)+ |
| 216.127 | 1 | 712.02 | C14 H16 N O | (M+H)+ |
| 427.238 | 1 | 353.65 | C28 H31 N2 O2 | (2M+H)+ |

**Predicted Isotope Match Table**

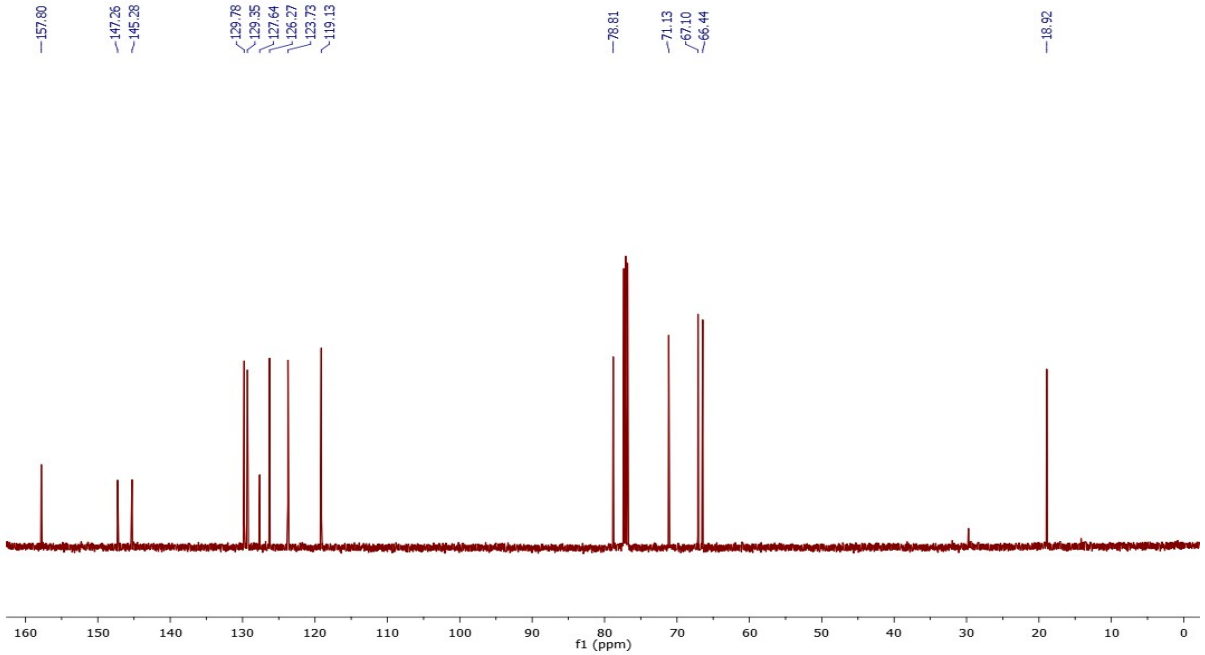
| Isotope | *m/z* | Calc m/z | Diff (ppm) | Abund % | Calc Abund % | Abund Sum % | Calc Abund Sum % |
|---|---|---|---|---|---|---|---|
| 1 | 214.1226 | 214.1226 | 0.22 | 100 | 100 | 83.09 | 85.4 |
| 2 | 215.1258 | 215.1259 | 0.42 | 18.12 | 15.73 | 15.05 | 13.43 |
| 3 | 216.127 | 216.1288 | 8.18 | 2.23 | 1.36 | 1.85 | 1.16 |

--- End Of Report ---

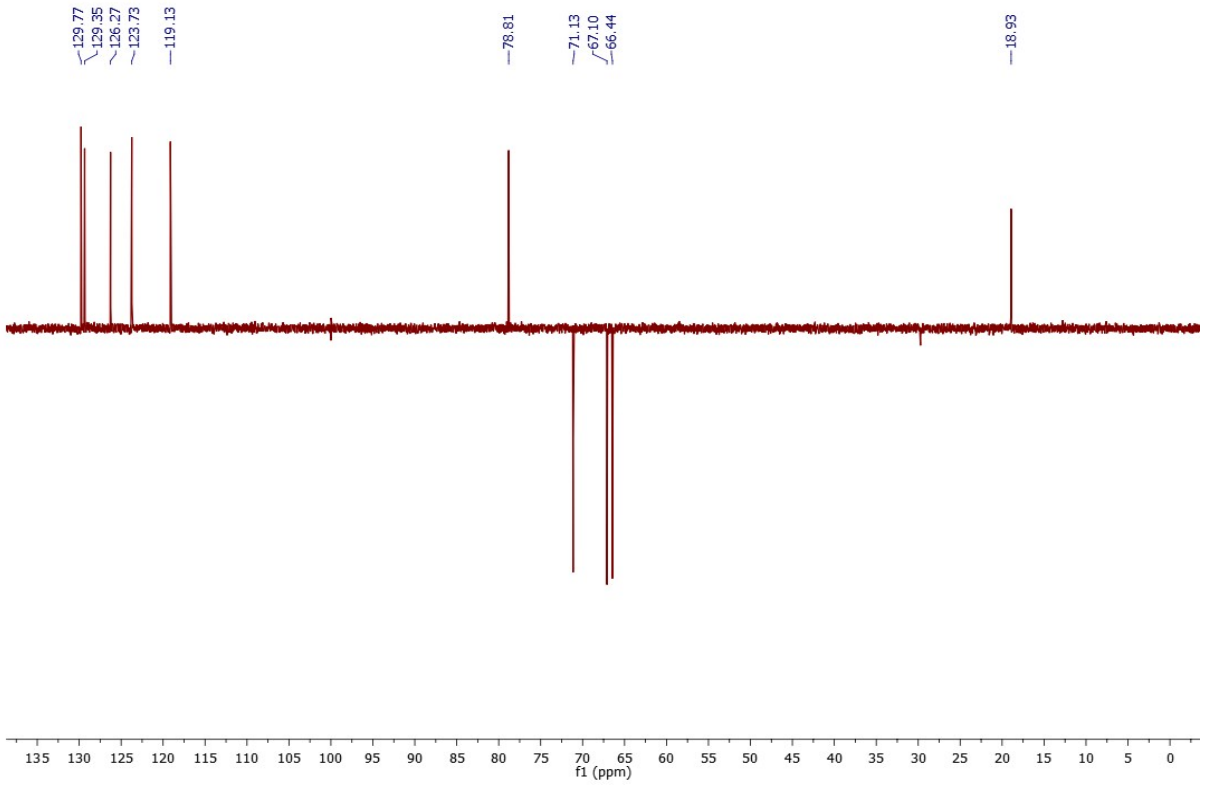
**$^1$H NMR of 2-(1,4-dioxan-2-yl)-4-methylquinoline (3ba)**



**$^{13}$C NMR of 2-(1,4-dioxan-2-yl)-4-methylquinoline (3ba)**



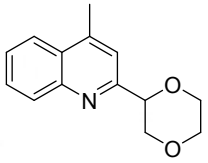

**DEPT of 2-(1,4-dioxan-2-yl)-4-methylquinoline (3ba)**



**HRMS of 2-(1,4-dioxan-2-yl)-4-methylquinoline (3ba)**

## Qualitative Compound Report

| | | | |
|---|---|---|---|
| **Data File** | E-174.d | **Sample Name** | E-174 |
| **Sample Type** | Sample | **Position** | Vial 7 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | vishal_12-01-13.m | **Acquired Time** | 04-02-2015 PM 1:32:13 |
| **IRM Calibration Status** | Success | **DA Method** | daily_report.m |
| **Comment** | | | |



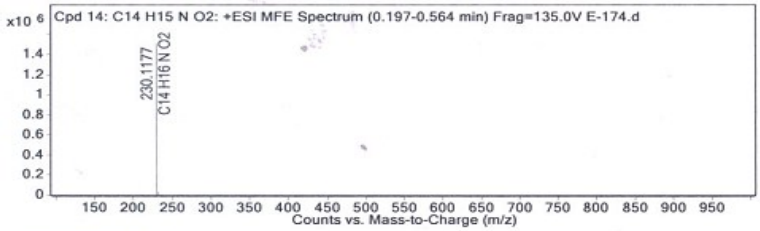

| | |
|---|---|
| **Sample Group** | **Info.** |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) |

**Compound Table**

| Compound Label | RT | Mass | Formula | MFG Formula | MFG Diff (ppm) | DB Formula |
|---|---|---|---|---|---|---|
| Cpd 14: C14 H15 N O2 | 0.286 | 229.1105 | C14 H15 N O2 | C14 H15 N O2 | -0.94 | C14 H15 N O2 |

| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 14: C14 H15 N O2 | 230.1177 | 0.286 | Find by Molecular Feature | 229.1105 |

MFE MS Spectrum




**MS Spectrum Peak List**

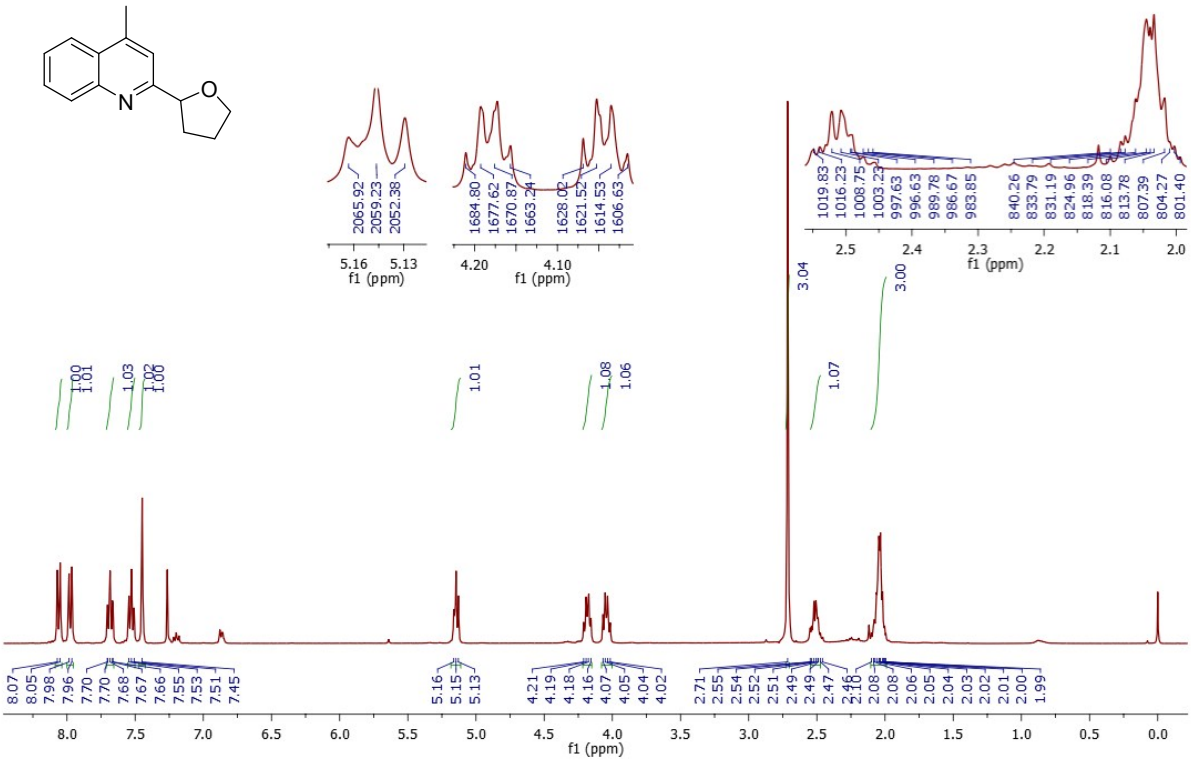
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 230.1177 | 1 | 1499903.75 | C14 H16 N O2 | (M+H)+ |
| 231.1215 | 1 | 216100.36 | C14 H16 N O2 | (M+H)+ |
| 232.1239 | 1 | 22905.55 | C14 H16 N O2 | (M+H)+ |
| 233.128 | 1 | 1682.26 | C14 H16 N O2 | (M+H)+ |

**Predicted Isotope Match Table**

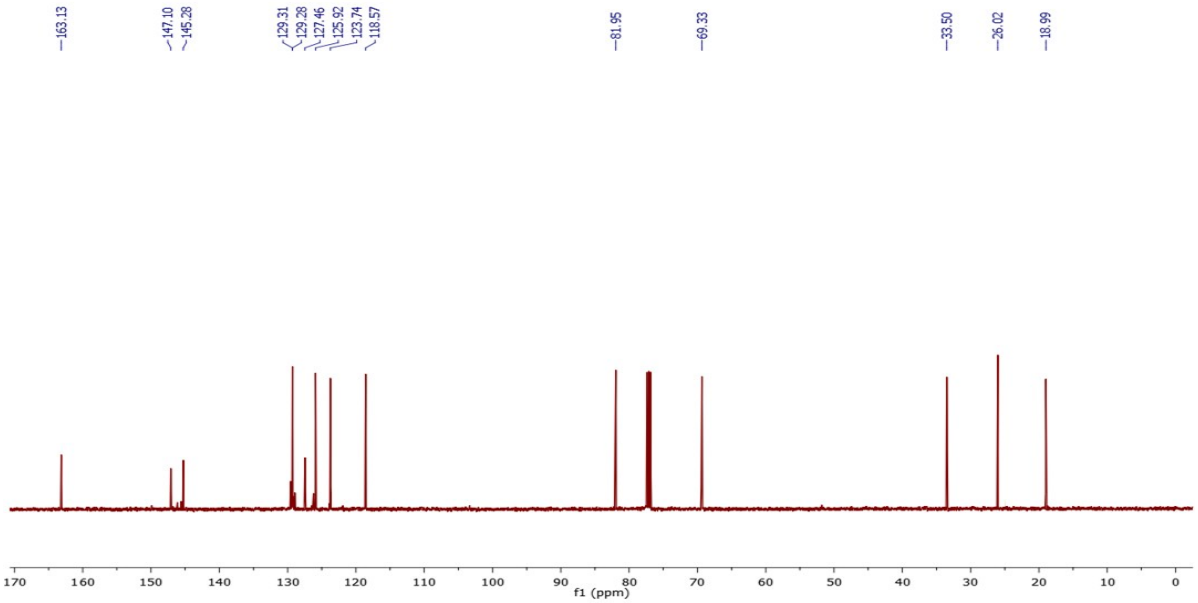
| Isotope | *m/z* | Calc m/z | Diff (ppm) | Abund % | Calc Abund % | Abund Sum % | Calc Abund Sum % |
|---|---|---|---|---|---|---|---|
| 1 | 230.1177 | 230.1176 | -0.61 | 100 | 100 | 86.17 | 85.14 |
| 2 | 231.1215 | 231.1208 | -3.04 | 14.41 | 15.77 | 12.42 | 13.42 |
| 3 | 232.1239 | 232.1235 | -2 | 1.53 | 1.57 | 1.32 | 1.34 |
| 4 | 233.128 | 233.126 | -8.19 | 0.11 | 0.12 | 0.1 | 0.1 |

--- End Of Report ---

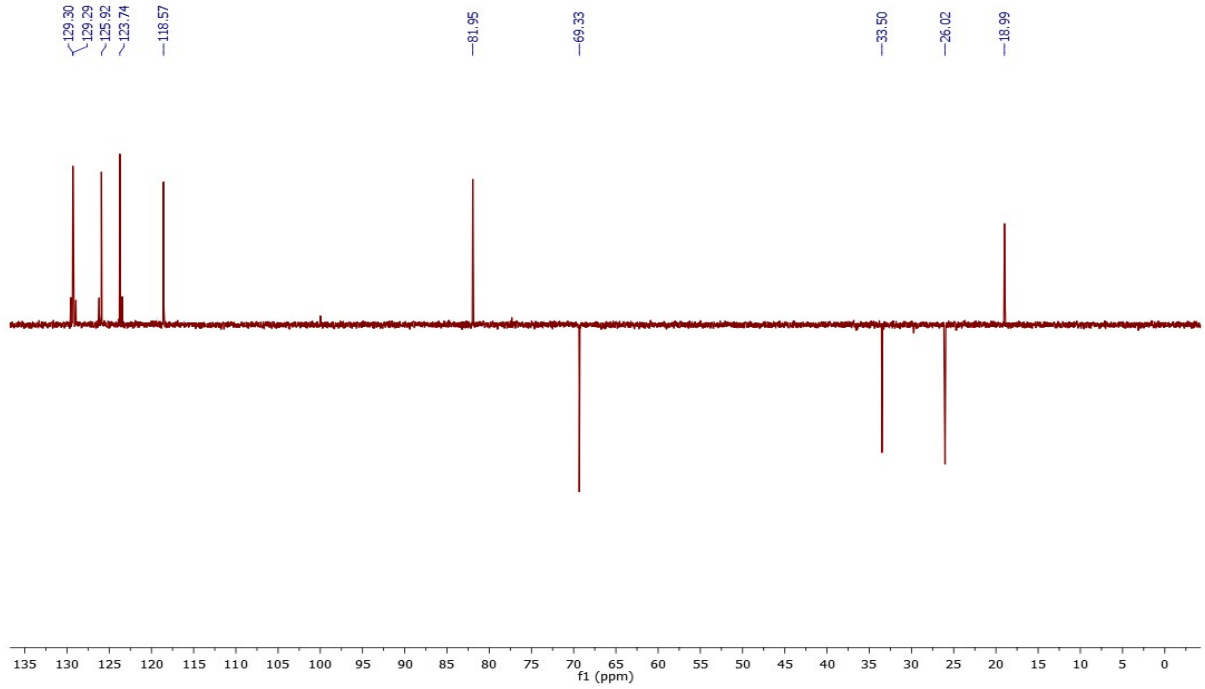
**$^1$H NMR of 4-methyl-2-(tetrahydrofuran-2-yl)quinoline (3bb)**



**$^{13}$C NMR of 4-methyl-2-(tetrahydrofuran-2-yl)quinoline (3bb)**



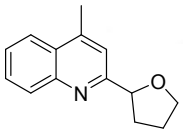

**DEPT of 4-methyl-2-(tetrahydrofuran-2-yl)quinoline (3bb)**



**HRMS of 4-methyl-2-(tetrahydrofuran-2-yl)quinoline (3bb)**

## Qualitative Compound Report

| | | | |
|---|---|---|---|
| **Data File** | E-178.d | **Sample Name** | E-178 |
| **Sample Type** | Sample | **Position** | Vial 8 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | vishal_12-01-13.m | **Acquired Time** | 04-02-2015 PM 1:36:30 |
| **IRM Calibration Status** | Success | **DA Method** | daily_report.m |
| **Comment** | | | |



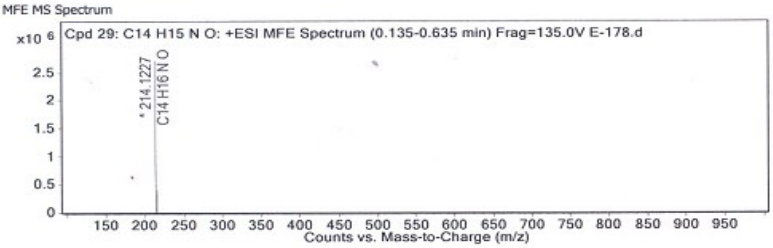

| | |
|---|---|
| **Sample Group** | **Info.** |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) |

**Compound Table**

| Compound Label | RT | Mass | Formula | MFG Formula | MFG Diff (ppm) | DB Formula |
|---|---|---|---|---|---|---|
| Cpd 29: C14 H15 N O | 0.288 | 213.1156 | C14 H15 N O | C14 H15 N O | -1.18 | C14 H15 N O |

| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 29: C14 H15 N O | 214.1227 | 0.288 | Find by Molecular Feature | 213.1156 |

MFE MS Spectrum




**MS Spectrum Peak List**

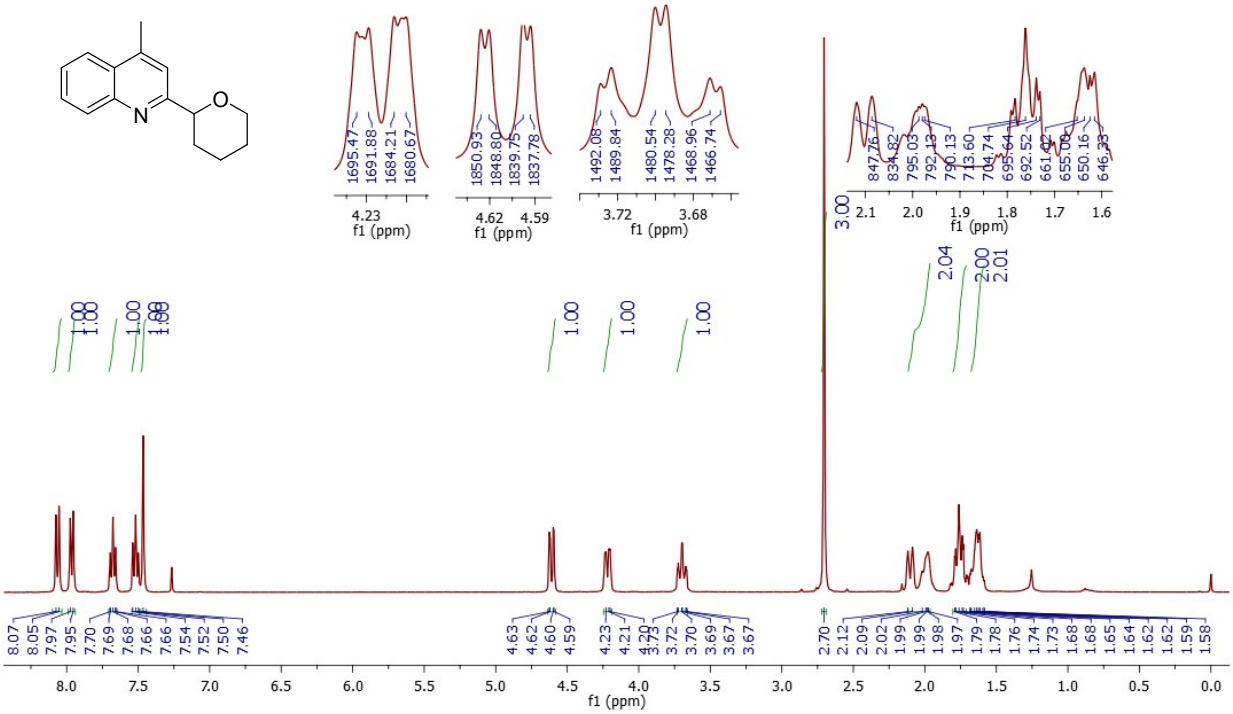
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 214.1227 | 1 | 2705281 | C14 H16 N O | (M+H)+ |
| 215.1271 | 1 | 404520.72 | C14 H16 N O | (M+H)+ |
| 216.1299 | 1 | 31478.53 | C14 H16 N O | (M+H)+ |
| 217.1315 | 1 | 2590.66 | C14 H16 N O | (M+H)+ |

**Predicted Isotope Match Table**

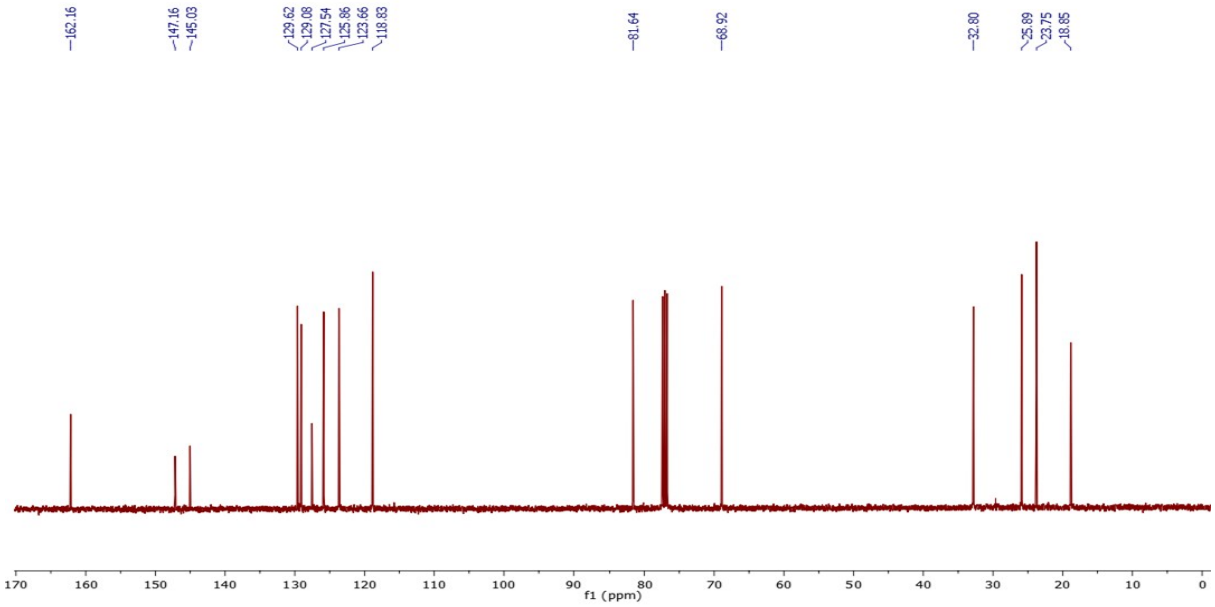
| Isotope | *m/z* | Calc m/z | Diff (ppm) | Abund % | Calc Abund % | Abund Sum % | Calc Abund Sum % |
|---|---|---|---|---|---|---|---|
| 1 | 214.1227 | 214.1226 | -0.42 | 100 | 100 | 86.05 | 85.34 |
| 2 | 215.1271 | 215.1259 | -5.86 | 14.95 | 15.73 | 12.87 | 13.42 |
| 3 | 216.1299 | 216.1288 | -5.32 | 1.16 | 1.36 | 1 | 1.16 |
| 4 | 217.1315 | 217.1315 | -0.03 | 0.1 | 0.08 | 0.08 | 0.07 |

--- End Of Report ---

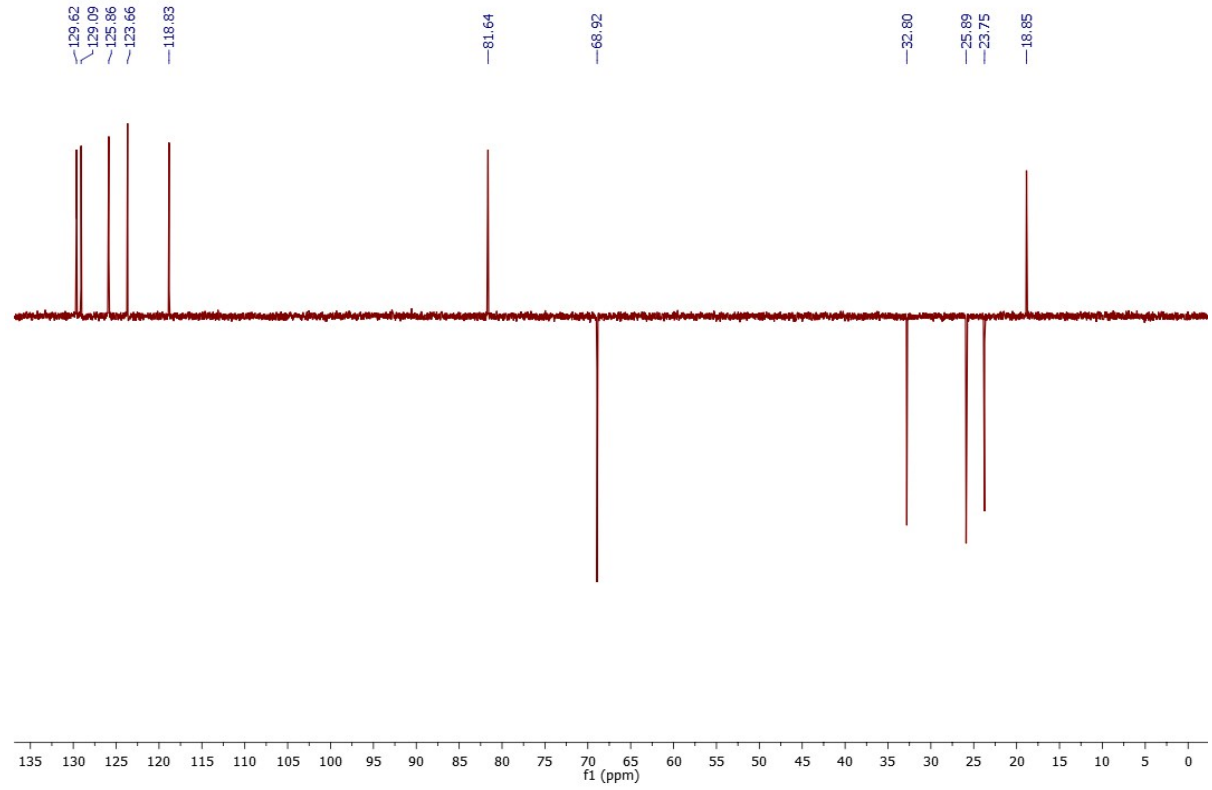
**$^{1}$H NMR of 4-methyl-2-(tetrahydro-2H-pyran-2-yl)quinoline (3bc)**



**$^{13}$C NMR of 4-methyl-2-(tetrahydro-2H-pyran-2-yl)quinoline (3bc)**



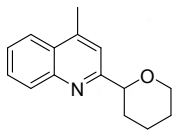

**DEPT of 4-methyl-2-(tetrahydro-2H-pyran-2-yl)quinoline (3bc)**



**HRMS of 4-methyl-2-(tetrahydro-2H-pyran-2-yl)quinoline (3bc)**

## Qualitative Compound Report

| | | | |
|---|---|---|---|
| **Data File** | E-177.d | **Sample Name** | E-177 |
| **Sample Type** | Sample | **Position** | Vial 13 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | vishal_12-01-13.m | **Acquired Time** | 04-02-2015 PM 2:02:33 |
| **IRM Calibration Status** | Success | **DA Method** | daily_report.m |
| **Comment** | | | |



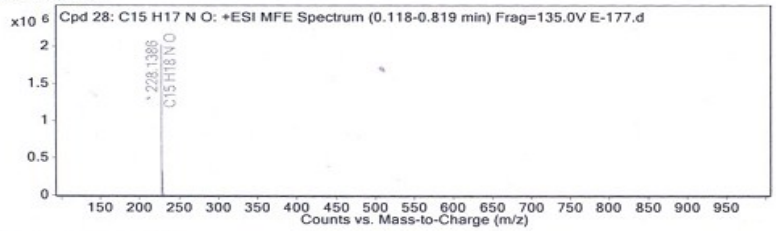
| | |
|---|---|
| **Sample Group** | **Info.** |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) |

**Compound Table**

| Compound Label | RT | Mass | Formula | MFG Formula | MFG Diff (ppm) | DB Formula |
|---|---|---|---|---|---|---|
| Cpd 28: C15 H17 N O | 0.29 | 227.1313 | C15 H17 N O | C15 H17 N O | -1.18 | C15 H17 N O |

| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 28: C15 H17 N O | 228.1386 | 0.29 | Find by Molecular Feature | 227.1313 |

MFE MS Spectrum




**MS Spectrum Peak List**

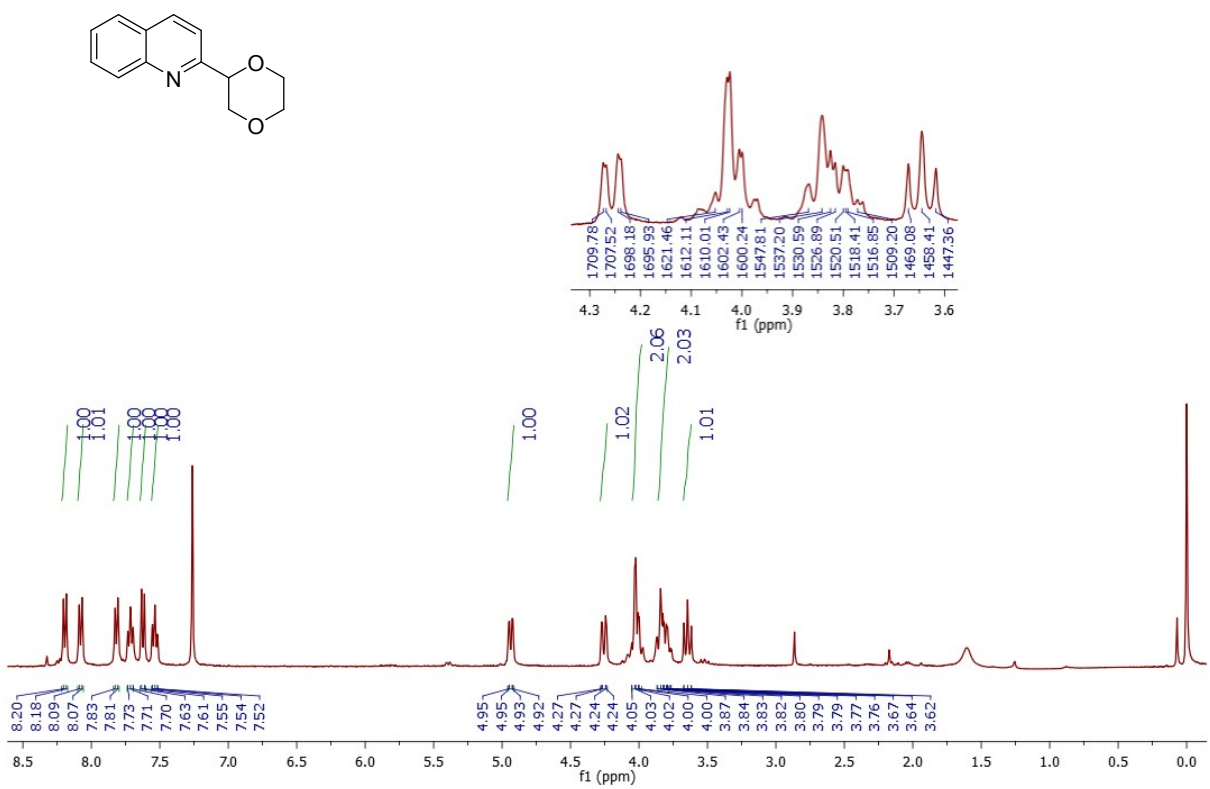
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 228.1386 | 1 | 2024989 | C15 H18 N O | (M+H)+ |
| 229.1416 | 1 | 324460.34 | C15 H18 N O | (M+H)+ |
| 230.1442 | 1 | 26987.7 | C15 H18 N O | (M+H)+ |
| 231.1471 | 1 | 2806.02 | C15 H18 N O | (M+H)+ |

**Predicted Isotope Match Table**

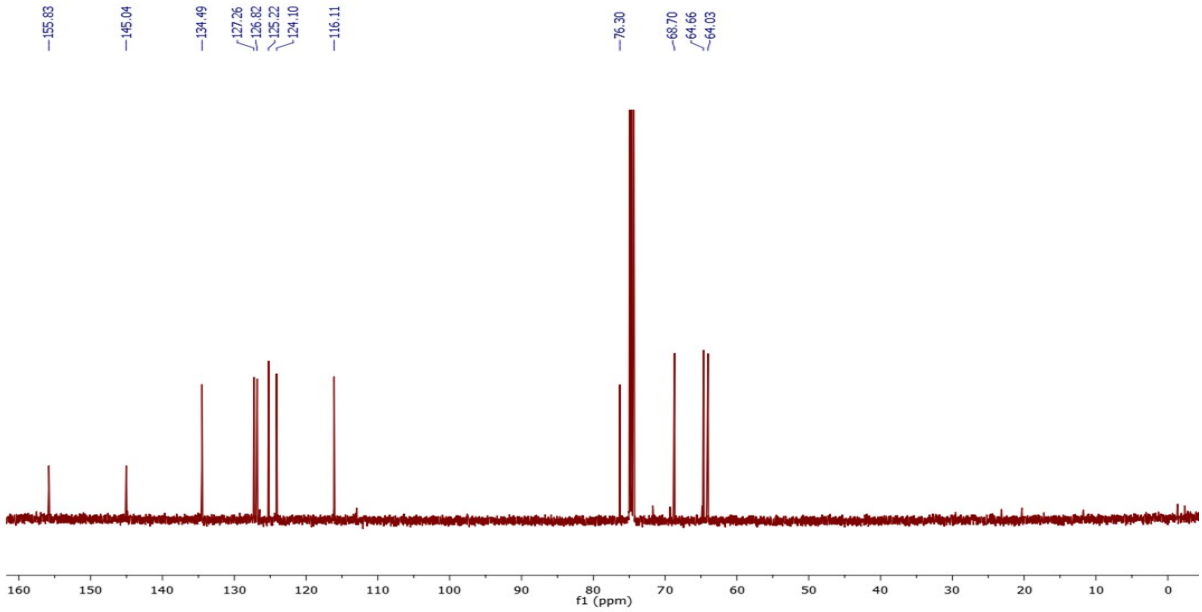
| Isotope | *m/z* | Calc m/z | Diff (ppm) | Abund % | Calc Abund % | Abund Sum % | Calc Abund Sum % |
|---|---|---|---|---|---|---|---|
| 1 | 228.1386 | 228.1383 | -1.33 | 100 | 100 | 85.11 | 84.41 |
| 2 | 229.1416 | 229.1415 | -0.44 | 16.02 | 16.83 | 13.64 | 14.21 |
| 3 | 230.1442 | 230.1445 | 1.16 | 1.33 | 1.53 | 1.13 | 1.29 |
| 4 | 231.1471 | 231.1473 | 0.56 | 0.14 | 0.1 | 0.12 | 0.08 |

--- End Of Report ---

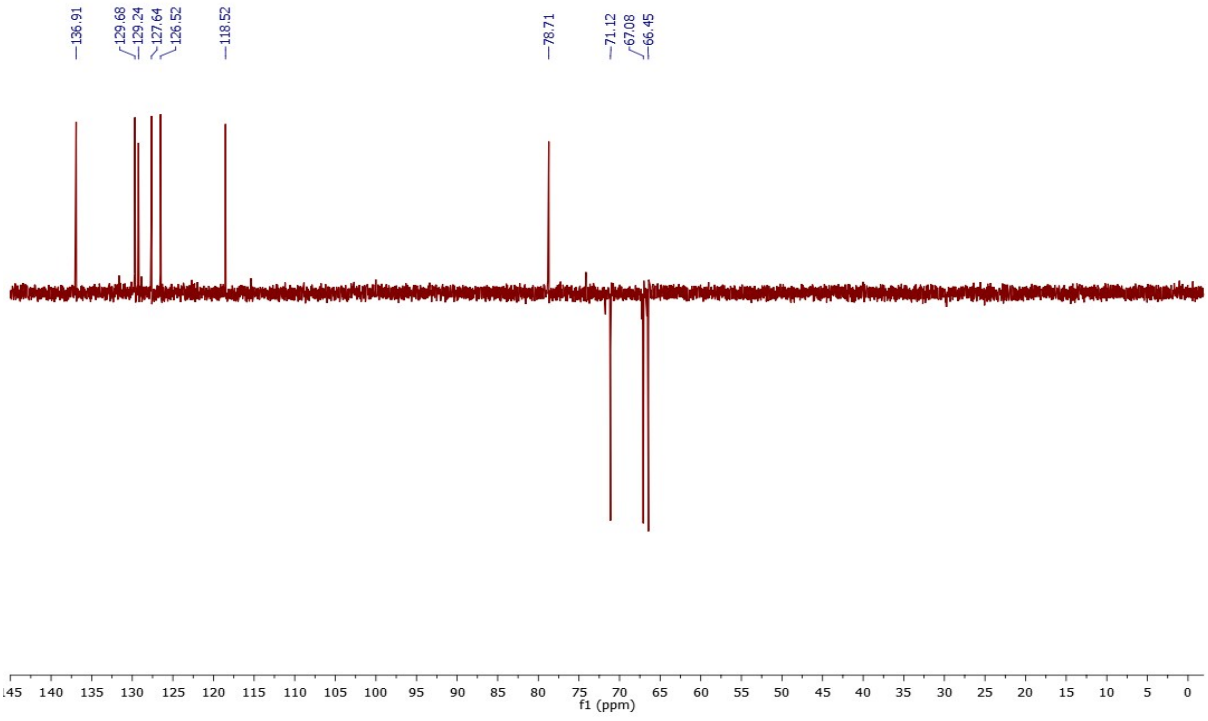
**$^1$H NMR of 2-(1,4-dioxan-2-yl)quinoline (3ca)**



**$^{13}$C NMR of 2-(1,4-dioxan-2-yl)quinoline (3ca)**



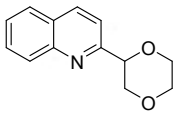

**DEPT of 2-(1,4-dioxan-2-yl)quinoline (3ca)**



**HRMS of 2-(1,4-dioxan-2-yl)quinoline (3ca)**

## Qualitative Compound Report

| | | | |
|---|---|---|---|
| **Data File** | E-134(I).d | **Sample Name** | E-134(I) |
| **Sample Type** | Sample | **Position** | Vial 7 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | vishal_12-01-13.m | **Acquired Time** | 10-02-2015 PM 12:23:21 |
| **IRM Calibration Status** | Success | **DA Method** | daily_report.m |
| **Comment** | | | |



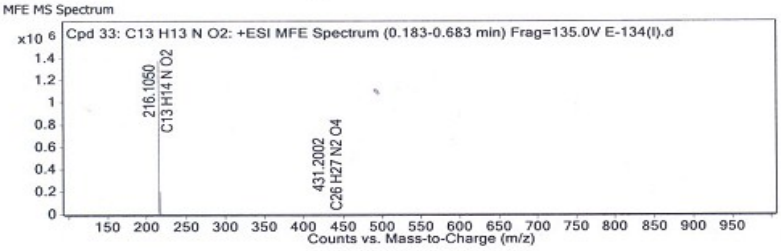
| | |
|---|---|
| **Sample Group** | **Info.** |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) |

**Compound Table**

| Compound Label | RT | Mass | Formula | MFG Formula | MFG Diff (ppm) | DB Formula |
|---|---|---|---|---|---|---|
| Cpd 33: C13 H13 N O2 | 0.28 | 215.0978 | C13 H13 N O2 | C13 H13 N O2 | -14.76 | C13 H13 N O2 |

| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 33: C13 H13 N O2 | 216.105 | 0.28 | Find by Molecular Feature | 215.0978 |

MFE MS Spectrum




**MS Spectrum Peak List**

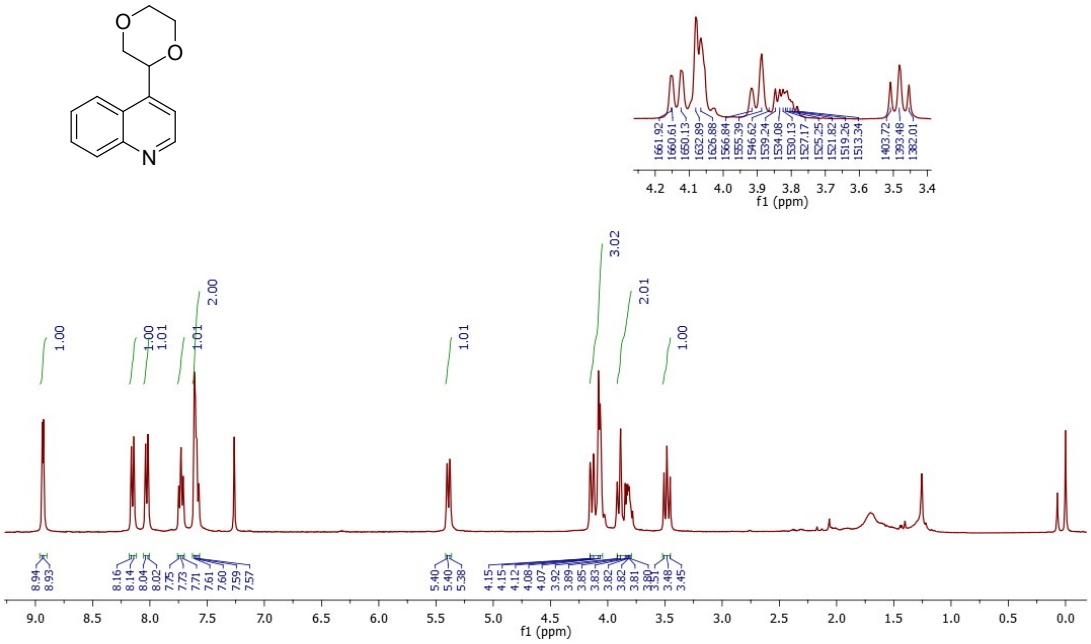
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 216.105 | 1 | 1373209.88 | C13 H14 N O2 | (M+H)+ |
| 217.1086 | 1 | 204491.08 | C13 H14 N O2 | (M+H)+ |
| 218.1117 | 1 | 18687.9 | C13 H14 N O2 | (M+H)+ |
| 219.1126 | 1 | 3300.62 | C13 H14 N O2 | (M+H)+ |
| 431.2002 | 1 | 440.42 | C26 H27 N2 O4 | (2M+H)+ |

**Predicted Isotope Match Table**

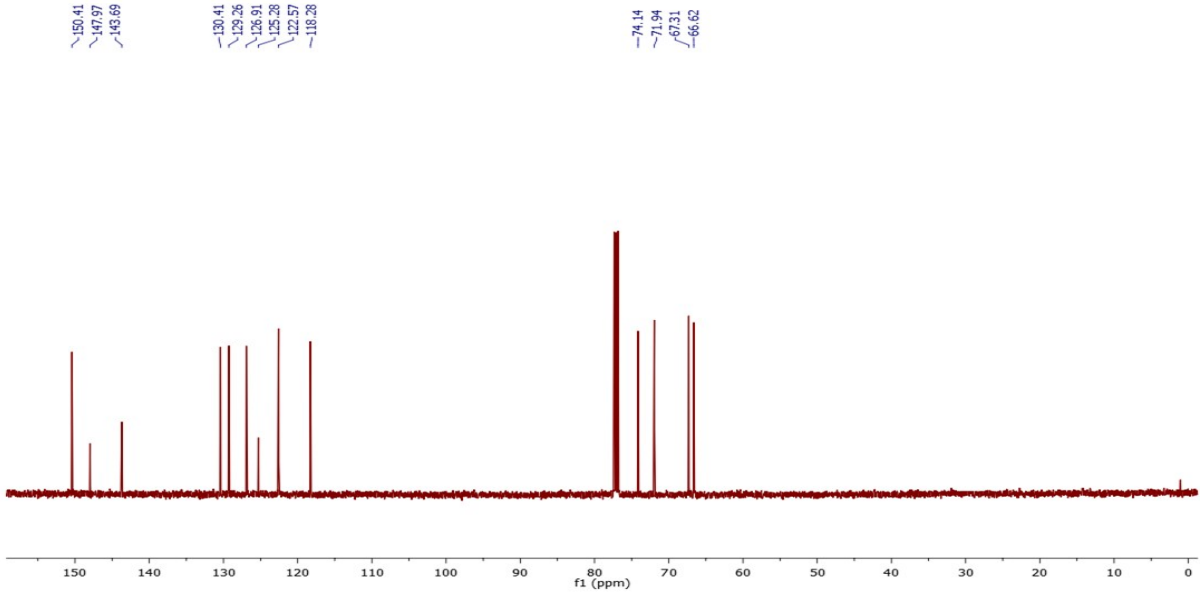
| Isotope | *m/z* | Calc m/z | Diff (ppm) | Abund % | Calc Abund % | Abund Sum % | Calc Abund Sum % |
|---|---|---|---|---|---|---|---|
| 1 | 216.105 | 216.1019 | -14.43 | 100 | 100 | 85.84 | 86.08 |
| 2 | 217.1086 | 217.1051 | -16.15 | 14.89 | 14.66 | 12.78 | 12.62 |
| 3 | 218.1117 | 218.1077 | -18.06 | 1.36 | 1.41 | 1.17 | 1.21 |
| 4 | 219.1126 | 219.1103 | -10.59 | 0.24 | 0.1 | 0.21 | 0.09 |

--- End Of Report ---

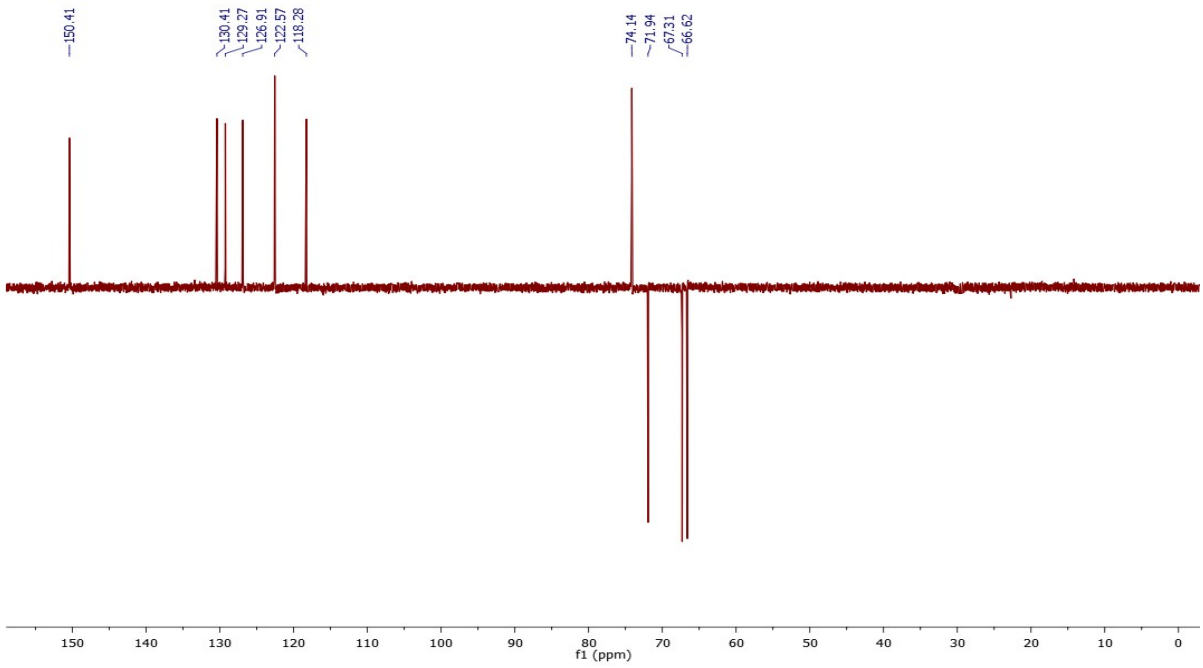
**$^1$H NMR of 4-(1,4-dioxan-2-yl)quinoline (3ca')**



**$^{13}$C NMR of 4-(1,4-dioxan-2-yl)quinoline (3ca')**



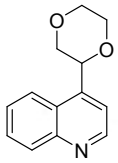

**DEPT of 4-(1,4-dioxan-2-yl)quinoline (3ca')**



**HRMS of 4-(1,4-dioxan-2-yl)quinoline (3ca')**

## Qualitative Compound Report

| | | | |
|---|---|---|---|
| **Data File** | E-134(11).d | **Sample Name** | E-134(11) |
| **Sample Type** | Sample | **Position** | Vial 9 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | vishal_12-01-13.m | **Acquired Time** | 04-02-2015 PM 1:40:48 |
| **IRM Calibration Status** | Success | **DA Method** | daily_report.m |
| **Comment** | | | |
| **Sample Group** | | **Info.** | |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) | | |

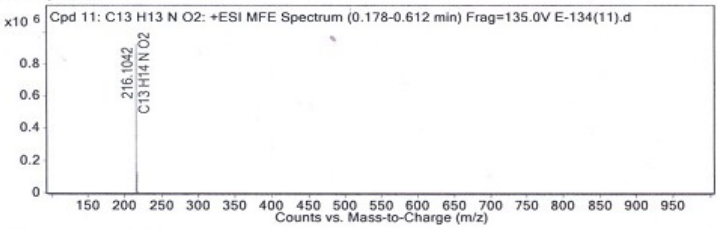



**Compound Table**

| Compound Label | RT | Mass | Formula | MFG Formula | MFG Diff (ppm) | DB Formula |
|---|---|---|---|---|---|---|
| Cpd 11: C13 H13 N O2 | 0.288 | 215.0969 | C13 H13 N O2 | C13 H13 N O2 | -10.54 | C13 H13 N O2 |

| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 11: C13 H13 N O2 | 216.1042 | 0.288 | Find by Molecular Feature | 215.0969 |

MFE MS Spectrum




**MS Spectrum Peak List**

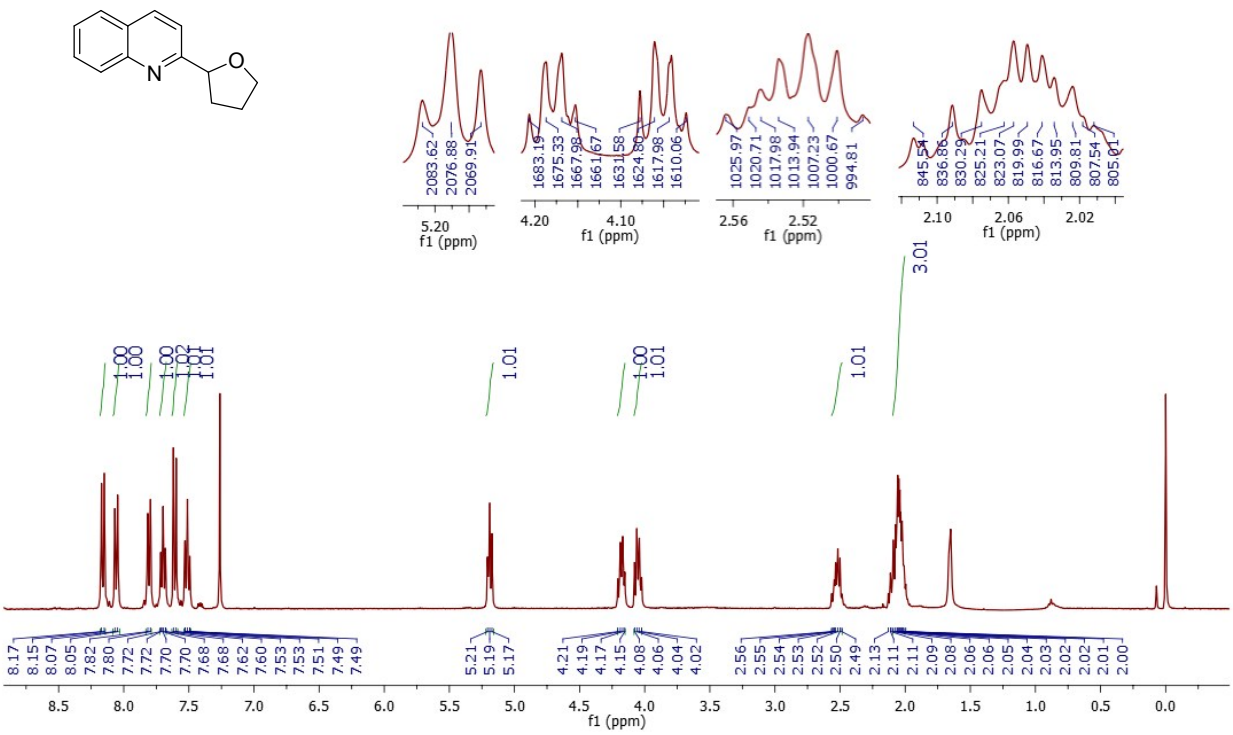
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 216.1042 | 1 | 924414 | C13 H14 N O2 | (M+H)+ |
| 217.1076 | 1 | 132205.89 | C13 H14 N O2 | (M+H)+ |
| 218.1093 | 1 | 12304.54 | C13 H14 N O2 | (M+H)+ |
| 219.1123 | 1 | 975.17 | C13 H14 N O2 | (M+H)+ |

**Predicted Isotope Match Table**

| Isotope | *m/z* | Calc m/z | Diff (ppm) | Abund % | Calc Abund % | Abund Sum % | Calc Abund Sum % |
|---|---|---|---|---|---|---|---|
| 1 | 216.1042 | 216.1019 | -10.42 | 100 | 100 | 86.4 | 86.08 |
| 2 | 217.1076 | 217.1051 | -11.29 | 14.3 | 14.66 | 12.36 | 12.62 |
| 3 | 218.1093 | 218.1077 | -7.11 | 1.33 | 1.41 | 1.15 | 1.21 |
| 4 | 219.1123 | 219.1103 | -9.02 | 0.11 | 0.1 | 0.09 | 0.09 |

--- End Of Report ---

**$^1$H NMR of 2-(tetrahydrofuran-2-yl)quinoline (3cb):**



**$^{13}$C NMR of 2-(tetrahydrofuran-2-yl)quinoline (3cb)**

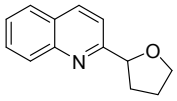
**DEPT of 2-(tetrahydrofuran-2-yl)quinoline (3cb)**

**HRMS of 2-(tetrahydrofuran-2-yl)quinoline (3cb)**

## Qualitative Compound Report

| | | | |
|---|---|---|---|
| **Data File** | E-142(I).d | **Sample Name** | E-142(I) |
| **Sample Type** | Sample | **Position** | Vial 14 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | vishal_12-01-13.m | **Acquired Time** | 04-02-2015 PM 2:06:51 |
| **IRM Calibration Status** | Success | **DA Method** | daily_report.m |
| **Comment** | | | |

**Sample Group** **Info.**
**Acquisition SW Version** 6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

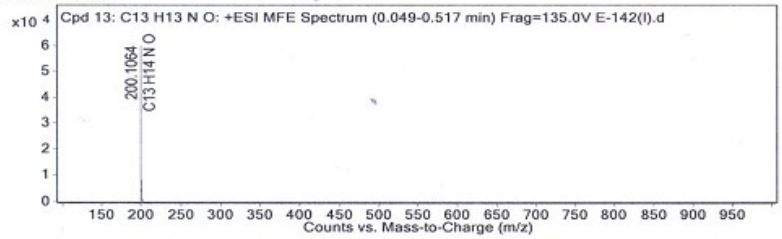


**Compound Table**

| Compound Label | RT | Mass | Formula | MFG Formula | MFG Diff (ppm) | DB Formula |
|---|---|---|---|---|---|---|
| Cpd 13: C13 H13 N O | 0.291 | 199.0991 | C13 H13 N O | C13 H13 N O | 2.96 | C13 H13 N O |

| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 13: C13 H13 N O | 200.1064 | 0.291 | Find by Molecular Feature | 199.0991 |

MFE MS Spectrum




**MS Spectrum Peak List**

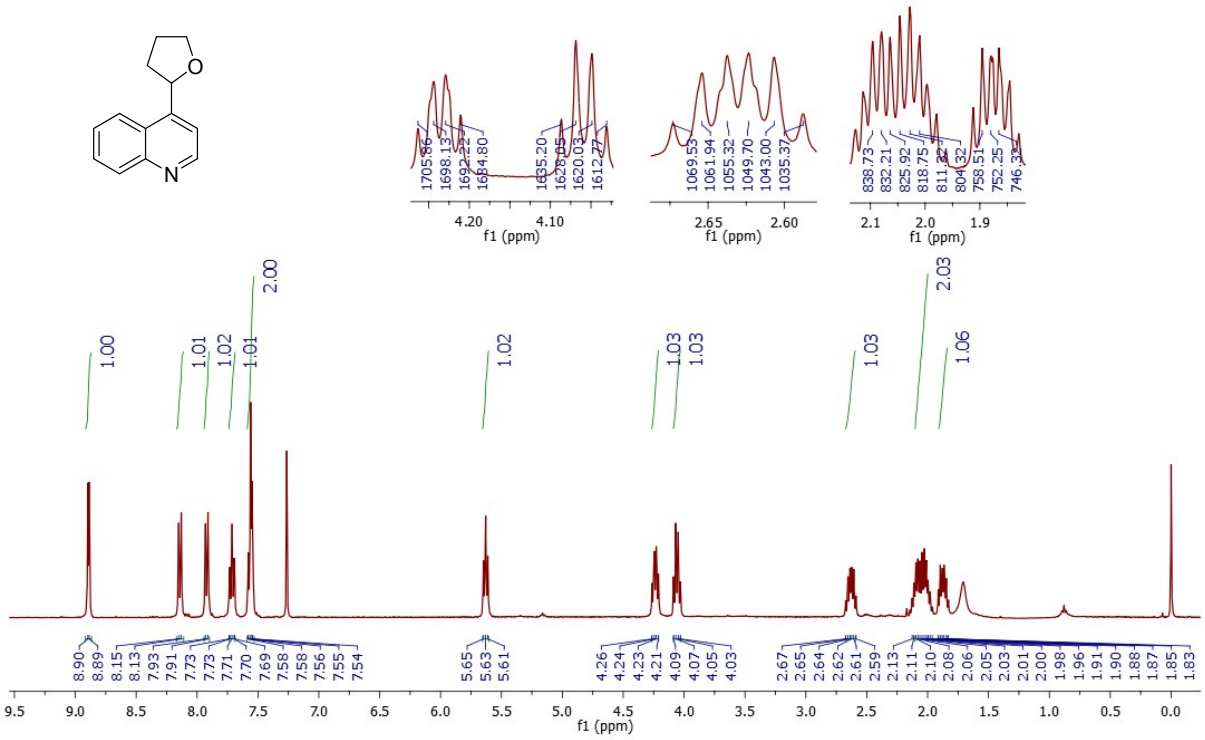
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 200.1064 | 1 | 60006.23 | C13 H14 N O | (M+H)+ |
| 201.1098 | 1 | 8546.98 | C13 H14 N O | (M+H)+ |
| 202.1104 | 1 | 1106 | C13 H14 N O | (M+H)+ |

**Predicted Isotope Match Table**

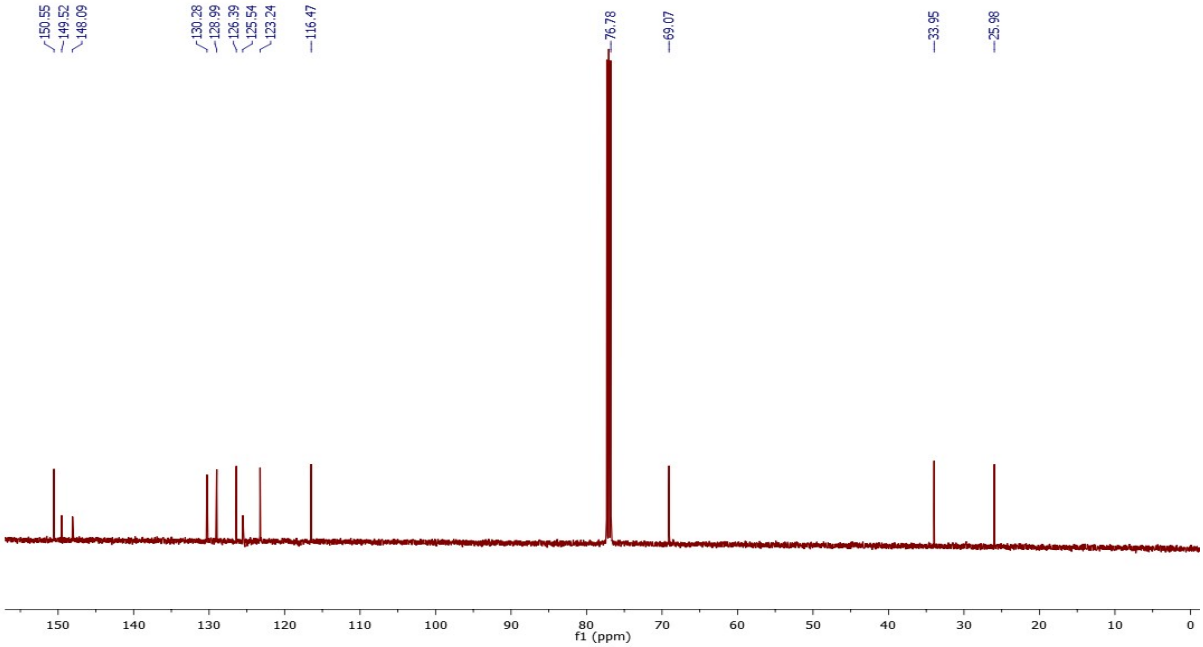
| Isotope | *m/z* | Calc m/z | Diff (ppm) | Abund % | Calc Abund % | Abund Sum % | Calc Abund Sum % |
|---|---|---|---|---|---|---|---|
| 1 | 200.1064 | 200.107 | 2.89 | 100 | 100 | 86.14 | 86.34 |
| 2 | 201.1098 | 201.1102 | 2.07 | 14.24 | 14.62 | 12.27 | 12.63 |
| 3 | 202.1104 | 202.1131 | 12.93 | 1.84 | 1.2 | 1.59 | 1.03 |

--- End Of Report ---

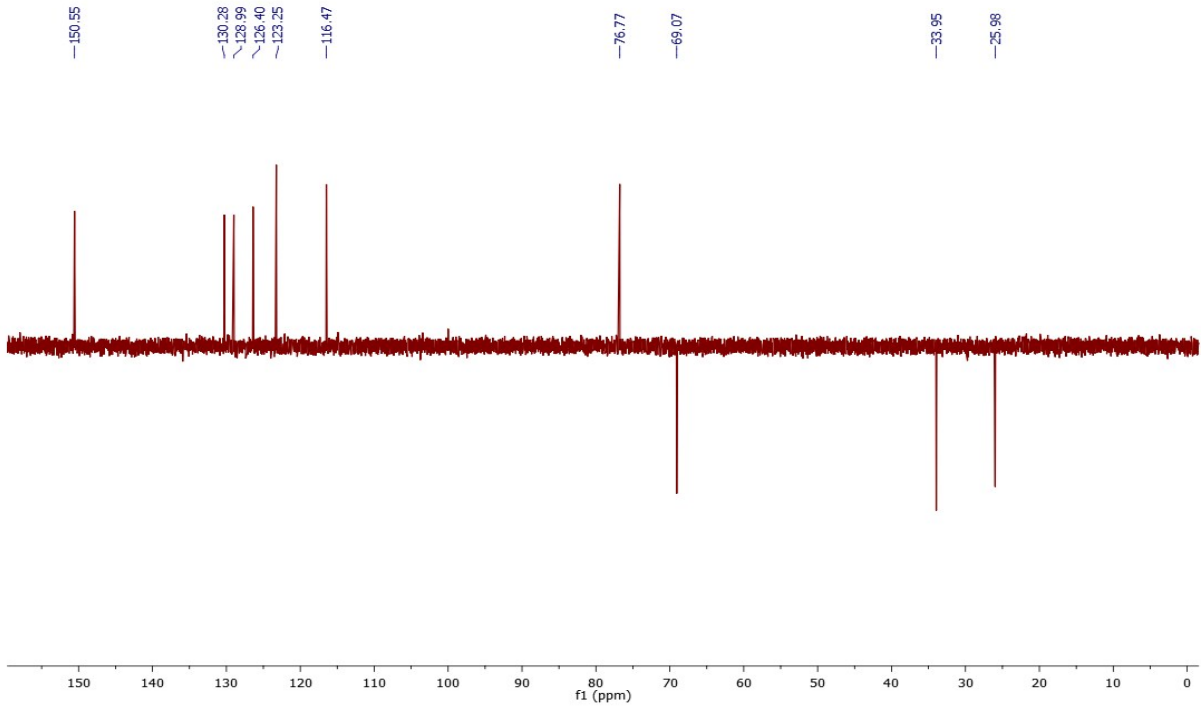
**[1]H NMR of 4-(tetrahydrofuran-2-yl)quinoline (3cb')**



**$^{13}$C NMR of 4-(tetrahydrofuran-2-yl)quinoline (3cb')**




**DEPT of 4-(tetrahydrofuran-2-yl)quinoline (3cb')**

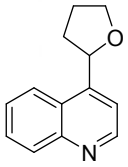


**HRMS of 4-(tetrahydrofuran-2-yl)quinoline (3cb')**

## Qualitative Compound Report

| | | | |
|---|---|---|---|
| **Data File** | E-142(II).d | **Sample Name** | E-142(II) |
| **Sample Type** | Sample | **Position** | Vial 16 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | vishal_12-01-13.m | **Acquired Time** | 12-01-2015 PM 1:47:20 |
| **IRM Calibration Status** | Success | **DA Method** | daily_report.m |
| **Comment** | | | |

**Sample Group** **Info.**
**Acquisition SW Version** 6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

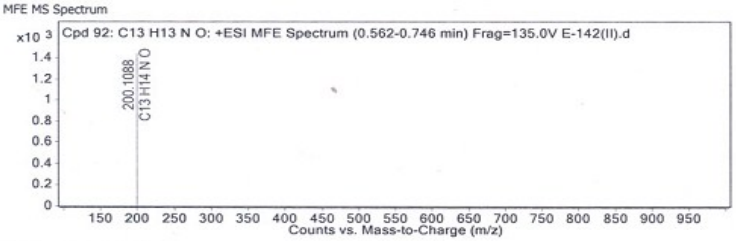



**Compound Table**

| Compound Label | RT | Mass | Formula | MFG Formula | MFG Diff (ppm) | DB Formula |
|---|---|---|---|---|---|---|
| Cpd 92: C13 H13 N O | 0.605 | 199.1015 | C13 H13 N O | C13 H13 N O | -9.09 | C13 H13 N O |

| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 92: C13 H13 N O | 200.1088 | 0.605 | Find by Molecular Feature | 199.1015 |

MFE MS Spectrum




**MS Spectrum Peak List**

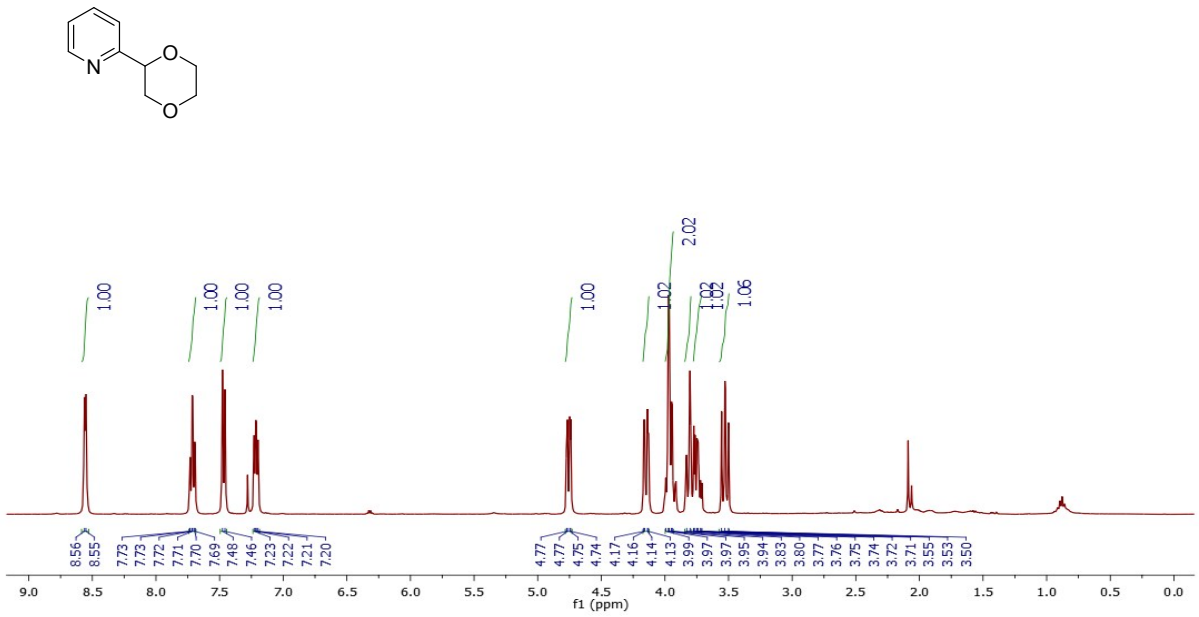
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 200.1088 | 1 | 1448.28 | C13 H14 N O | (M+H)+ |

**Predicted Isotope Match Table**

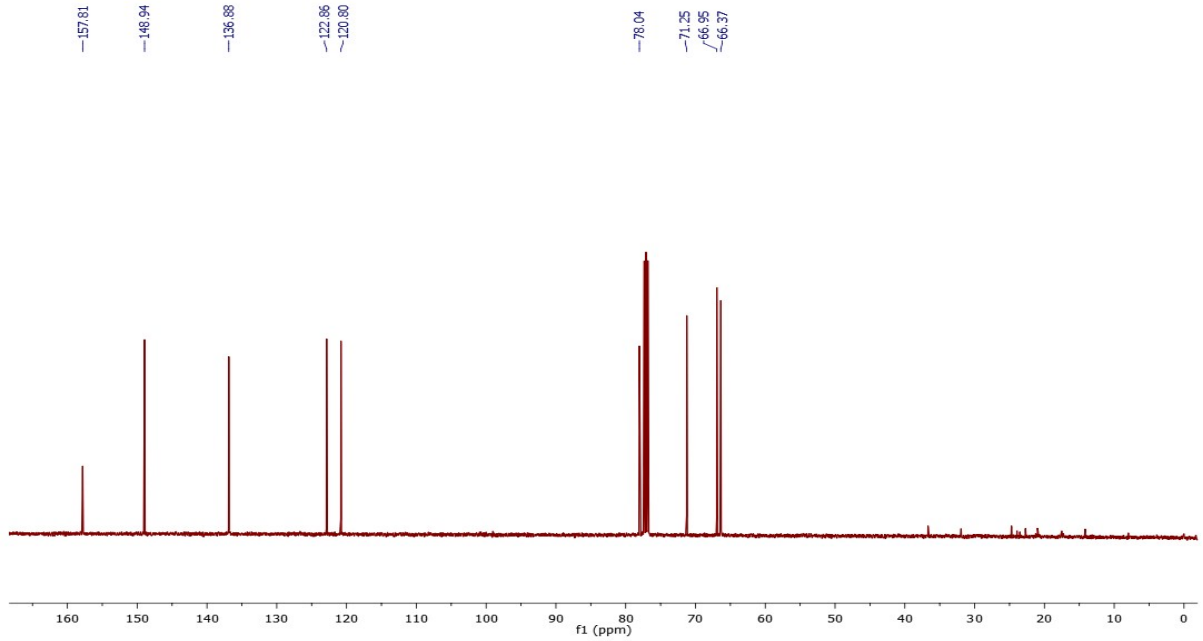
| Isotope | *m/z* | Calc m/z | Diff (ppm) | Abund % | Calc Abund % | Abund Sum % | Calc Abund Sum % |
|---|---|---|---|---|---|---|---|
| 1 | 200.1088 | 200.107 | -9.05 | 100 | 100 | 100 | 100 |

--- End Of Report ---

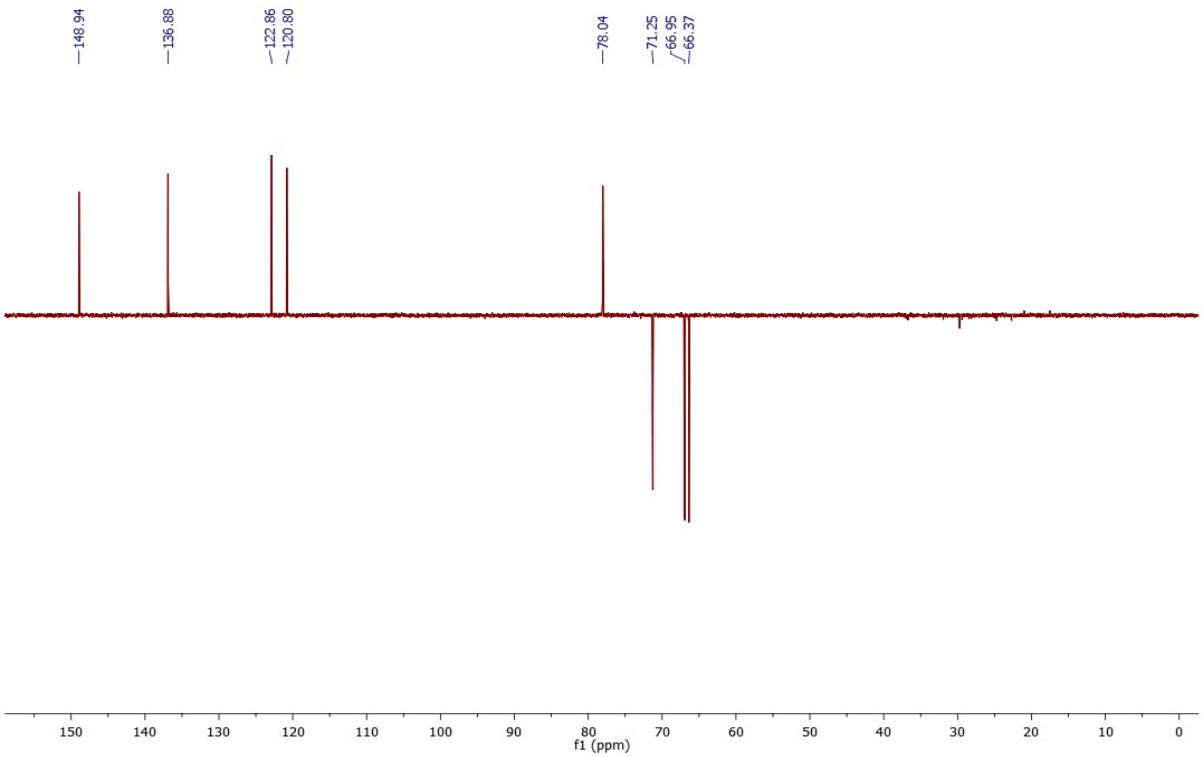
**$^{1}$H NMR of 2-(1,4-dioxan-2-yl)pyridine (3da)**



**$^{13}$C NMR of 2-(1,4-dioxan-2-yl)pyridine (3da)**



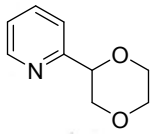

**DEPT of 2-(1,4-dioxan-2-yl)pyridine (3da)**



**HRMS of 2-(1,4-dioxan-2-yl)pyridine (3da)**

## Qualitative Compound Report

| | | | |
|---|---|---|---|
| **Data File** | E-143(I).d | **Sample Name** | E-143(I) |
| **Sample Type** | Sample | **Position** | Vial 4 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | vishal_12-01-13.m | **Acquired Time** | 26-12-2014 PM 5:48:39 |
| **IRM Calibration Status** | Success | **DA Method** | daily_report.m |
| **Comment** | | | |



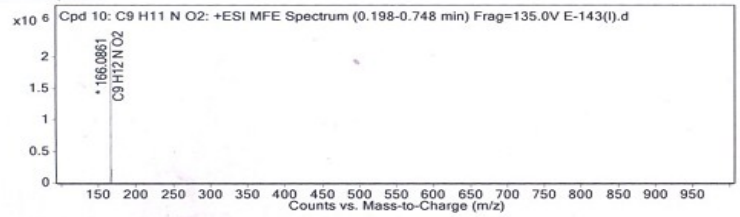
| | |
|---|---|
| **Sample Group** | **Info.** |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) |

**Compound Table**

| Compound Label | RT | Mass | Formula | MFG Formula | MFG Diff (ppm) | DB Formula |
|---|---|---|---|---|---|---|
| Cpd 10: C9 H11 N O2 | 0.292 | 165.0789 | C9 H11 N O2 | C9 H11 N O2 | 0.67 | C9 H11 N O2 |

| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 10: C9 H11 N O2 | 166.0861 | 0.292 | Find by Molecular Feature | 165.0789 |

MFE MS Spectrum




**MS Spectrum Peak List**

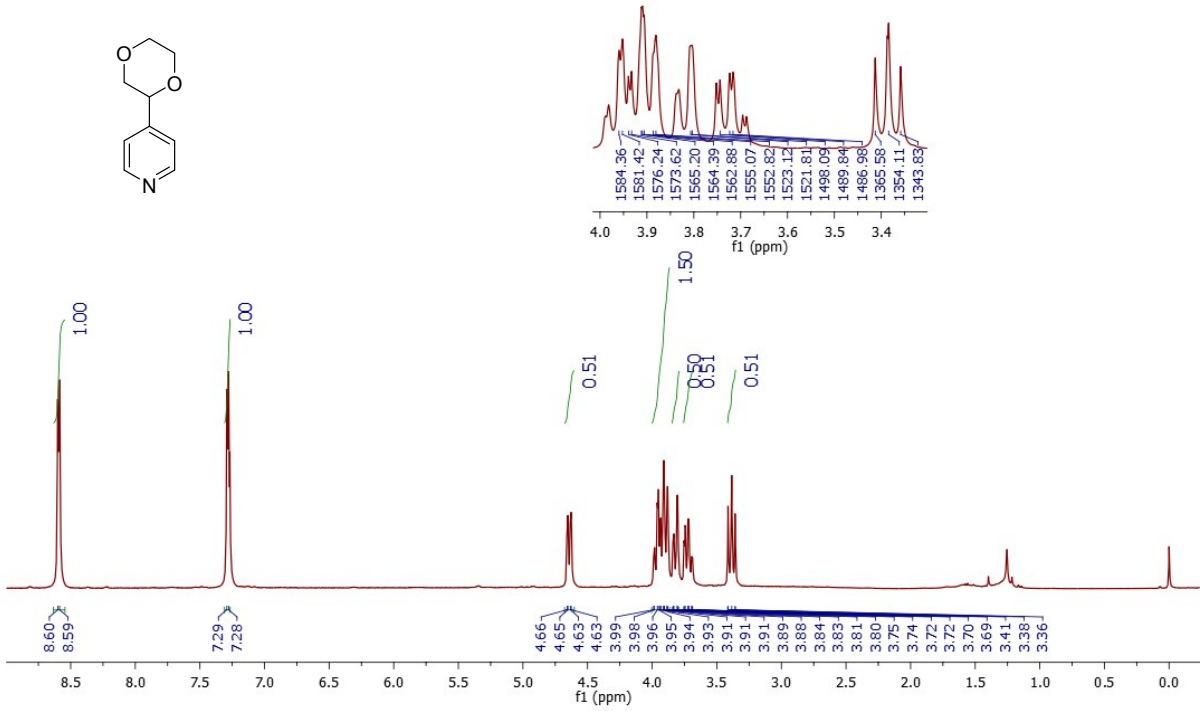
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 166.0861 | 1 | 2240720.75 | C9 H12 N O2 | (M+H)+ |
| 167.09 | 1 | 209115.8 | C9 H12 N O2 | (M+H)+ |
| 168.0921 | 1 | 13691.96 | C9 H12 N O2 | (M+H)+ |
| 169.0956 | 1 | 1565.61 | C9 H12 N O2 | (M+H)+ |

**Predicted Isotope Match Table**

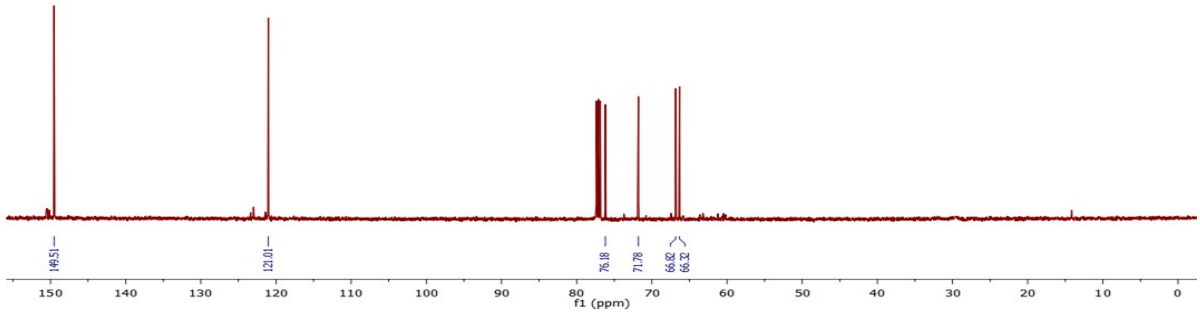
| Isotope | *m/z* | Calc m/z | Diff (ppm) | Abund % | Calc Abund % | Abund Sum % | Calc Abund Sum % |
|---|---|---|---|---|---|---|---|
| 1 | 166.0861 | 166.0863 | 1.09 | 100 | 100 | 90.9 | 89.88 |
| 2 | 167.09 | 167.0894 | -3.6 | 9.33 | 10.31 | 8.48 | 9.27 |
| 3 | 168.0921 | 168.0916 | -3.1 | 0.61 | 0.89 | 0.56 | 0.8 |
| 4 | 169.0956 | 169.0942 | -8.52 | 0.07 | 0.06 | 0.06 | 0.05 |

--- End Of Report ---

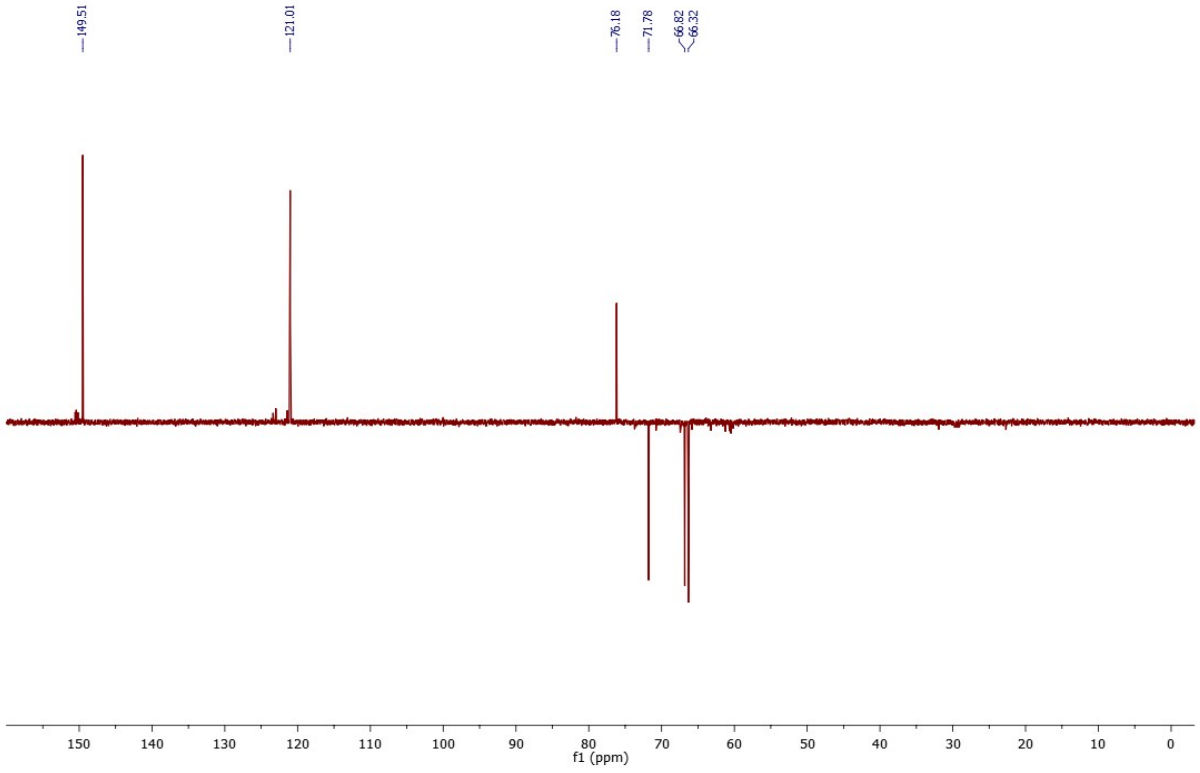
**$^{1}$H NMR of 4-(1,4-dioxan-2-yl)pyridine (3da')**



**$^{13}$C NMR of 4-(1,4-dioxan-2-yl)pyridine (3da')**



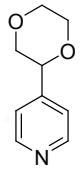

**DEPT of 4-(1,4-dioxan-2-yl)pyridine (3da')**



**HRMS of 4-(1,4-dioxan-2-yl)pyridine (3da')**

## Qualitative Compound Report

| | | | |
|---|---|---|---|
| **Data File** | E-143(II).d | **Sample Name** | E-143(II) |
| **Sample Type** | Sample | **Position** | Vial 8 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | vishal_12-01-13.m | **Acquired Time** | 10-02-2015 PM 12:27:38 |
| **IRM Calibration Status** | Success | **DA Method** | daily_report.m |
| **Comment** | | | |



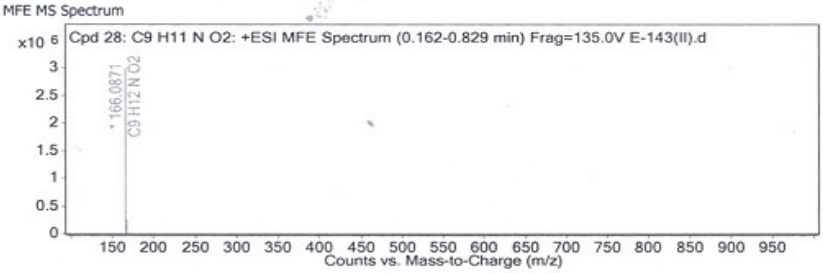
| | |
|---|---|
| **Sample Group** | **Info.** |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) |

**Compound Table**

| Compound Label | RT | Mass | Formula | MFG Formula | MFG Diff (ppm) | DB Formula |
|---|---|---|---|---|---|---|
| Cpd 28: C9 H11 N O2 | 0.279 | 165.08 | C9 H11 N O2 | C9 H11 N O2 | -6.42 | C9 H11 N O2 |

| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 28: C9 H11 N O2 | 166.0871 | 0.279 | Find by Molecular Feature | 165.08 |

MFE MS Spectrum




**MS Spectrum Peak List**

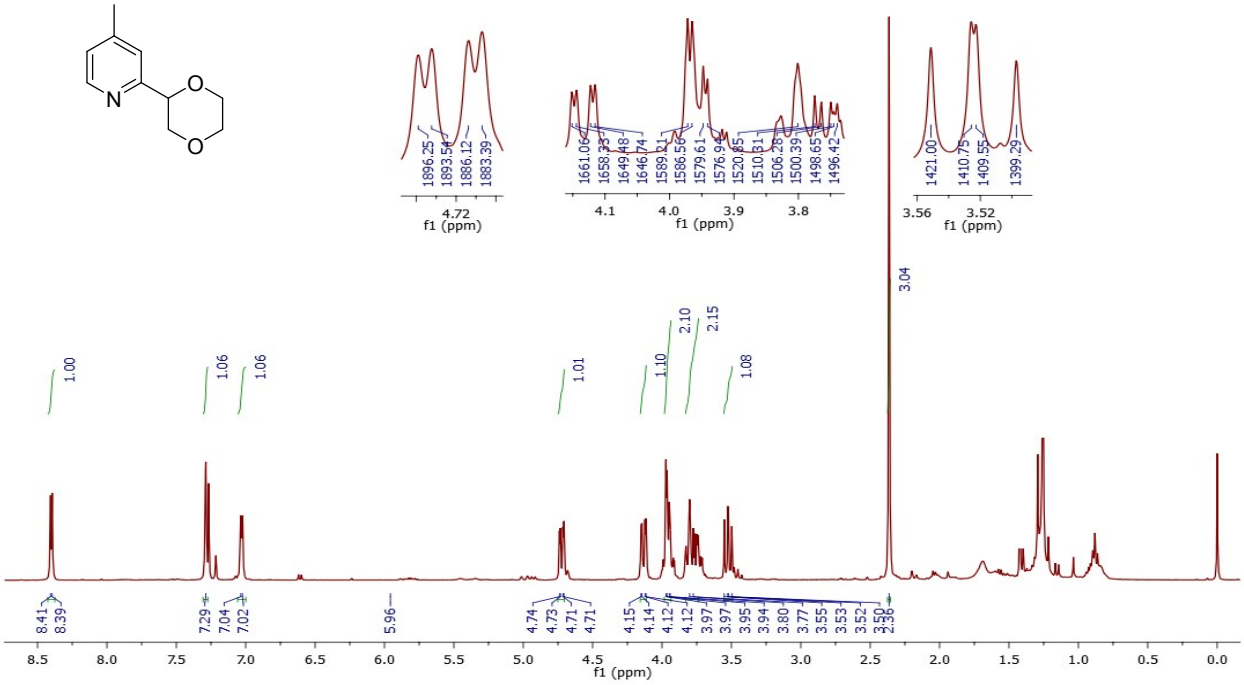
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 166.0871 | 1 | 3003842.5 | C9 H12 N O2 | (M+H)+ |
| 167.0931 | 1 | 261764.97 | C9 H12 N O2 | (M+H)+ |
| 168.0947 | 1 | 20601.63 | C9 H12 N O2 | (M+H)+ |

**Predicted Isotope Match Table**

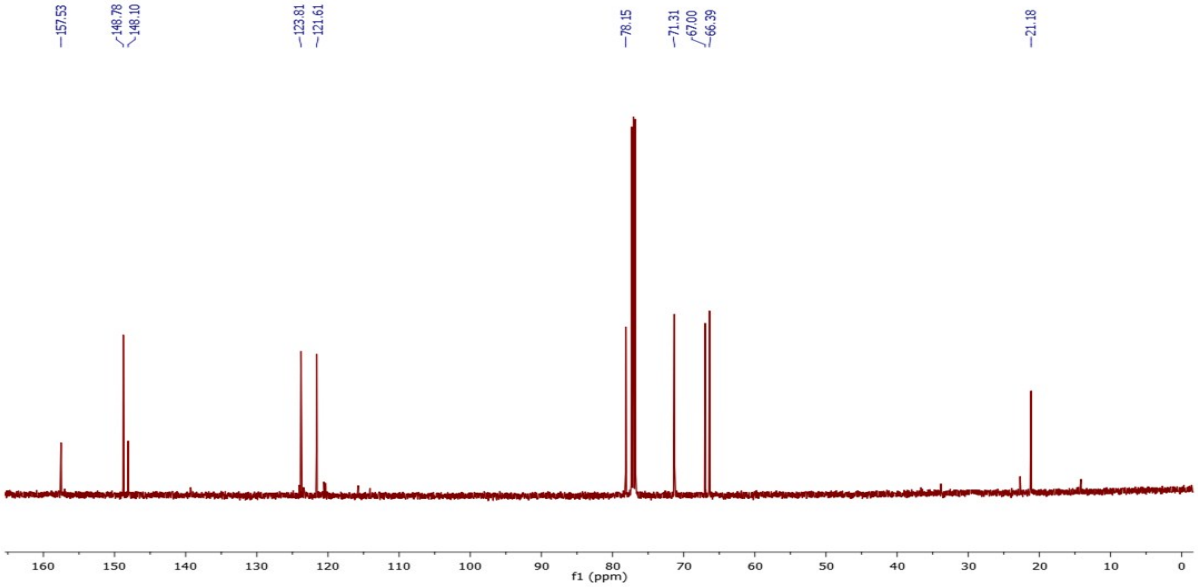
| Isotope | *m/z* | Calc m/z | Diff (ppm) | Abund % | Calc Abund % | Abund Sum % | Calc Abund Sum % |
|---|---|---|---|---|---|---|---|
| 1 | 166.0871 | 166.0863 | -4.9 | 100 | 100 | 91.41 | 89.93 |
| 2 | 167.0931 | 167.0894 | -22.19 | 8.71 | 10.31 | 7.97 | 9.27 |
| 3 | 168.0947 | 168.0916 | -18.41 | 0.69 | 0.89 | 0.63 | 0.8 |

--- End Of Report ---

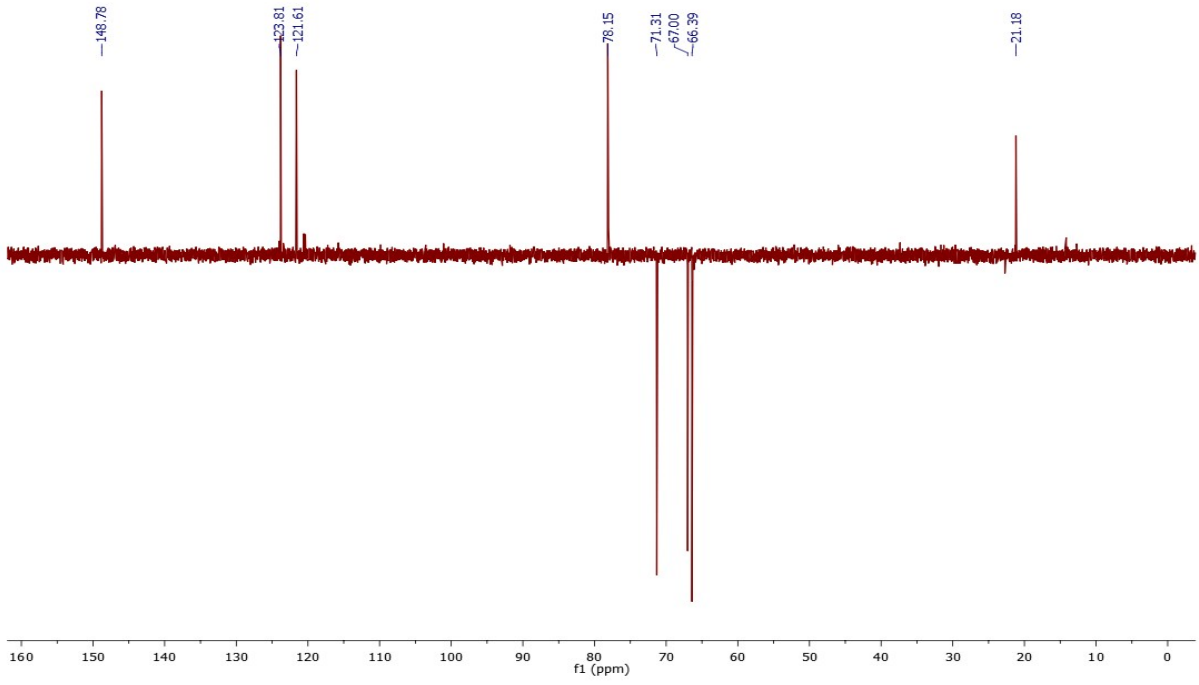
**[1]H NMR of 2-(1,4-dioxan-2-yl)-4-methylpyridine (3ea)**



**$^{13}$C NMR of 2-(1,4-dioxan-2-yl)-4-methylpyridine (3ea)**



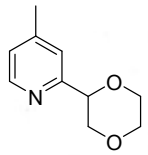

**DEPT of 2-(1,4-dioxan-2-yl)-4-methylpyridine (3ea)**



**HRMS of 2-(1,4-dioxan-2-yl)-4-methylpyridine (3ea)**

## Qualitative Compound Report

| | | | |
|---|---|---|---|
| **Data File** | E-170.d | **Sample Name** | E-170 |
| **Sample Type** | Sample | **Position** | Vial 12 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | vishal_12-01-13.m | **Acquired Time** | 04-02-2015 PM 1:58:15 |
| **IRM Calibration Status** | Success | **DA Method** | daily_report.m |
| **Comment** | | | |



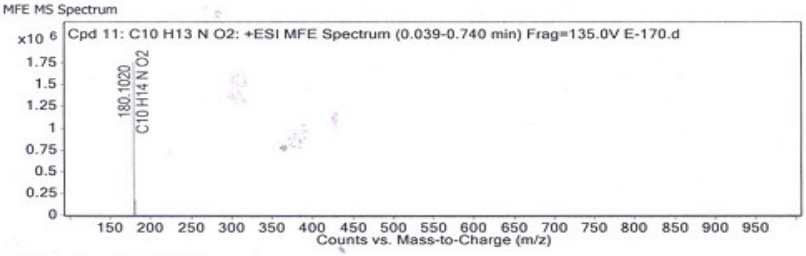

| | |
|---|---|
| **Sample Group** | **Info.** |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) |

**Compound Table**

| Compound Label | RT | Mass | Formula | MFG Formula | MFG Diff (ppm) | DB Formula |
|---|---|---|---|---|---|---|
| Cpd 11: C10 H13 N O2 | 0.292 | 179.0948 | C10 H13 N O2 | C10 H13 N O2 | -0.87 | C10 H13 N O2 |

| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 11: C10 H13 N O2 | 180.102 | 0.292 | Find by Molecular Feature | 179.0948 |

MFE MS Spectrum




**MS Spectrum Peak List**

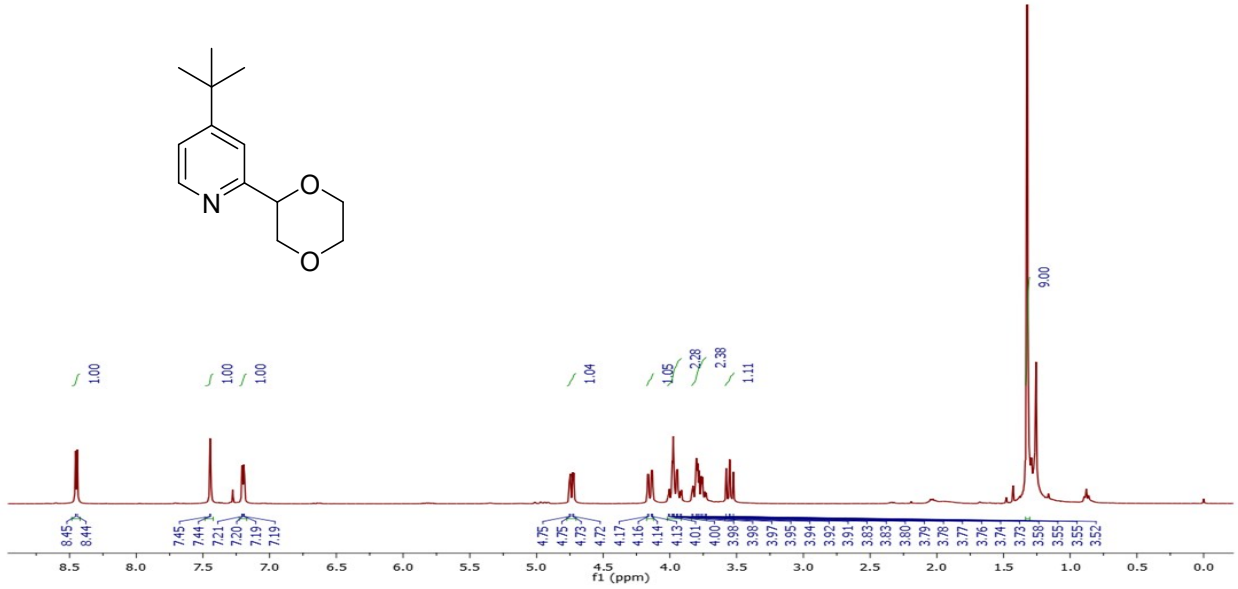
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 180.102 | 1 | 1760240.38 | C10 H14 N O2 | (M+H)+ |
| 181.1058 | 1 | 181487.97 | C10 H14 N O2 | (M+H)+ |
| 182.108 | 1 | 14387.18 | C10 H14 N O2 | (M+H)+ |
| 183.1066 | 1 | 1322.15 | C10 H14 N O2 | (M+H)+ |

**Predicted Isotope Match Table**

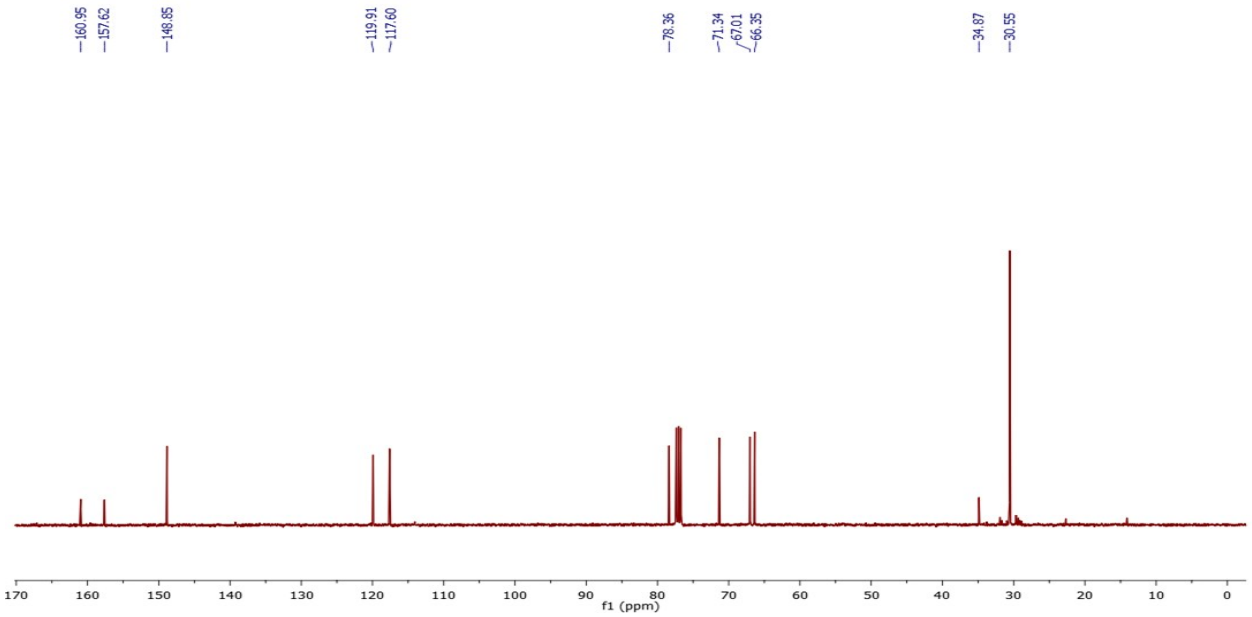
| Isotope | *m/z* | Calc m/z | Diff (ppm) | Abund % | Calc Abund % | Abund Sum % | Calc Abund Sum % |
|---|---|---|---|---|---|---|---|
| 1 | 180.102 | 180.1019 | -0.58 | 100 | 100 | 89.93 | 88.9 |
| 2 | 181.1058 | 181.1051 | -3.58 | 10.31 | 11.42 | 9.27 | 10.15 |
| 3 | 182.108 | 182.1074 | -3.12 | 0.82 | 1 | 0.74 | 0.89 |
| 4 | 183.1066 | 183.1099 | 18.4 | 0.08 | 0.07 | 0.07 | 0.06 |

--- End Of Report ---

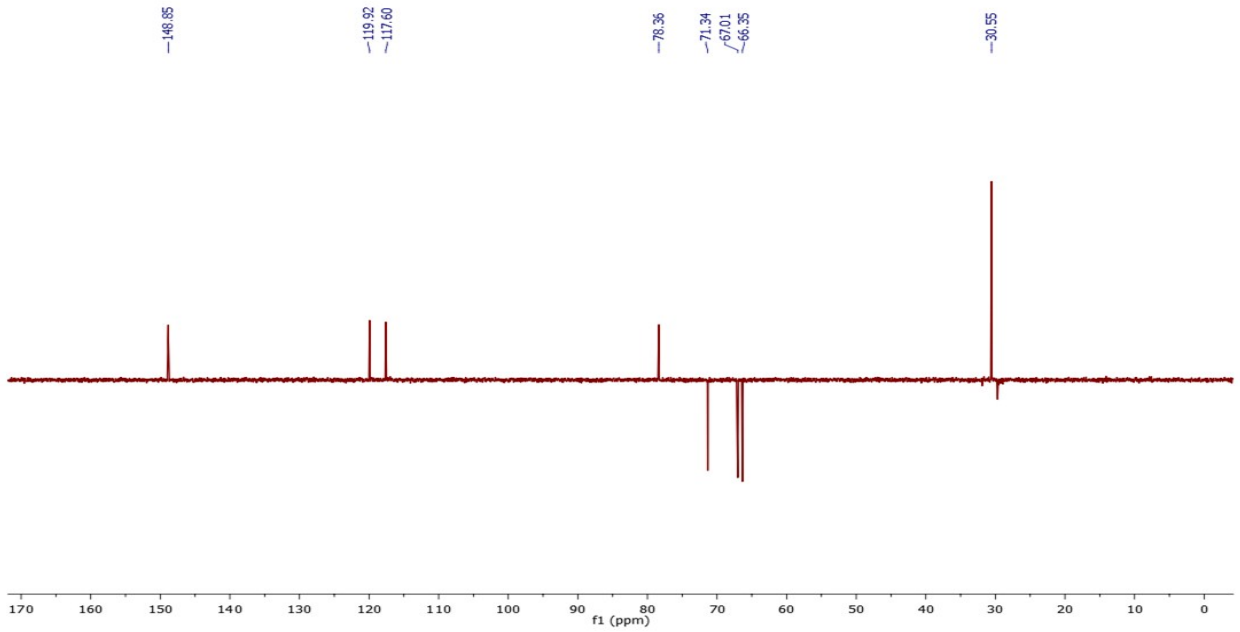
**$^{1}$H NMR of 4-(tert-butyl)-2-(1,4-dioxan-2-yl)pyridine (3fa)**



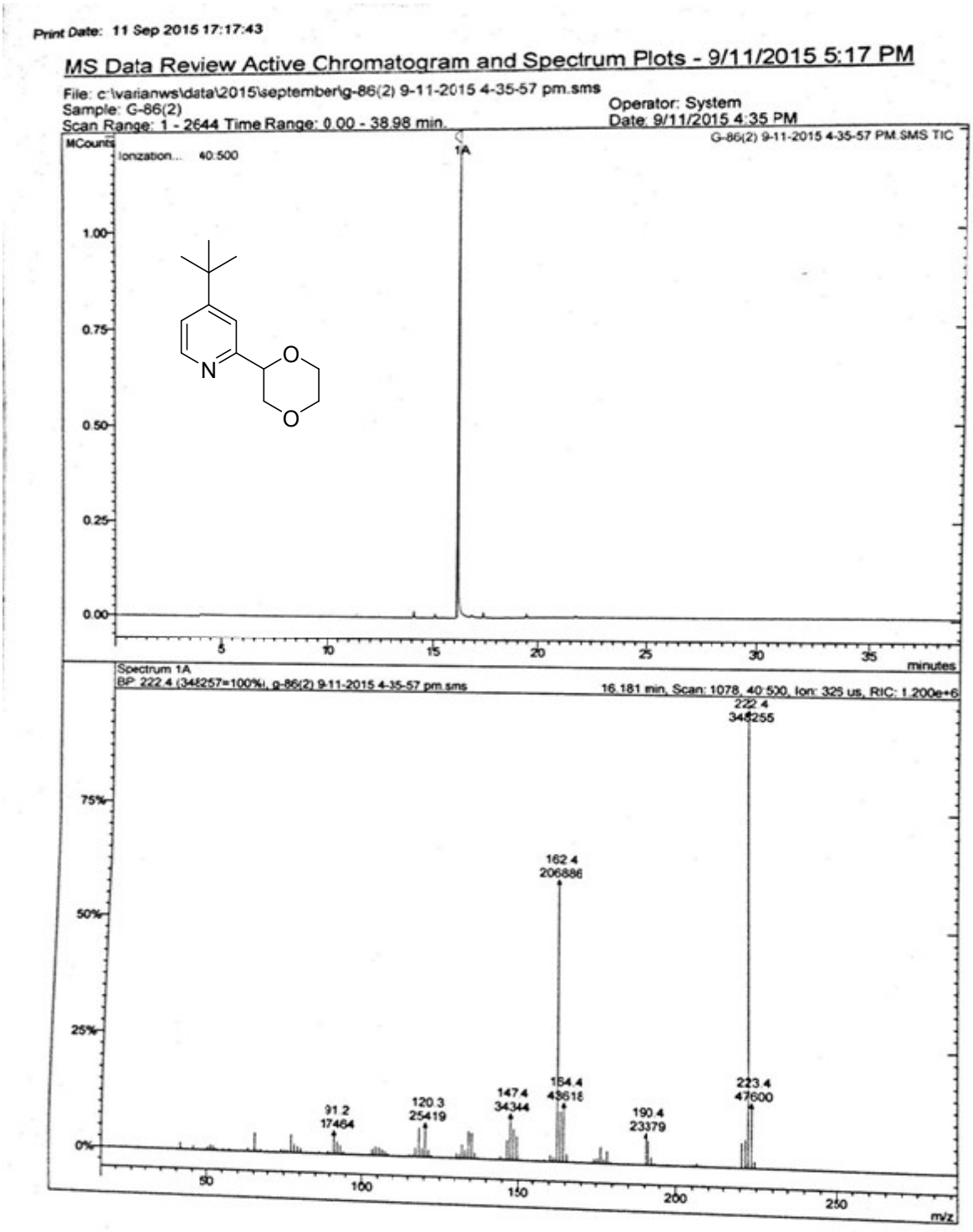
**$^{13}$C NMR of 4-(tert-butyl)-2-(1,4-dioxan-2-yl)pyridine (3fa)**



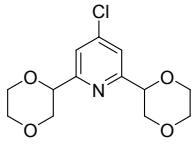

**DEPT of 4-(tert-butyl)-2-(1,4-dioxan-2-yl)pyridine (3fa)**

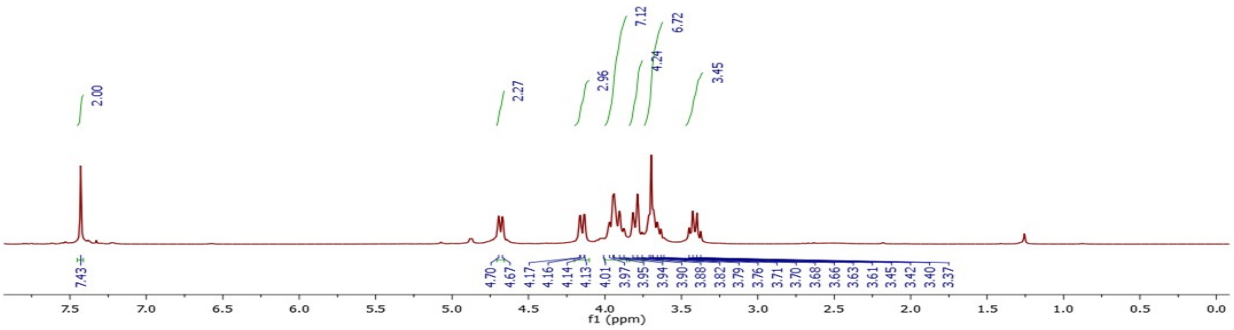


**GC-MS of 4-(tert-butyl)-2-(1,4-dioxan-2-yl)pyridine (3fa)**

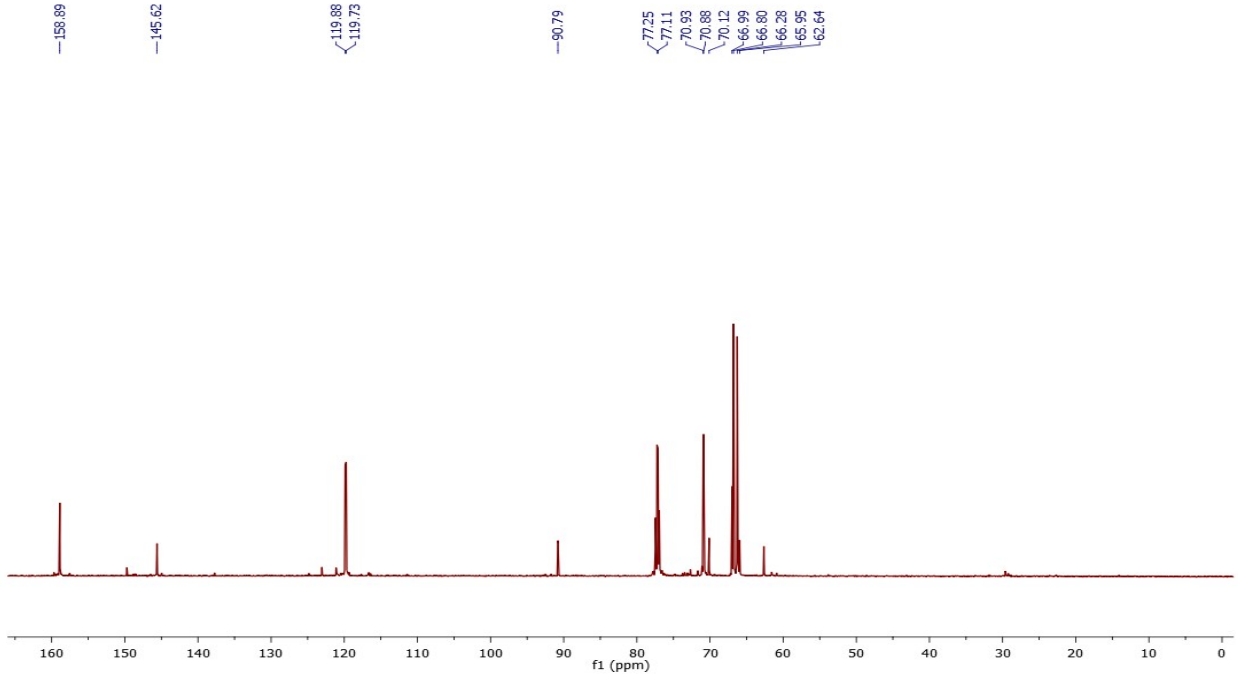


**$^{1}$H NMR of 4-chloro-2,6-di(1,4-dioxan-2-yl)pyridine (3ga)**

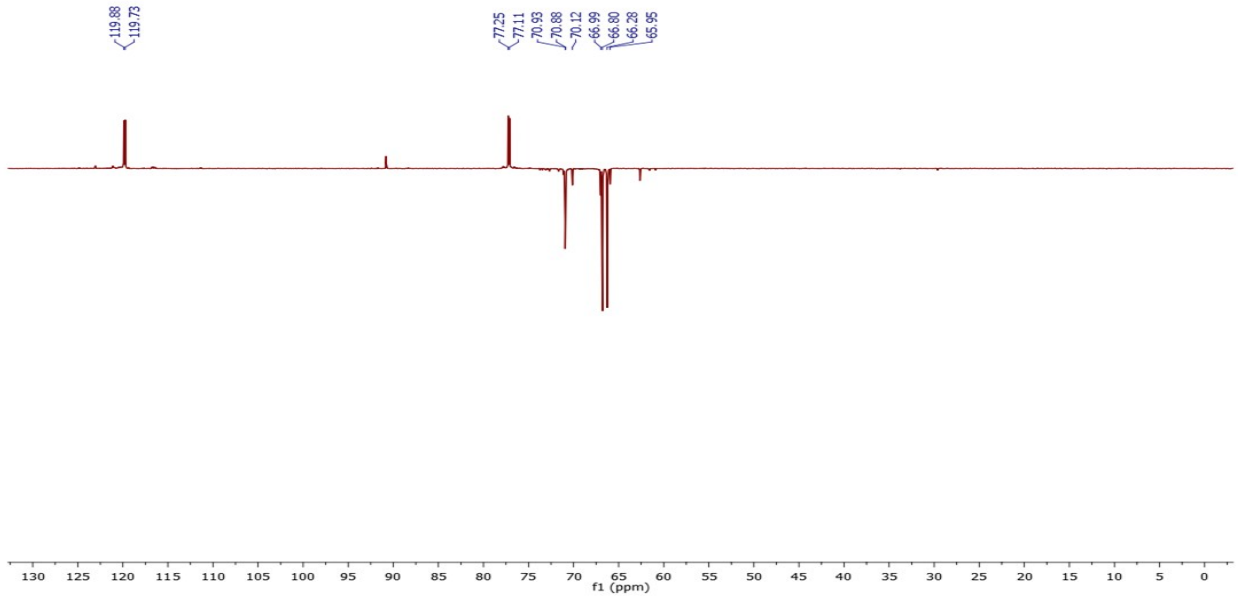


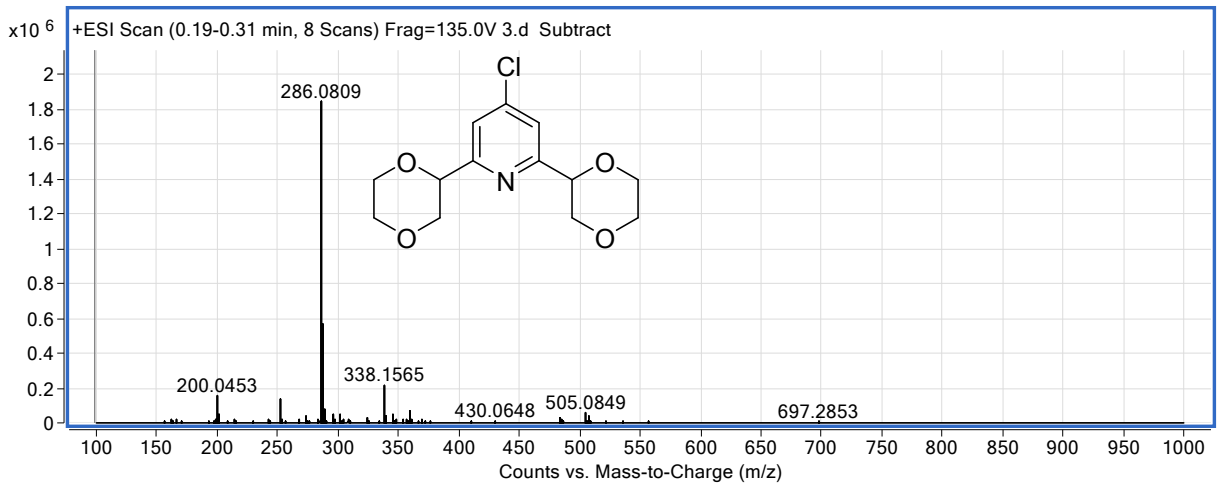
**$^{13}$C NMR of 44-chloro-2,6-di(1,4-dioxan-2-yl)pyridine (3ga)**



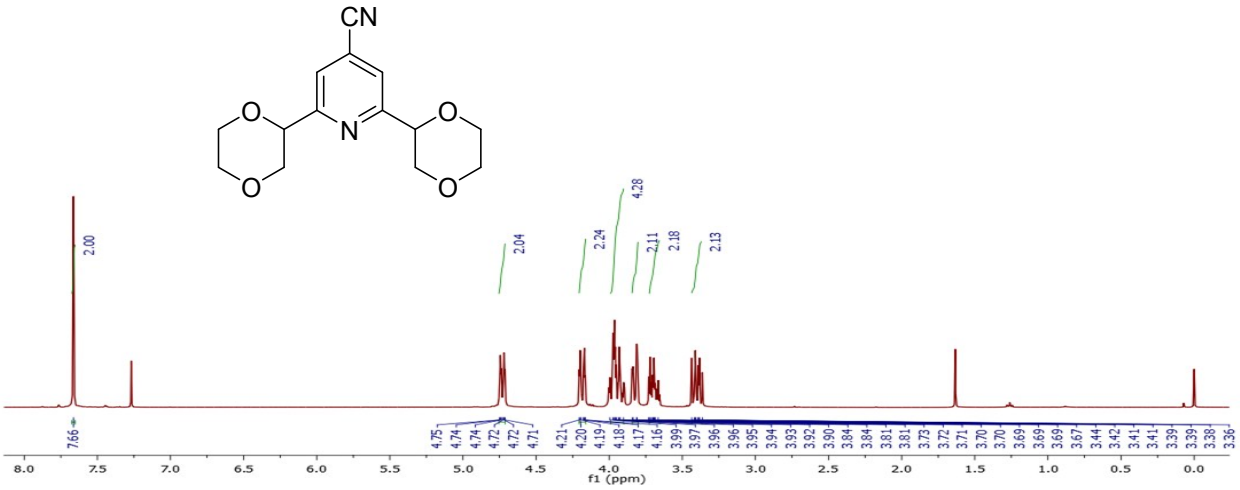

**DEPT of 4-chloro-2,6-di(1,4-dioxan-2-yl)pyridine (3ga)**



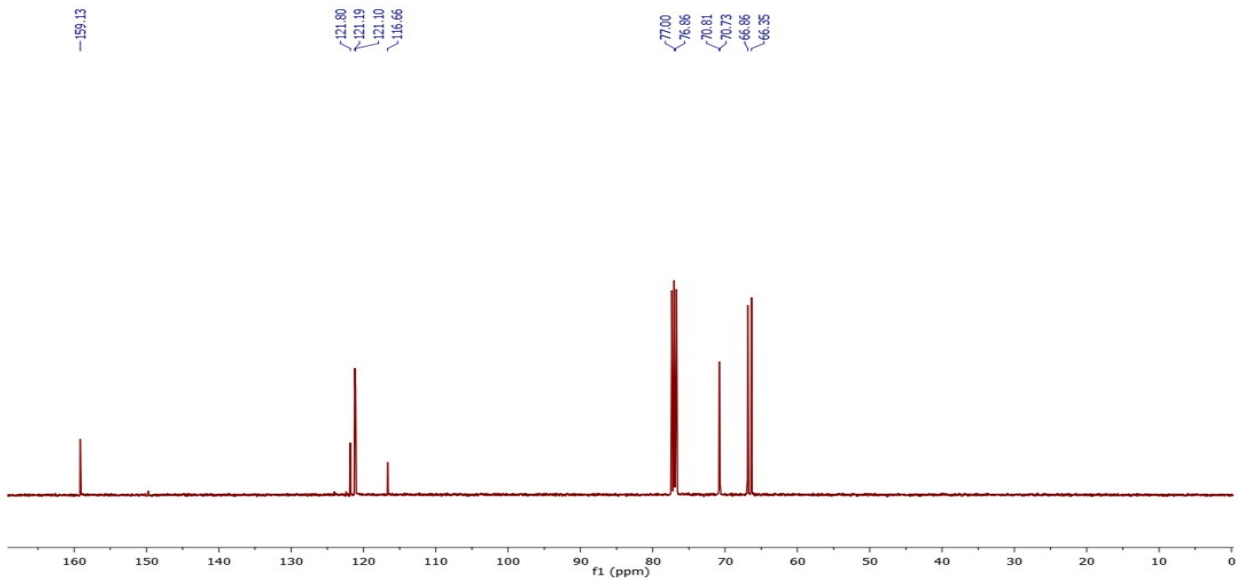
## LC-MS of 4-chloro-2,6-di(1,4-dioxan-2-yl)pyridine (3ga)



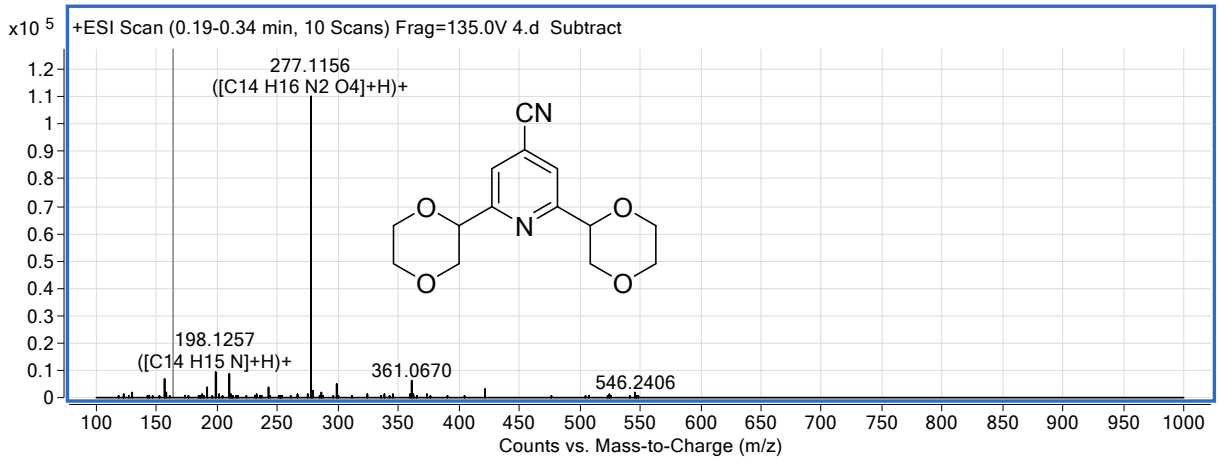

## $^1$H NMR of 2,6-di(1,4-dioxan-2-yl)isonicotinonitrile (3ha)



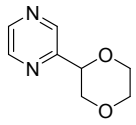
## $^{13}$C NMR of 2,6-di(1,4-dioxan-2-yl)isonicotinonitrile (3ha)

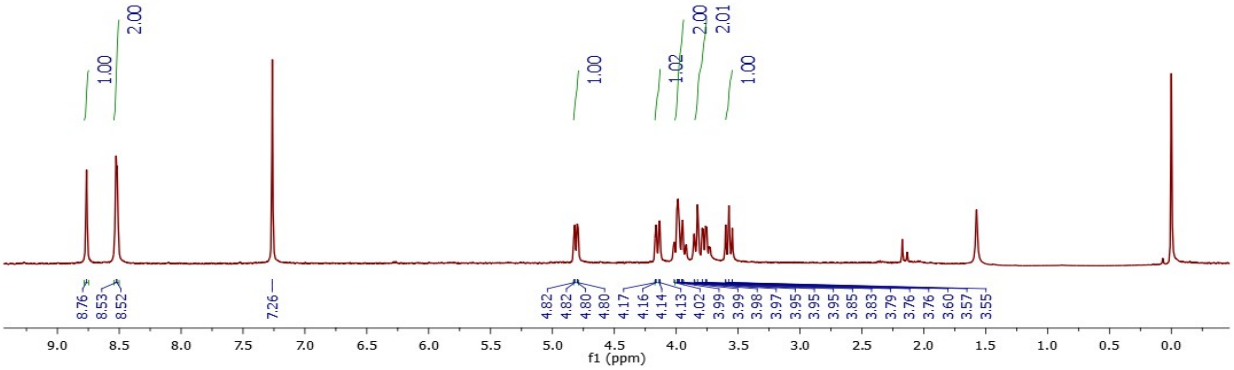



## LC-MS of 2,6-di(1,4-dioxan-2-yl)isonicotinonitrile (3ha)

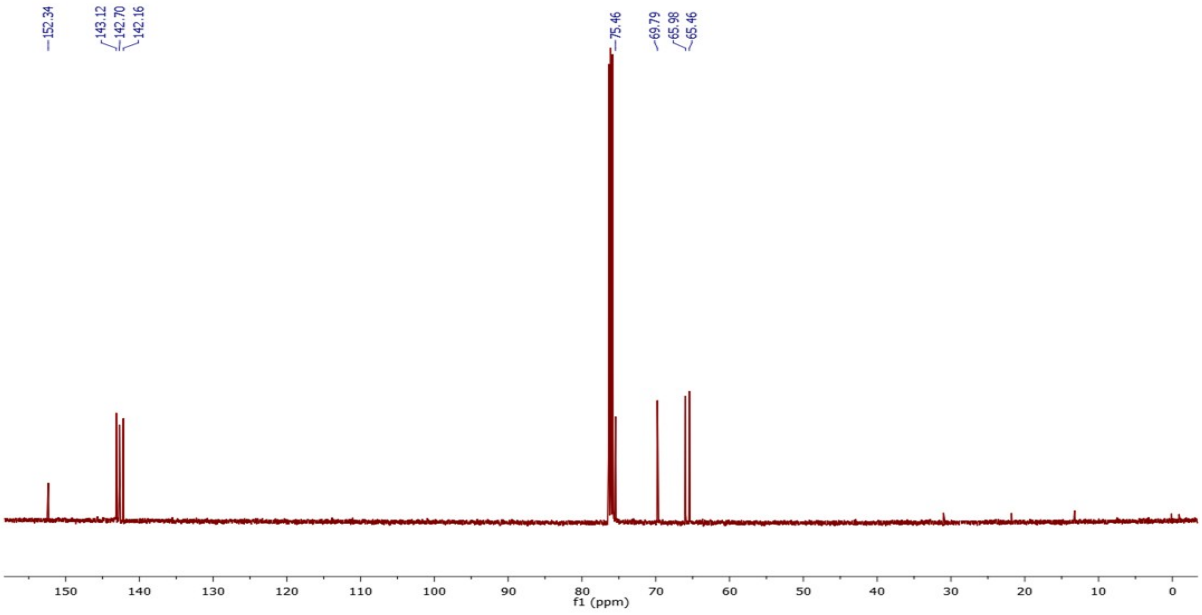


**$^1$H NMR of 2-(1,4-dioxan-2-yl)pyrazine (3ia)**

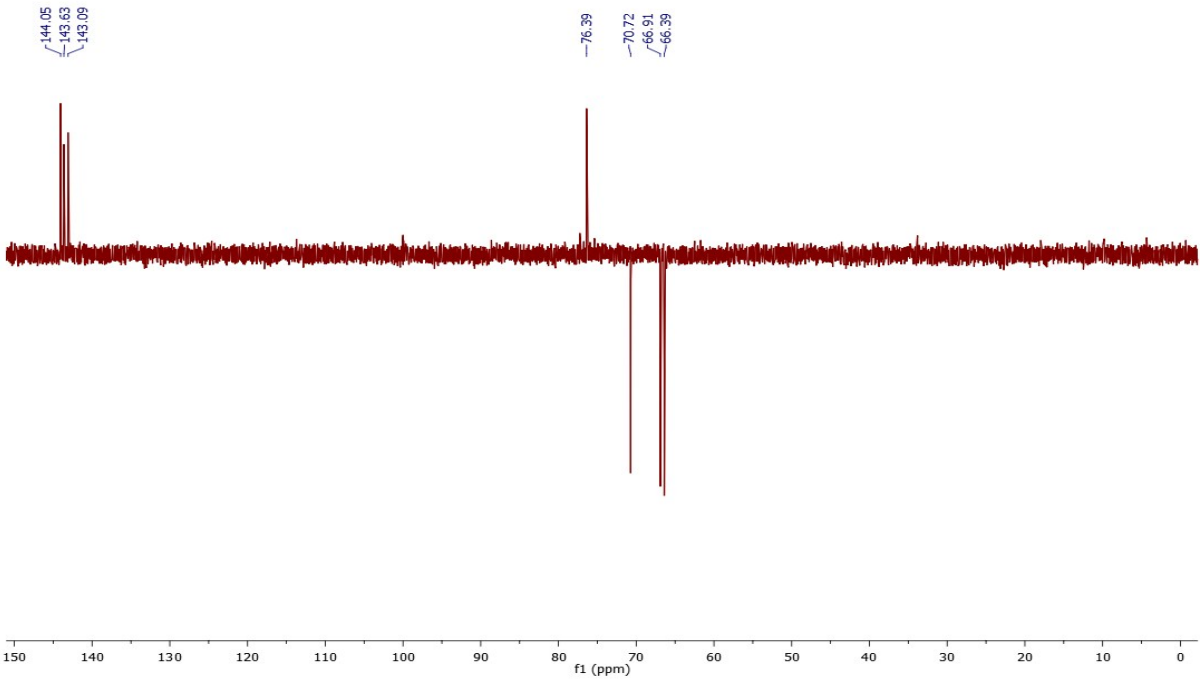


**$^{13}$C NMR of 2-(1,4-dioxan-2-yl)pyrazine (3ia)**




**DEPT of 2-(1,4-dioxan-2-yl)pyrazine (3ia)**

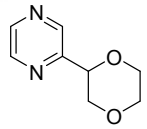


**HRMS of 2-(1,4-dioxan-2-yl)pyrazine (3ia)**

## Qualitative Compound Report

| | | | |
|---|---|---|---|
| **Data File** | E-94.d | **Sample Name** | E-94 |
| **Sample Type** | Sample | **Position** | Vial 20 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | vishal_12-01-13.m | **Acquired Time** | 07-02-2015 PM 1:01:41 |
| **IRM Calibration Status** | Success | **DA Method** | daily_report.m |
| **Comment** | | | |

| | |
|---|---|
| **Sample Group** | **Info.** |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) |

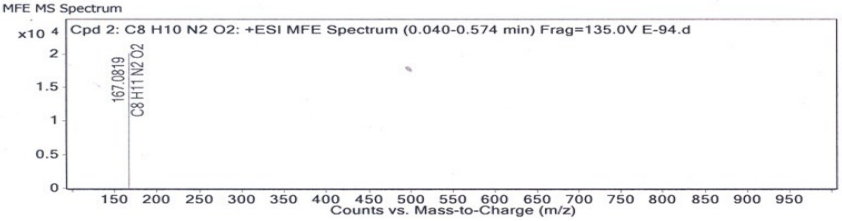



**Compound Table**

| Compound Label | RT | Mass | Formula | MFG Formula | MFG Diff (ppm) | DB Formula |
|---|---|---|---|---|---|---|
| Cpd 2: C8 H10 N2 O2 | 0.274 | 166.0749 | C8 H10 N2 O2 | C8 H10 N2 O2 | -3.76 | C8 H10 N2 O2 |

| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 2: C8 H10 N2 O2 | 167.0819 | 0.274 | Find by Molecular Feature | 166.0749 |

MFE MS Spectrum




**MS Spectrum Peak List**

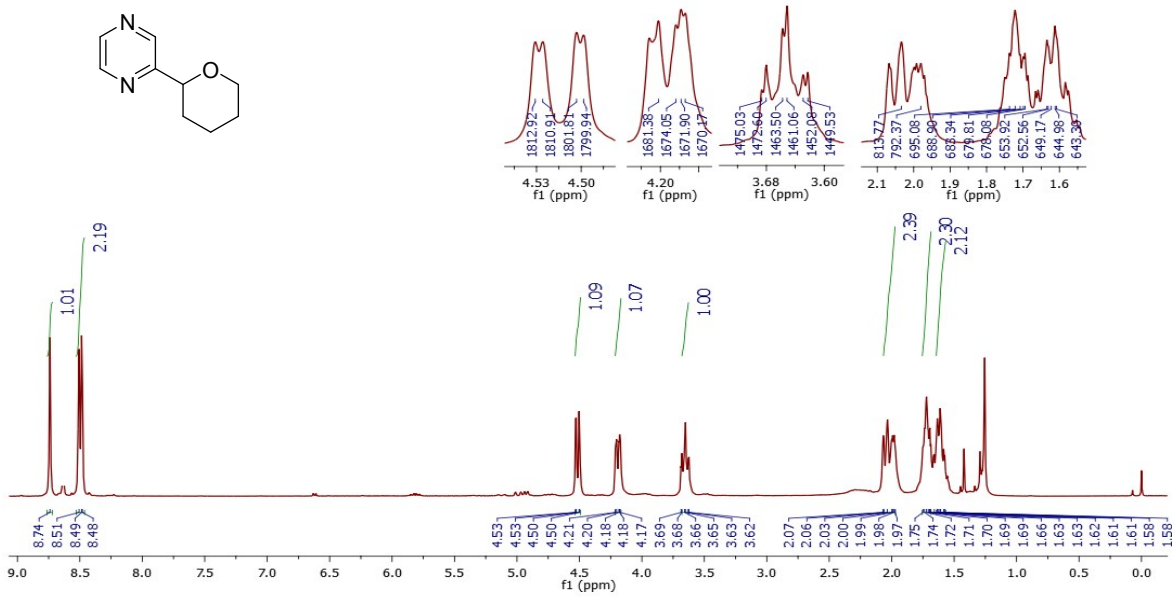
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 167.0819 | 1 | 20138.78 | C8 H11 N2 O2 | (M+H)+ |
| 168.0871 | 1 | 2421.31 | C8 H11 N2 O2 | (M+H)+ |

**Predicted Isotope Match Table**

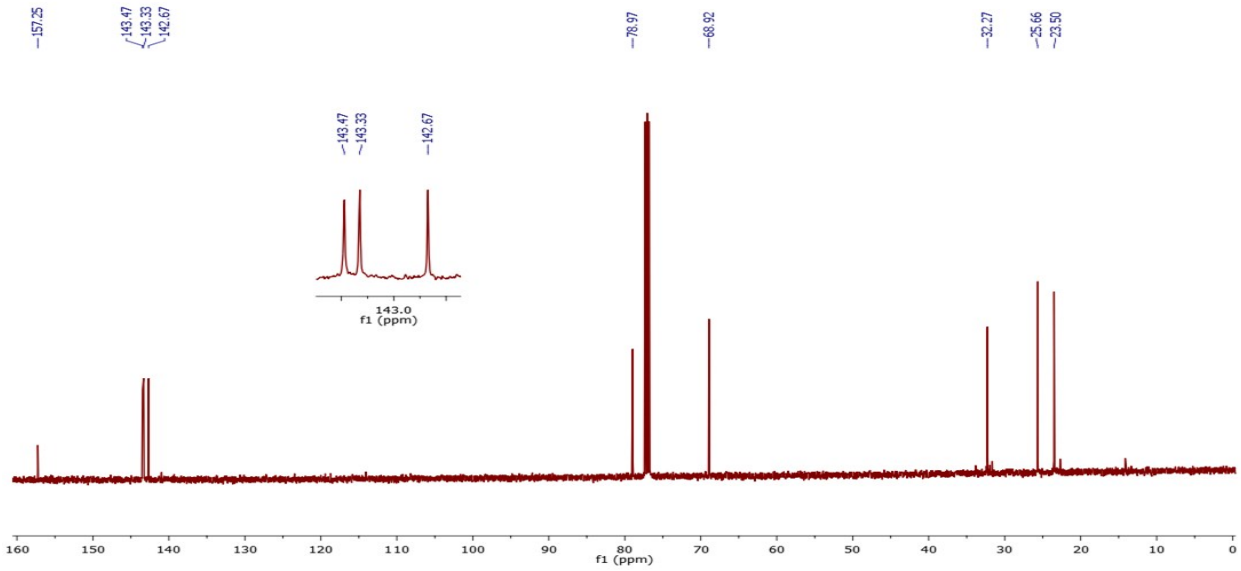
| Isotope | *m/z* | Calc m/z | Diff (ppm) | Abund % | Calc Abund % | Abund Sum % | Calc Abund Sum % |
|---|---|---|---|---|---|---|---|
| 1 | 167.0819 | 167.0815 | -2.29 | 100 | 100 | 89.27 | 91.25 |
| 2 | 168.0871 | 168.0844 | -15.64 | 12.02 | 9.59 | 10.73 | 8.75 |

--- End Of Report ---

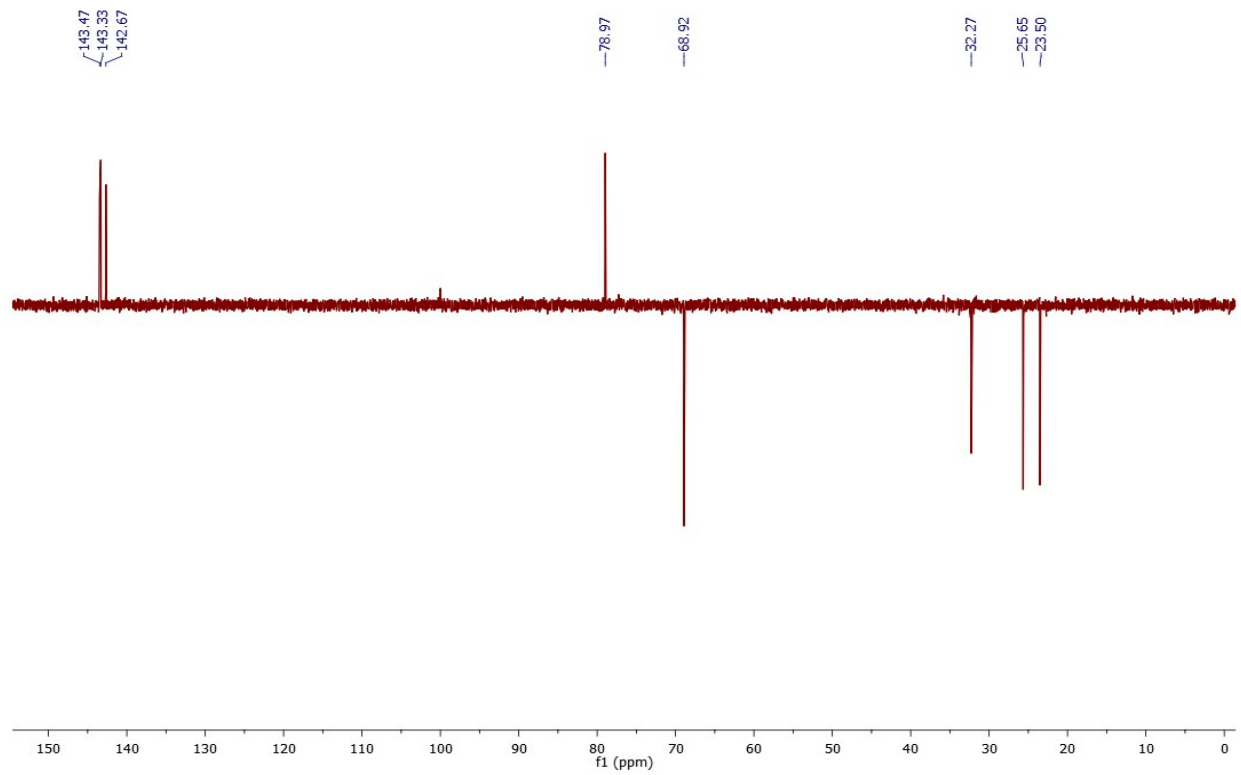
**[1]H NMR of 2-(tetrahydro-2H-pyran-2-yl)pyrazine (3ic)**



**$^{13}$C NMR of 2-(tetrahydro-2H-pyran-2-yl)pyrazine (3ic)**




**DEPT of 2-(tetrahydro-2H-pyran-2-yl)pyrazine (3ic)**

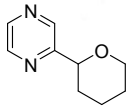


**HRMS of 2-(tetrahydro-2H-pyran-2-yl)pyrazine (3ic)**

## Qualitative Compound Report

| | | | |
|---|---|---|---|
| **Data File** | E-127.d | **Sample Name** | E-127 |
| **Sample Type** | Sample | **Position** | Vial 19 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | vishal_12-01-13.m | **Acquired Time** | 04-02-2015 PM 2:35:55 |
| **IRM Calibration Status** | Success | **DA Method** | daily_report.m |
| **Comment** | | | |

| | |
|---|---|
| **Sample Group** | **Info.** |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) |

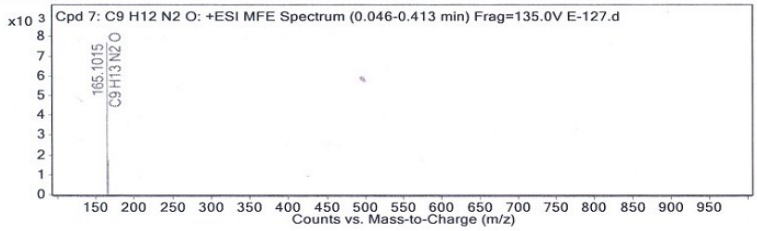



**Compound Table**

| Compound Label | RT | Mass | Formula | MFG Formula | MFG Diff (ppm) | DB Formula |
|---|---|---|---|---|---|---|
| Cpd 7: C9 H12 N2 O | 0.283 | 164.0926 | C9 H12 N2 O | C9 H12 N2 O | 14.32 | C9 H12 N2 O |

| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 7: C9 H12 N2 O | 165.1015 | 0.283 | Find by Molecular Feature | 164.0926 |

MFE MS Spectrum




**MS Spectrum Peak List**

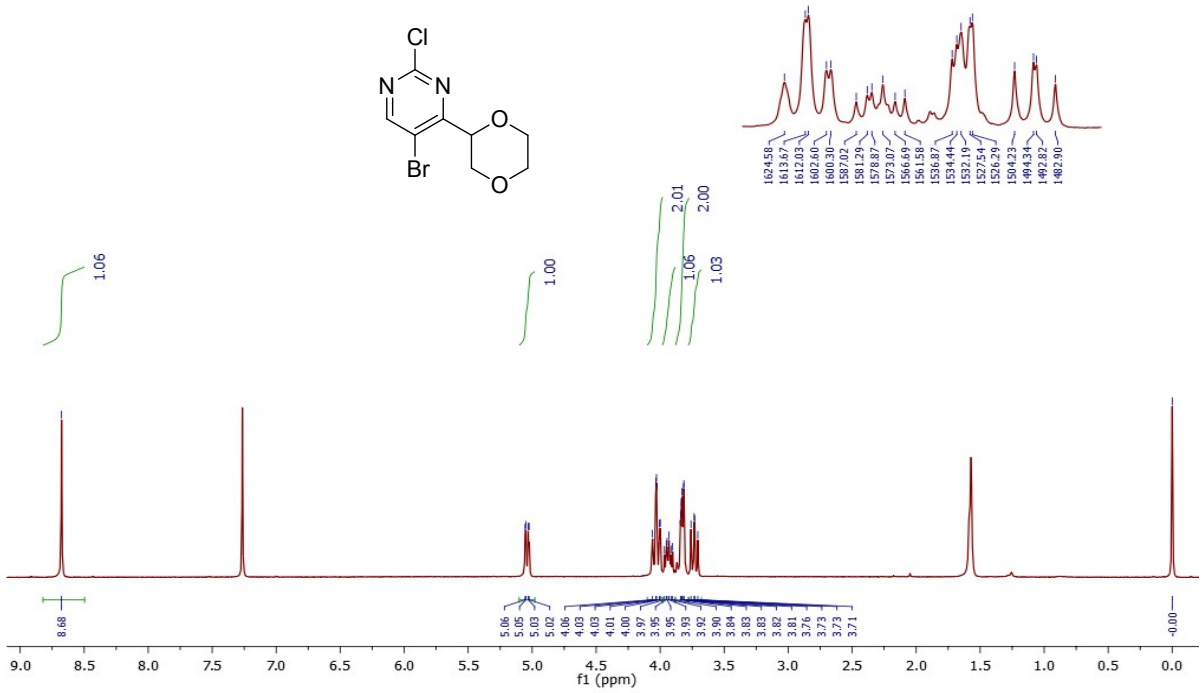
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 165.1015 | 1 | 7720.58 | C9 H13 N2 O | (M+H)+ |
| 166.0958 | 1 | 1755.7 | C9 H13 N2 O | (M+H)+ |

**Predicted Isotope Match Table**

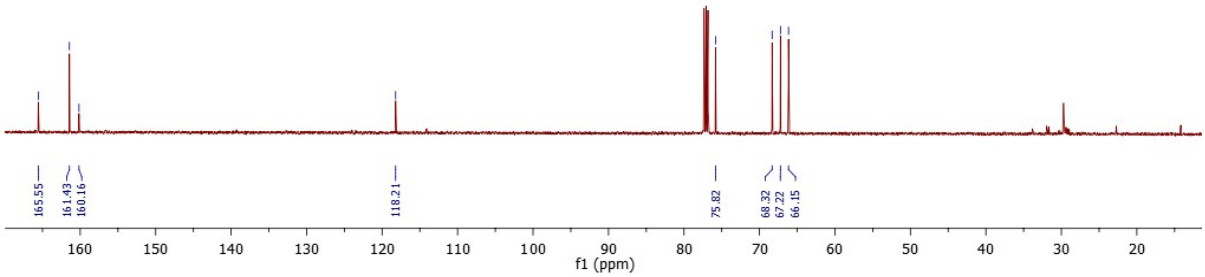
| Isotope | *m/z* | Calc m/z | Diff (ppm) | Abund % | Calc Abund % | Abund Sum % | Calc Abund Sum % |
|---|---|---|---|---|---|---|---|
| 1 | 165.1015 | 165.1022 | 4.56 | 100 | 100 | 81.47 | 90.37 |
| 2 | 166.0958 | 166.1052 | 56.43 | 22.74 | 10.65 | 18.53 | 9.63 |

--- End Of Report ---

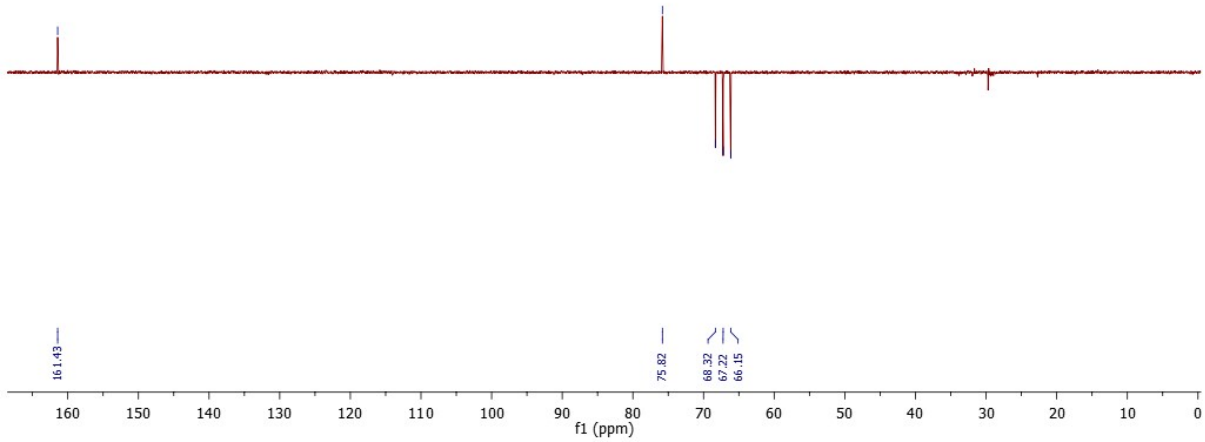
**$^{1}$H NMR of 5-bromo-2-chloro-4-(1,4-dioxan-2-yl)pyrimidine (3ja)**



**$^{13}$C NMR of 5-bromo-2-chloro-4-(1,4-dioxan-2-yl)pyrimidine (3ja)**



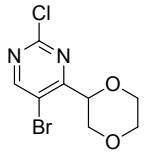

**DEPT NMR of 5-bromo-2-chloro-4-(1,4-dioxan-2-yl)pyrimidine (3ja)**



**HRMS of 5-bromo-2-chloro-4-(1,4-dioxan-2-yl)pyrimidine (3ja)**

## Qualitative Compound Report

| | | | |
|---|---|---|---|
| **Data File** | 2cl5BrPy-DO.d | **Sample Name** | 2cl5BrPy-DO |
| **Sample Type** | Sample | **Position** | Vial 17 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | vishal_12-01-13.m | **Acquired Time** | 03-02-2015 PM 2:43:05 |
| **IRM Calibration Status** | Success | **DA Method** | daily_report.m |
| **Comment** | | | |
| **Sample Group** | | **Info.** | |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) | | |

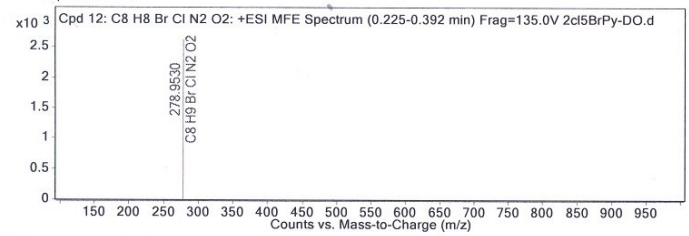



**Compound Table**

| Compound Label | RT | Mass | Formula | MFG Formula | MFG Diff (ppm) | DB Formula |
|---|---|---|---|---|---|---|
| Cpd 12: C8 H8 Br Cl N2 O2 | 0.292 | 277.9457 | C8 H8 Br Cl N2 O2 | C8 H8 Br Cl N2 O2 | 0.33 | C8 H8 Br Cl N2 O2 |

| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 12: C8 H8 Br Cl N2 O2 | 278.953 | 0.292 | Find by Molecular Feature | 277.9457 |

MFE MS Spectrum




**MS Spectrum Peak List**

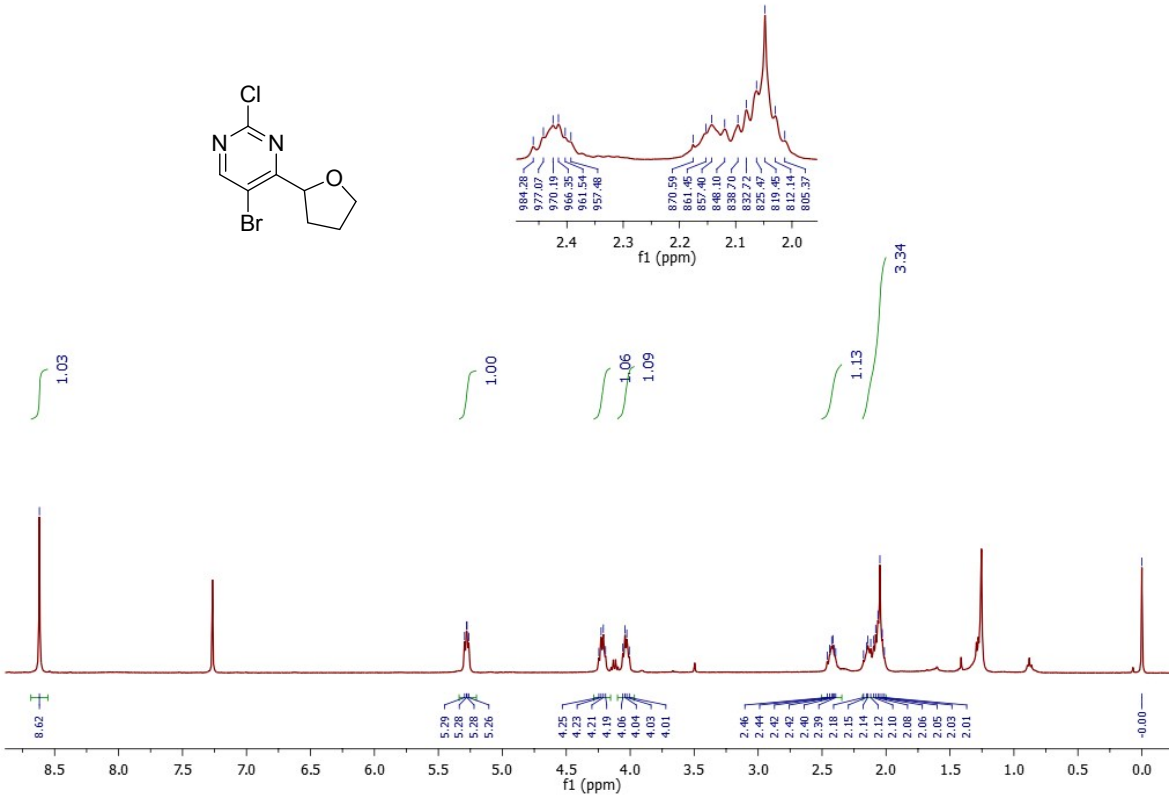
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 278.953 | 1 | 2612.92 | C8 H9 Br Cl N2 O2 | (M+H)+ |

**Predicted Isotope Match Table**

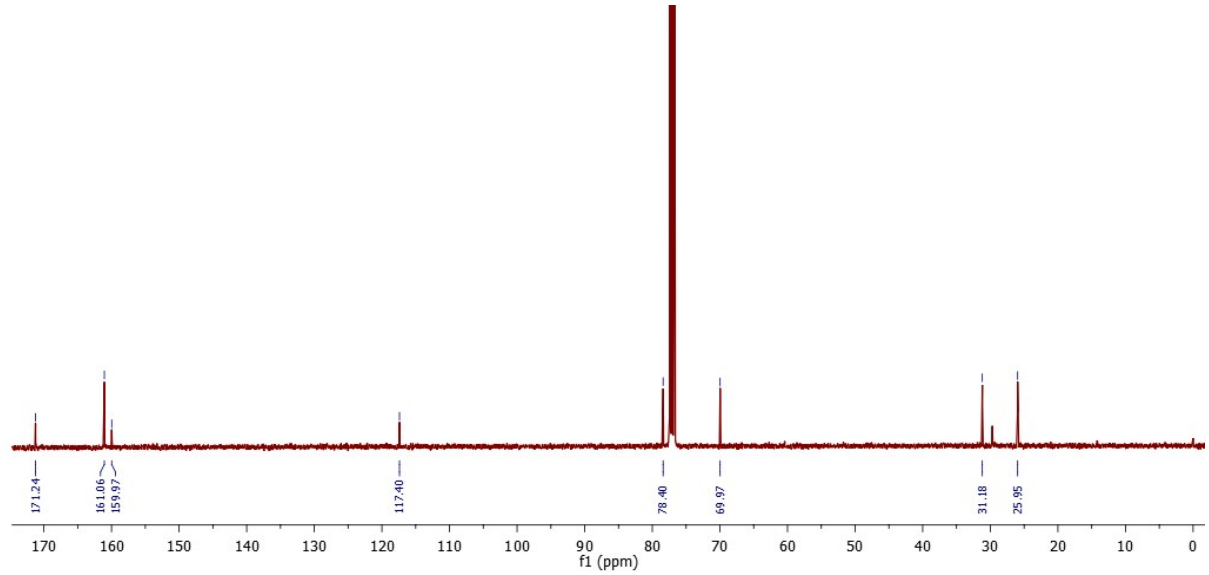
| Isotope | *m/z* | Calc m/z | Diff (ppm) | Abund % | Calc Abund % | Abund Sum % | Calc Abund Sum % |
|---|---|---|---|---|---|---|---|
| 1 | 278.953 | 278.953 | 0.32 | 100 | 100 | 100 | 100 |

--- End Of Report ---

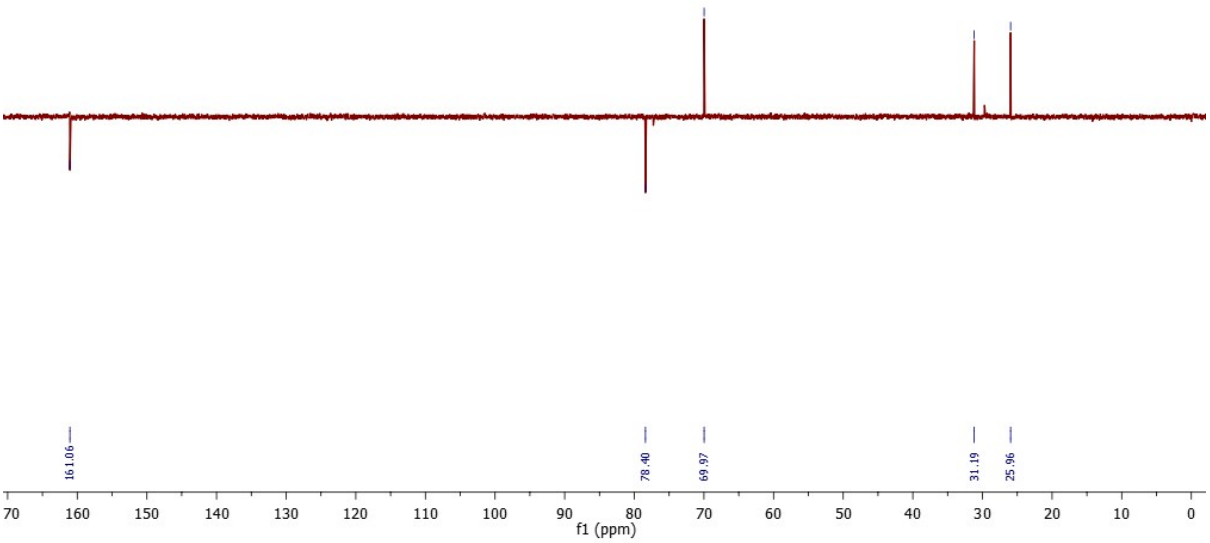
**$^{1}$H NMR of 5-bromo-2-chloro-4-(tetrahydrofuran-2-yl)pyrimidine (3jb)**



**$^{13}$C NMR of 5-bromo-2-chloro-4-(tetrahydrofuran-2-yl)pyrimidine (3jb)**




**DEPT of 5-bromo-2-chloro-4-(tetrahydrofuran-2-yl)pyrimidine (3jb)**

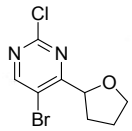


## HRMS of 5-bromo-2-chloro-4-(tetrahydrofuran-2-yl)pyrimidine (3jb)

### Qualitative Compound Report

| | | | |
|---|---|---|---|
| **Data File** | 2cl5Br-THF.d | **Sample Name** | 2cl5Br-THF |
| **Sample Type** | Sample | **Position** | Vial 18 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | vishal_12-01-13.m | **Acquired Time** | 03-02-2015 PM 2:47:22 |
| **IRM Calibration Status** | Success | **DA Method** | daily_report.m |
| **Comment** | | | |

| | |
|---|---|
| **Sample Group** | **Info.** |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) |

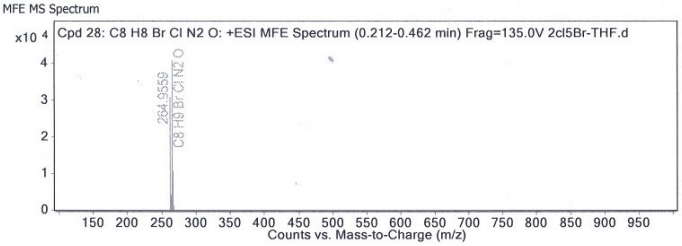



**Compound Table**

| Compound Label | RT | Mass | Formula | MFG Formula | MFG Diff (ppm) | DB Formula |
|---|---|---|---|---|---|---|
| Cpd 28: C8 H8 Br Cl N2 O | 0.287 | 261.9509 | C8 H8 Br Cl N2 O | C8 H8 Br Cl N2 O | 0 | C8 H8 Br Cl N2 O |

| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 28: C8 H8 Br Cl N2 O | 262.958 | 0.287 | Find by Molecular Feature | 261.9509 |

MFE MS Spectrum




**MS Spectrum Peak List**

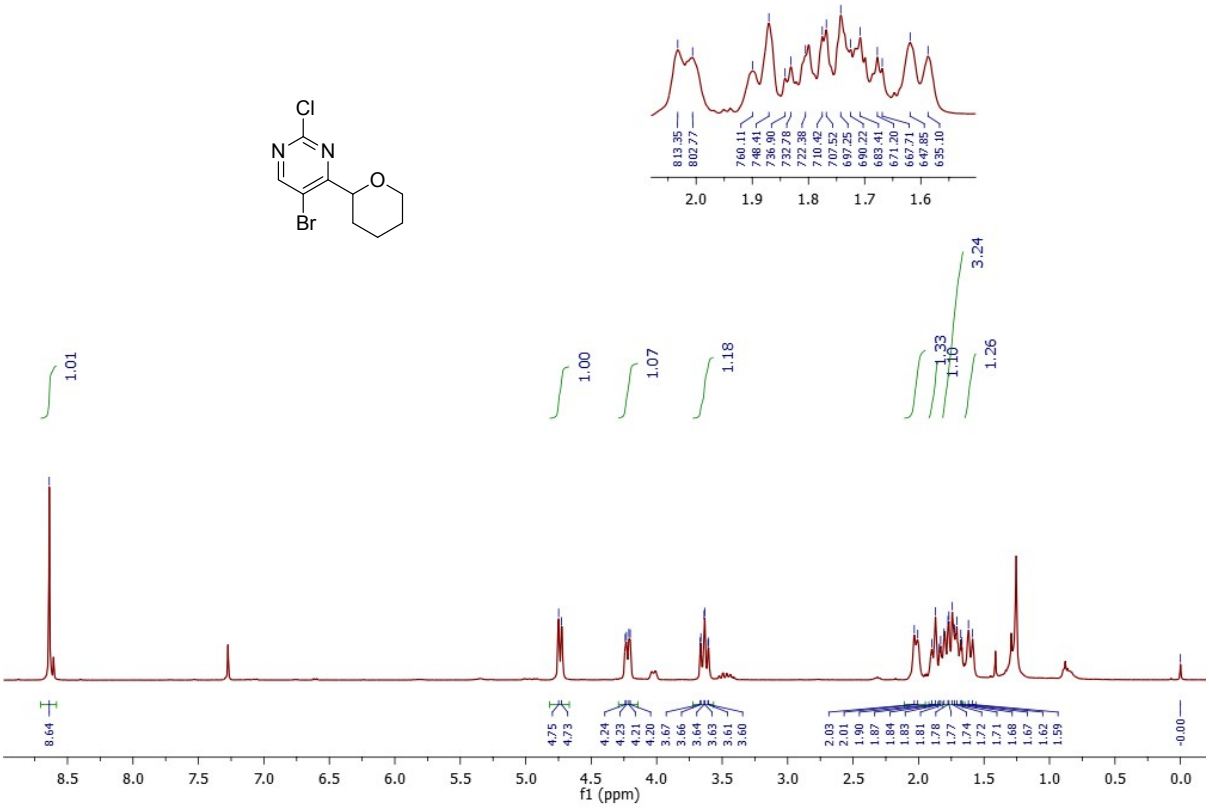
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 262.958 | 1 | 30909.55 | C8 H9 Br Cl N2 O | (M+H)+ |
| 263.9613 | 1 | 4232.67 | C8 H9 Br Cl N2 O | (M+H)+ |
| 264.9559 | 1 | 41059.67 | C8 H9 Br Cl N2 O | (M+H)+ |
| 265.9594 | 1 | 5015 | C8 H9 Br Cl N2 O | (M+H)+ |
| 266.9532 | 1 | 10600.69 | C8 H9 Br Cl N2 O | (M+H)+ |
| 267.9564 | 1 | 1083.53 | C8 H9 Br Cl N2 O | (M+H)+ |

**Predicted Isotope Match Table**

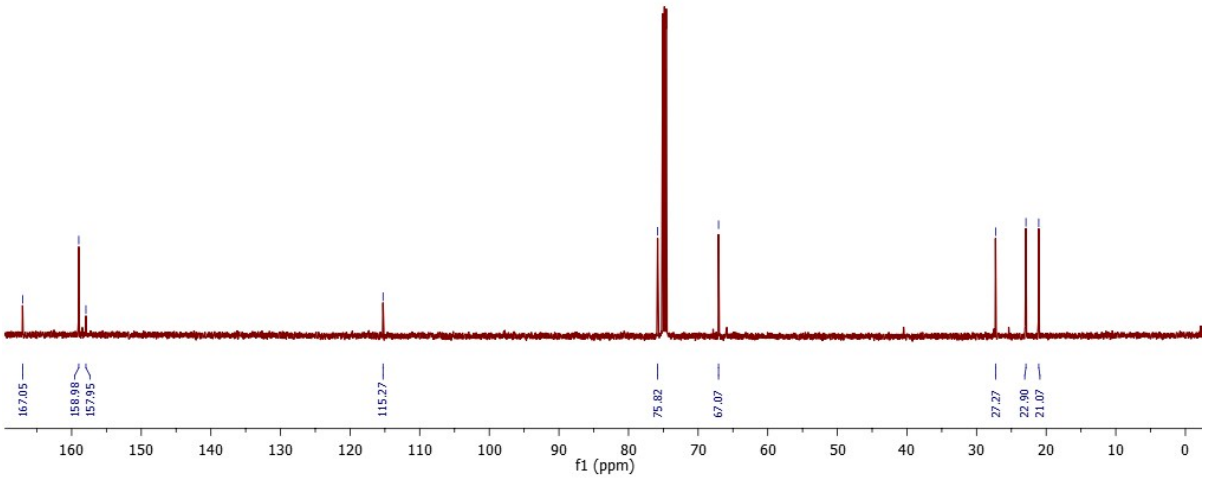
| Isotope | *m/z* | Calc m/z | Diff (ppm) | Abund % | Calc Abund % | Abund Sum % | Calc Abund Sum % |
|---|---|---|---|---|---|---|---|
| 1 | 262.958 | 262.9581 | 0.41 | 75.28 | 76.99 | 33.27 | 34.88 |
| 2 | 263.9613 | 263.961 | -1.03 | 10.31 | 7.33 | 4.56 | 3.32 |
| 3 | 264.9559 | 264.9559 | -0.05 | 100 | 100 | 44.2 | 45.31 |
| 4 | 265.9594 | 265.9588 | -2.31 | 12.21 | 9.5 | 5.4 | 4.31 |
| 5 | 266.9532 | 266.9533 | 0.62 | 25.82 | 24.57 | 11.41 | 11.13 |
| 6 | 267.9564 | 267.9561 | -1.09 | 2.64 | 2.31 | 1.17 | 1.05 |

--- End Of Report ---

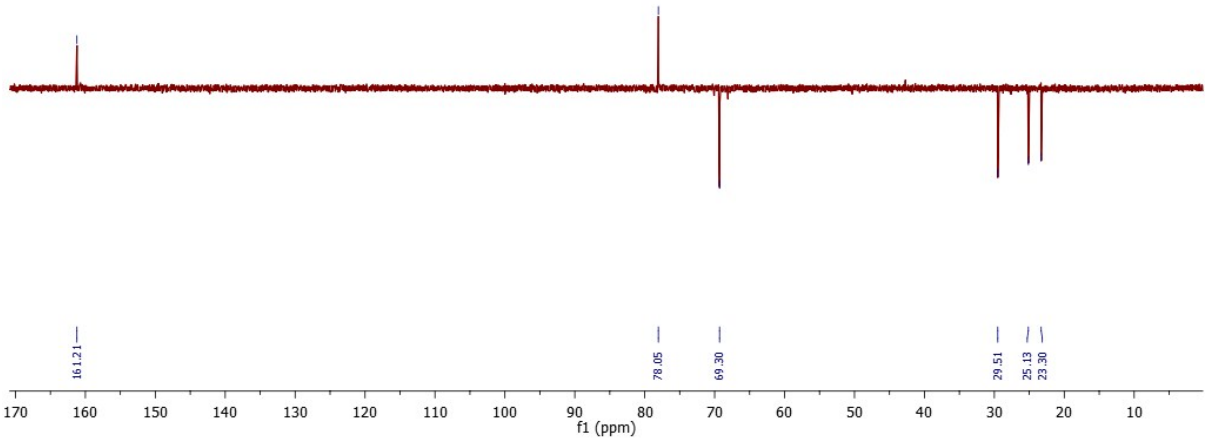
**$^{1}$H NMR of 5-bromo-2-chloro-4-(tetrahydro-2H-pyran-2-yl)pyrimidine (3jc)**



**$^{13}$C NMR of 5-bromo-2-chloro-4-(tetrahydro-2H-pyran-2-yl)pyrimidine (3jc)**



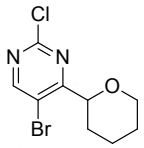

**DEPT of 5-bromo-2-chloro-4-(tetrahydro-2H-pyran-2-yl)pyrimidine (3jc)**



**HRMS of 5-bromo-2-chloro-4-(tetrahydro-2H-pyran-2-yl)pyrimidine (3jc)**

## Qualitative Compound Report

| | | | |
|---|---|---|---|
| **Data File** | 2cl5BrPy-THP.d | **Sample Name** | 2cl5BrPy-THP |
| **Sample Type** | Sample | **Position** | Vial 10 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | vishal_12-01-13.m | **Acquired Time** | 03-02-2015 PM 2:04:10 |
| **IRM Calibration Status** | Success | **DA Method** | daily_report.m |
| **Comment** | | | |
| **Sample Group** | | **Info.** | |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) | | |

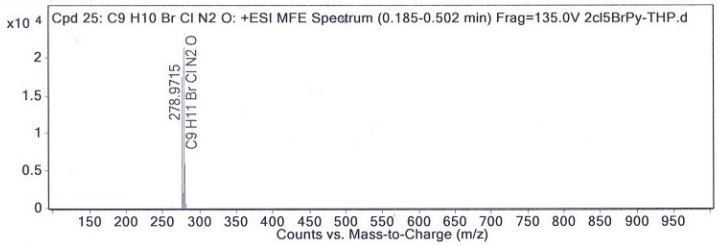



**Compound Table**

| Compound Label | RT | Mass | Formula | MFG Formula | MFG Diff (ppm) | DB Formula |
|---|---|---|---|---|---|---|
| Cpd 25: C9 H10 Br Cl N2 O | 0.289 | 275.9666 | C9 H10 Br Cl N2 O | C9 H10 Br Cl N2 O | -0.43 | C9 H10 Br Cl N2 O |

| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 25: C9 H10 Br Cl N2 O | 276.9739 | 0.289 | Find by Molecular Feature | 275.9666 |

MFE MS Spectrum




**MS Spectrum Peak List**

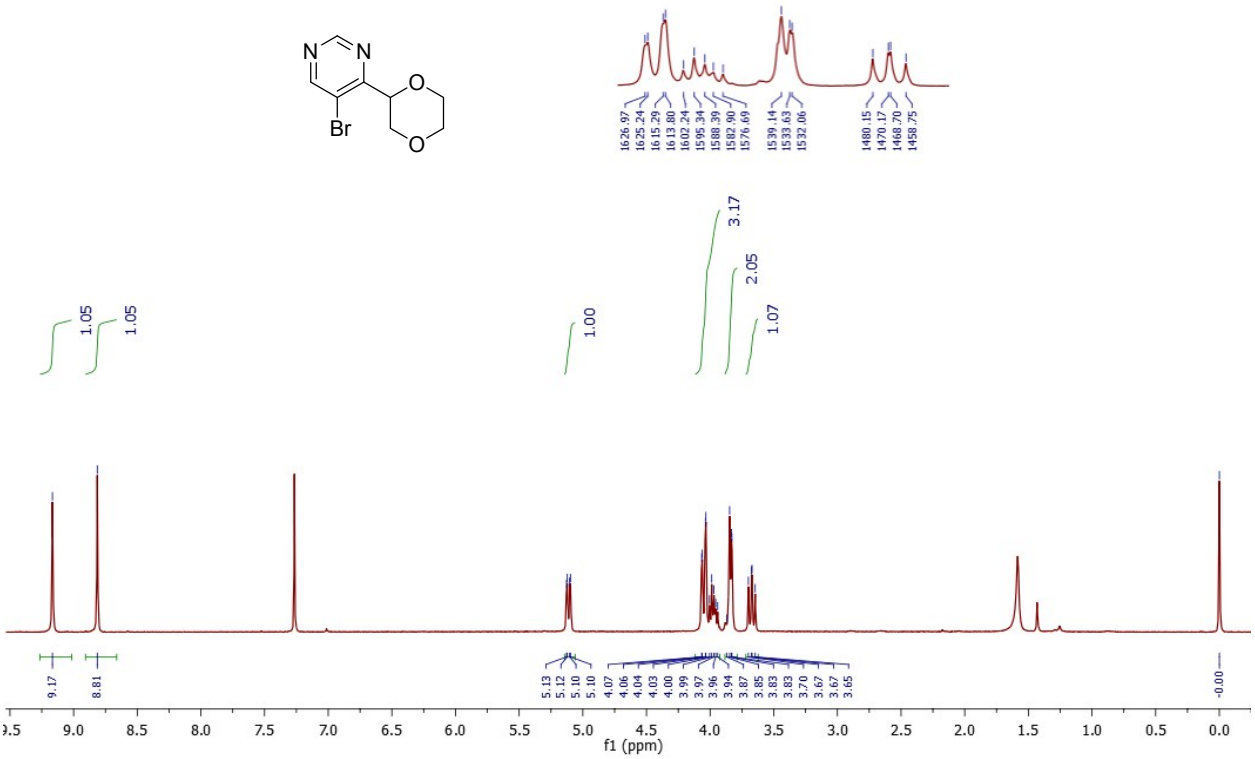
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 276.9739 | 1 | 17662.66 | C9 H11 Br Cl N2 O | (M+H)+ |
| 277.9766 | 1 | 2047.6 | C9 H11 Br Cl N2 O | (M+H)+ |
| 278.9715 | 1 | 21542.73 | C9 H11 Br Cl N2 O | (M+H)+ |
| 279.9756 | 1 | 2400.75 | C9 H11 Br Cl N2 O | (M+H)+ |
| 280.9694 | 1 | 5911.1 | C9 H11 Br Cl N2 O | (M+H)+ |
| 281.9714 | 1 | 614.84 | C9 H11 Br Cl N2 O | (M+H)+ |

**Predicted Isotope Match Table**

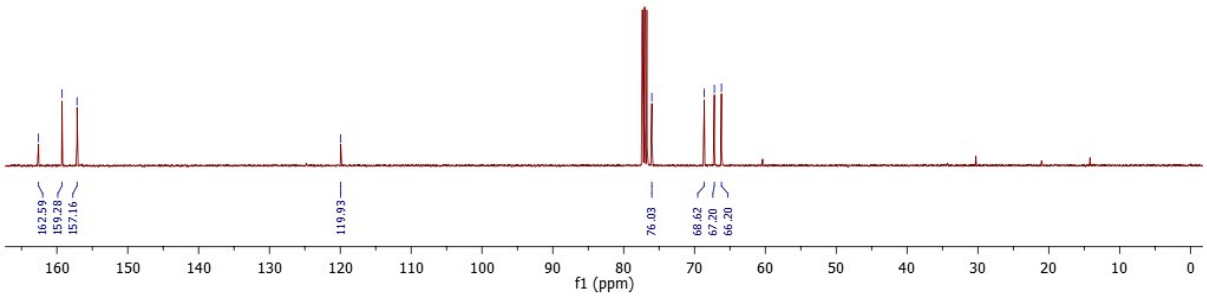
| Isotope | *m/z* | Calc m/z | Diff (ppm) | Abund % | Calc Abund % | Abund Sum % | Calc Abund Sum % |
|---|---|---|---|---|---|---|---|
| 1 | 276.9739 | 276.9738 | -0.41 | 81.99 | 76.93 | 35.2 | 34.51 |
| 2 | 277.9766 | 277.9767 | 0.56 | 9.5 | 8.18 | 4.08 | 3.67 |
| 3 | 278.9715 | 278.9716 | 0.06 | 100 | 100 | 42.93 | 44.85 |
| 4 | 279.9756 | 279.9745 | -4.13 | 11.14 | 10.6 | 4.78 | 4.75 |
| 5 | 280.9694 | 280.969 | -1.26 | 27.44 | 24.66 | 11.78 | 11.06 |
| 6 | 281.9714 | 281.9718 | 1.53 | 2.85 | 2.58 | 1.23 | 1.16 |

--- End Of Report ---

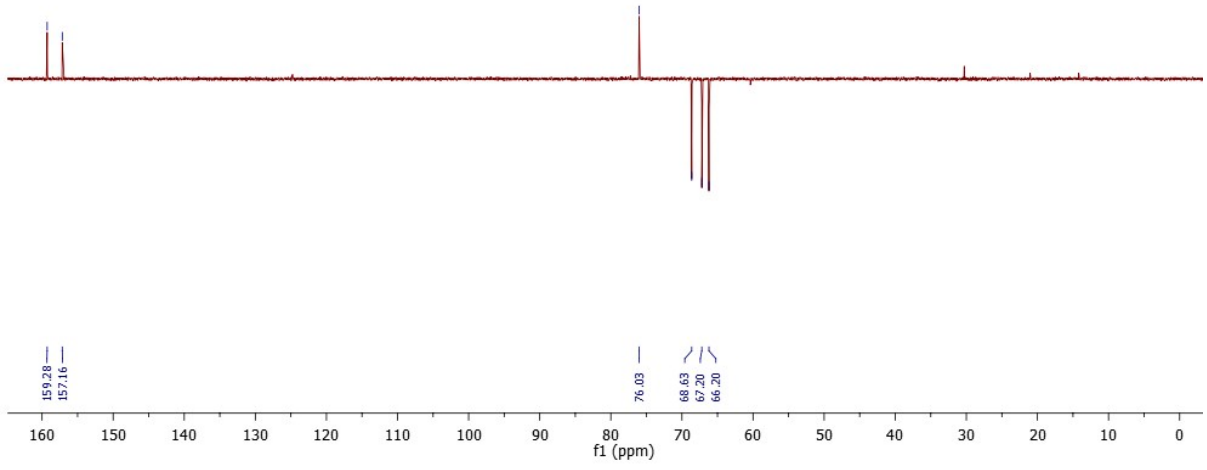
**$^{1}$H NMR of 5-bromo-4-(1,4-dioxan-2-yl)pyrimidine (3ka)**



**$^{13}$C NMR 5-bromo-4-(1,4-dioxan-2-yl)pyrimidine (3ka)**



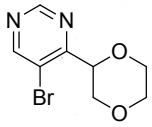

**DEPT NMR of 5-bromo-4-(1,4-dioxan-2-yl)pyrimidine (3ka)**



## HRMS of 5-bromo-4-(1,4-dioxan-2-yl)pyrimidine (3ka)

### Qualitative Compound Report

| | | | |
|---|---|---|---|
| **Data File** | 5BrPy-DO.d | **Sample Name** | 5BrPy-DO |
| **Sample Type** | Sample | **Position** | Vial 11 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | vishal_12-01-13.m | **Acquired Time** | 03-02-2015 PM 2:08:29 |
| **IRM Calibration Status** | Success | **DA Method** | daily_report.m |
| **Comment** | | | |



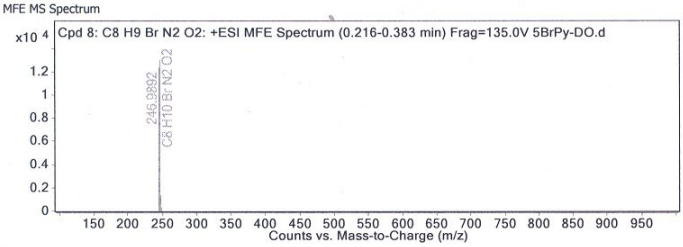

| | |
|---|---|
| **Sample Group** | **Info.** |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) |

**Compound Table**

| Compound Label | RT | Mass | Formula | MFG Formula | MFG Diff (ppm) | DB Formula |
|---|---|---|---|---|---|---|
| Cpd 8: C8 H9 Br N2 O2 | 0.284 | 243.9839 | C8 H9 Br N2 O2 | C8 H9 Br N2 O2 | 3.27 | C8 H9 Br N2 O2 |

| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 8: C8 H9 Br N2 O2 | 244.9913 | 0.284 | Find by Molecular Feature | 243.9839 |

MFE MS Spectrum




**MS Spectrum Peak List**

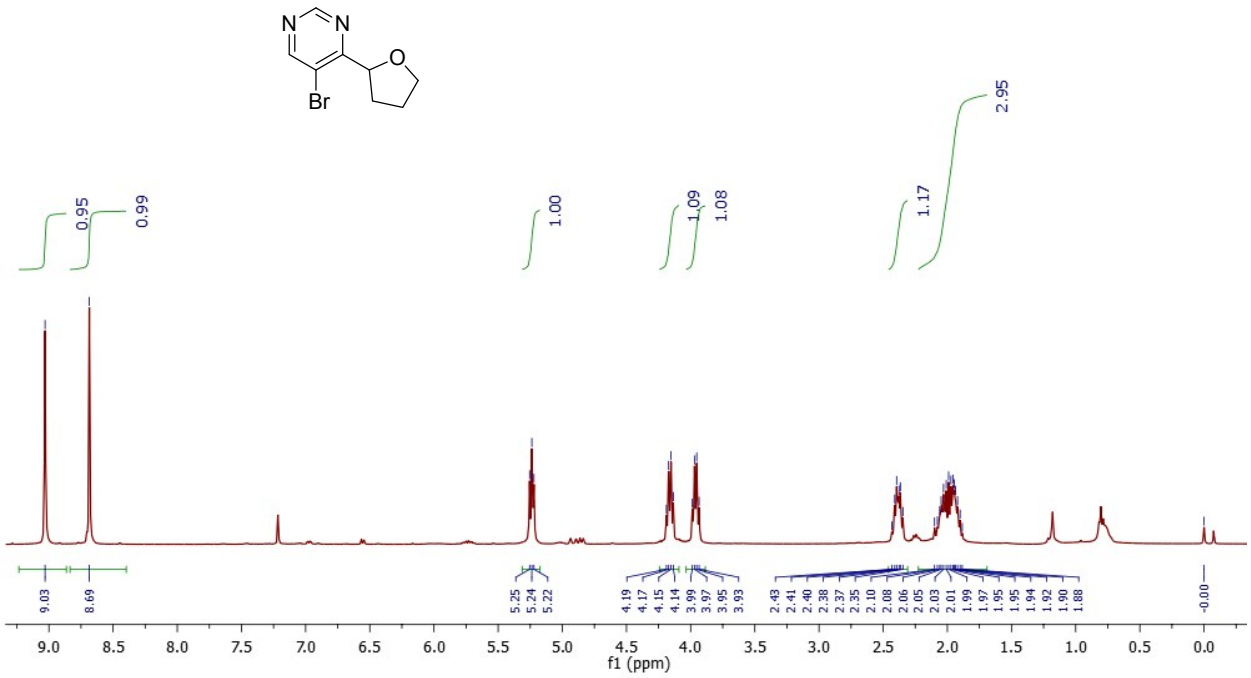
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 244.9913 | 1 | 12318.17 | C8 H10 Br N2 O2 | (M+H)+ |
| 245.9947 | 1 | 1327.64 | C8 H10 Br N2 O2 | (M+H)+ |
| 246.9892 | 1 | 13025.44 | C8 H10 Br N2 O2 | (M+H)+ |
| 247.9918 | 1 | 1360.56 | C8 H10 Br N2 O2 | (M+H)+ |
| 248.9933 | 1 | 317 | C8 H10 Br N2 O2 | (M+H)+ |

**Predicted Isotope Match Table**

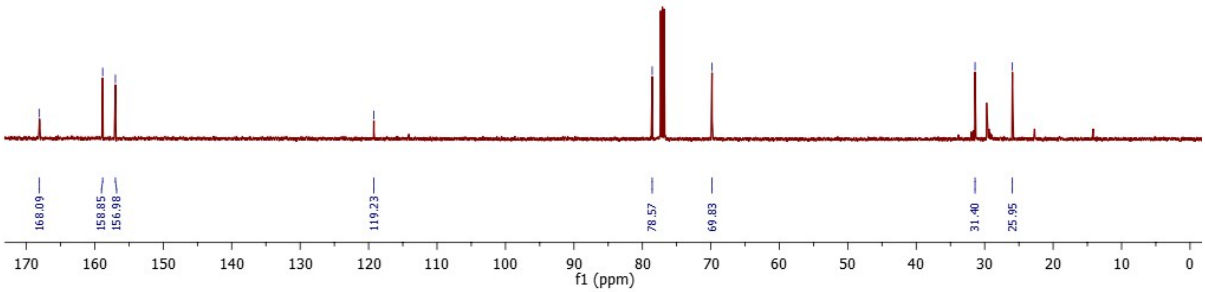
| Isotope | *m/z* | Calc m/z | Diff (ppm) | Abund % | Calc Abund % | Abund Sum % | Calc Abund Sum % |
|---|---|---|---|---|---|---|---|
| 1 | 244.9913 | 244.992 | 3.12 | 94.57 | 100 | 43.45 | 45.91 |
| 2 | 245.9947 | 245.9949 | 0.86 | 10.19 | 9.57 | 4.68 | 4.4 |
| 3 | 246.9892 | 246.99 | 3.38 | 100 | 98.1 | 45.95 | 45.03 |
| 4 | 247.9918 | 247.9929 | 4.47 | 10.45 | 9.36 | 4.8 | 4.3 |
| 5 | 248.9933 | 248.995 | 6.65 | 2.43 | 0.8 | 1.12 | 0.37 |

--- End Of Report ---

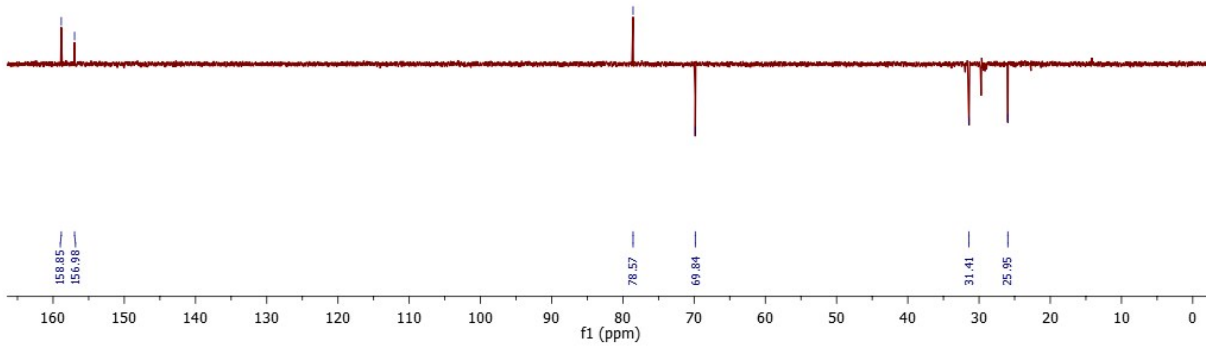
**$^{1}$H NMR of 5-bromo-4-(tetrahydrofuran-2-yl)pyrimidine (3kb)**



**$^{13}$C NMR of 5-bromo-4-(tetrahydrofuran-2-yl)pyrimidine (3kb)**



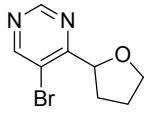

**DEPT NMR of 5-bromo-4-(tetrahydrofuran-2-yl)pyrimidine (3kb)**



**HRMS of 5-bromo-4-(tetrahydrofuran-2-yl)pyrimidine (3kb)**

## Qualitative Compound Report

| | | | |
|---|---|---|---|
| **Data File** | 5BrPy-THF.d | **Sample Name** | 5BrPy-THF |
| **Sample Type** | Sample | **Position** | Vial 12 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | vishal_12-01-13.m | **Acquired Time** | 03-02-2015 PM 2:17:09 |
| **IRM Calibration Status** | Success | **DA Method** | daily_report.m |
| **Comment** | | | |



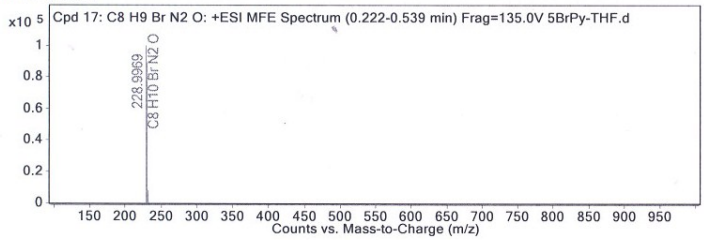

| | |
|---|---|
| **Sample Group** | **Info.** |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) |

**Compound Table**

| Compound Label | RT | Mass | Formula | MFG Formula | MFG Diff (ppm) | DB Formula |
|---|---|---|---|---|---|---|
| Cpd 17: C8 H9 Br N2 O | 0.288 | 227.9896 | C8 H9 Br N2 O | C8 H9 Br N2 O | 0.86 | C8 H9 Br N2 O |

| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 17: C8 H9 Br N2 O | 228.9969 | 0.288 | Find by Molecular Feature | 227.9896 |

MFE MS Spectrum




**MS Spectrum Peak List**

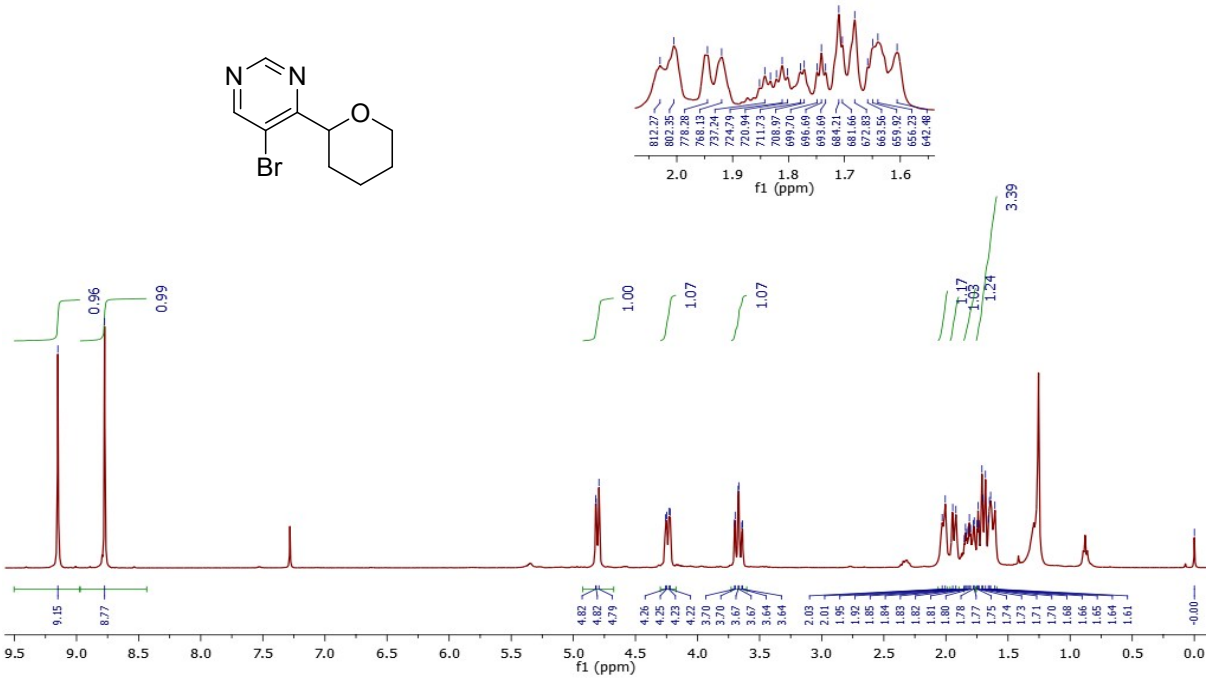
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 228.9969 | 1 | 99914.37 | C8 H10 Br N2 O | (M+H)+ |
| 229.9998 | 1 | 8836.79 | C8 H10 Br N2 O | (M+H)+ |
| 230.9949 | 1 | 89198.13 | C8 H10 Br N2 O | (M+H)+ |
| 231.9975 | 1 | 7721.43 | C8 H10 Br N2 O | (M+H)+ |
| 233.0001 | 1 | 692.19 | C8 H10 Br N2 O | (M+H)+ |

**Predicted Isotope Match Table**

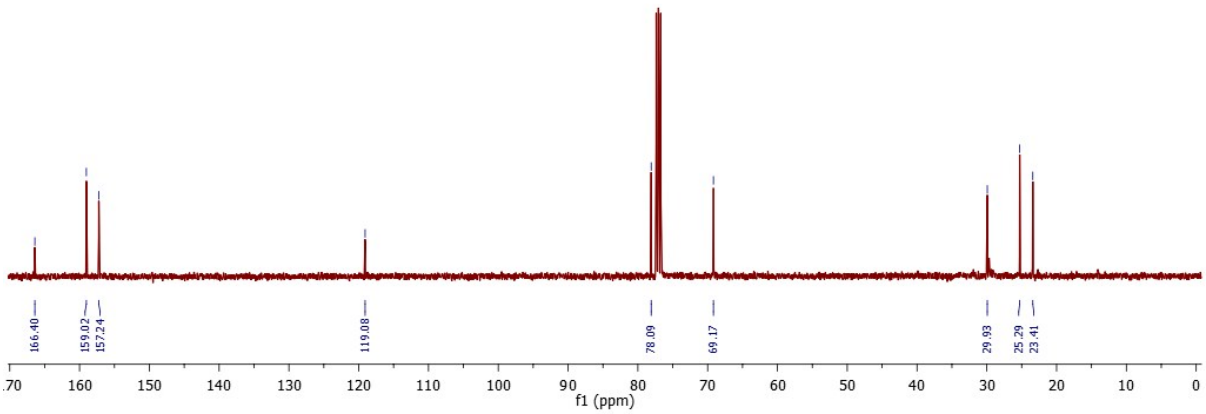
| Isotope | *m/z* | Calc m/z | Diff (ppm) | Abund % | Calc Abund % | Abund Sum % | Calc Abund Sum % |
|---|---|---|---|---|---|---|---|
| 1 | 228.9969 | 228.9971 | 0.78 | 100 | 100 | 48.42 | 46.01 |
| 2 | 229.9998 | 230 | 0.75 | 8.84 | 9.54 | 4.28 | 4.39 |
| 3 | 230.9949 | 230.9951 | 0.85 | 89.27 | 97.89 | 43.22 | 45.04 |
| 4 | 231.9975 | 231.998 | 1.91 | 7.73 | 9.31 | 3.74 | 4.28 |
| 5 | 233.0001 | 233.0003 | 0.77 | 0.69 | 0.6 | 0.34 | 0.27 |

--- End Of Report ---

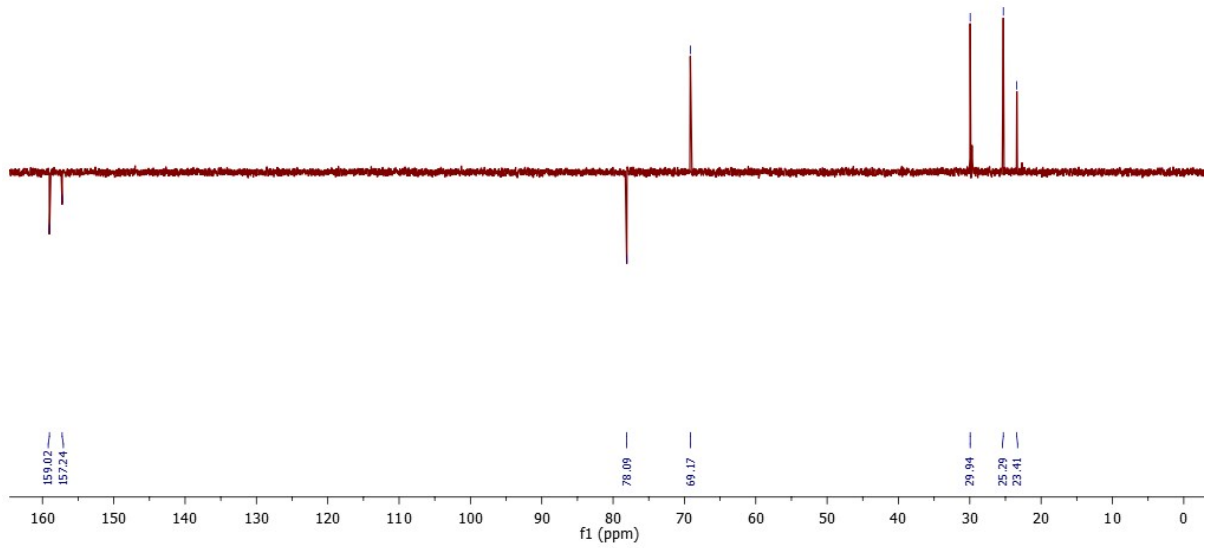
**$^1$H NMR of 5-bromo-4-(tetrahydro-2*H*-pyran-2-yl)pyrimidine (3kc)**



**$^{13}$C NMR of 5-bromo-4-(tetrahydro-2*H*-pyran-2-yl)pyrimidine (3kc)**



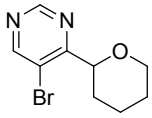

**DEPT of 5-bromo-4-(tetrahydro-2*H*-pyran-2-yl)pyrimidine (3kc)**



## HRMS of 5-bromo-4-(tetrahydro-2*H*-pyran-2-yl)pyrimidine (3kc)

### Qualitative Compound Report

| | | | |
|---|---|---|---|
| **Data File** | 5brpy-thp.d | **Sample Name** | 5brpy-thp |
| **Sample Type** | Sample | **Position** | Vial 5 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | vishal_12-01-13.m | **Acquired Time** | 09-02-2015 PM 12:11:42 |
| **IRM Calibration Status** | Success | **DA Method** | daily_report.m |
| **Comment** | | | |
| **Sample Group** | | **Info.** | |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) | | |

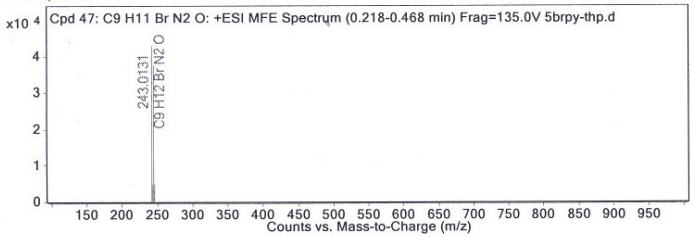



**Compound Table**

| Compound Label | RT | Mass | Formula | MFG Formula | MFG Diff (ppm) | DB Formula |
|---|---|---|---|---|---|---|
| Cpd 47: C9 H11 Br N2 O | 0.282 | 242.0059 | C9 H11 Br N2 O | C9 H11 Br N2 O | -1.86 | C9 H11 Br N2 O |

| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 47: C9 H11 Br N2 O | 243.0131 | 0.282 | Find by Molecular Feature | 242.0059 |

MFE MS Spectrum




**MS Spectrum Peak List**

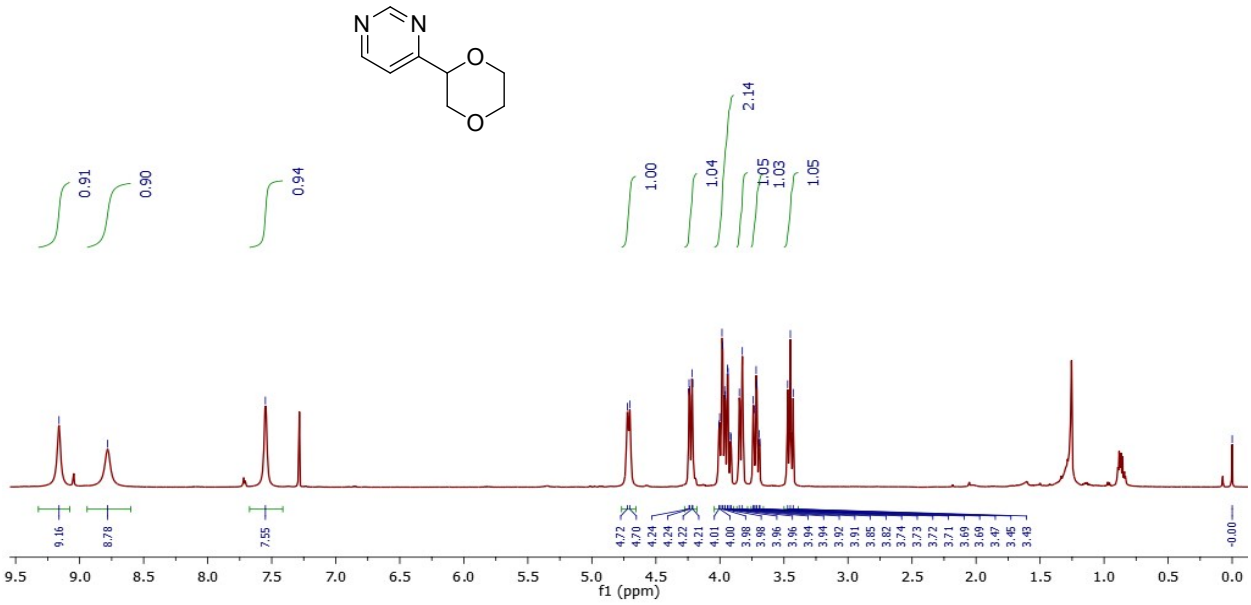
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 243.0131 | 1 | 42967.11 | C9 H12 Br N2 O | (M+H)+ |
| 244.0164 | 1 | 4588.85 | C9 H12 Br N2 O | (M+H)+ |
| 245.0112 | 1 | 37509.39 | C9 H12 Br N2 O | (M+H)+ |
| 246.0146 | 1 | 4911.13 | C9 H12 Br N2 O | (M+H)+ |
| 247.019 | 1 | 515.14 | C9 H12 Br N2 O | (M+H)+ |

**Predicted Isotope Match Table**

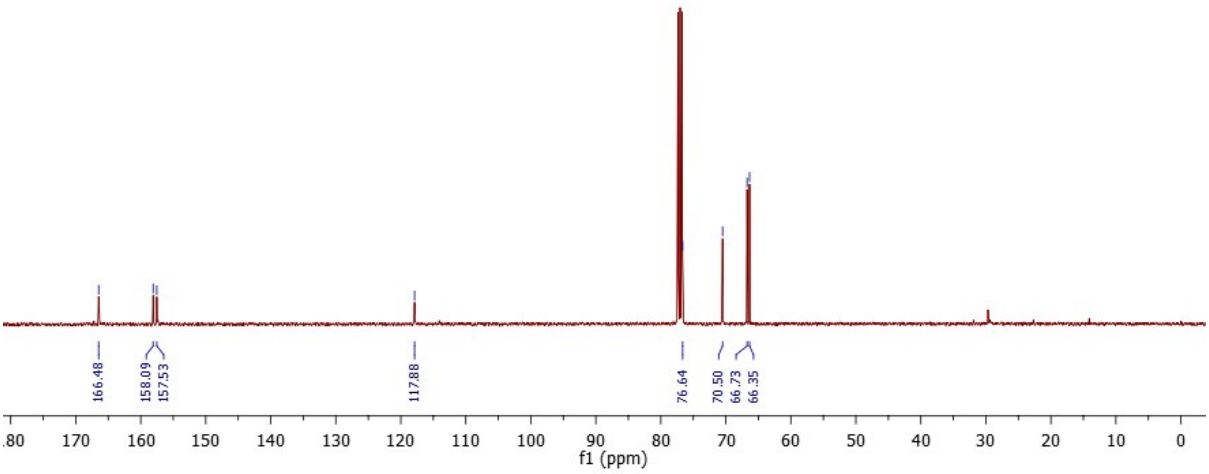
| Isotope | *m/z* | Calc m/z | Diff (ppm) | Abund % | Calc Abund % | Abund Sum % | Calc Abund Sum % |
|---|---|---|---|---|---|---|---|
| 1 | 243.0131 | 243.0128 | -1.39 | 100 | 100 | 47.48 | 45.51 |
| 2 | 244.0164 | 244.0157 | -2.7 | 10.68 | 10.64 | 5.07 | 4.84 |
| 3 | 245.0112 | 245.0108 | -1.89 | 87.3 | 98 | 41.45 | 44.6 |
| 4 | 246.0146 | 246.0137 | -3.62 | 11.43 | 10.39 | 5.43 | 4.73 |
| 5 | 247.019 | 247.0161 | -11.76 | 1.2 | 0.7 | 0.57 | 0.32 |

--- End Of Report ---

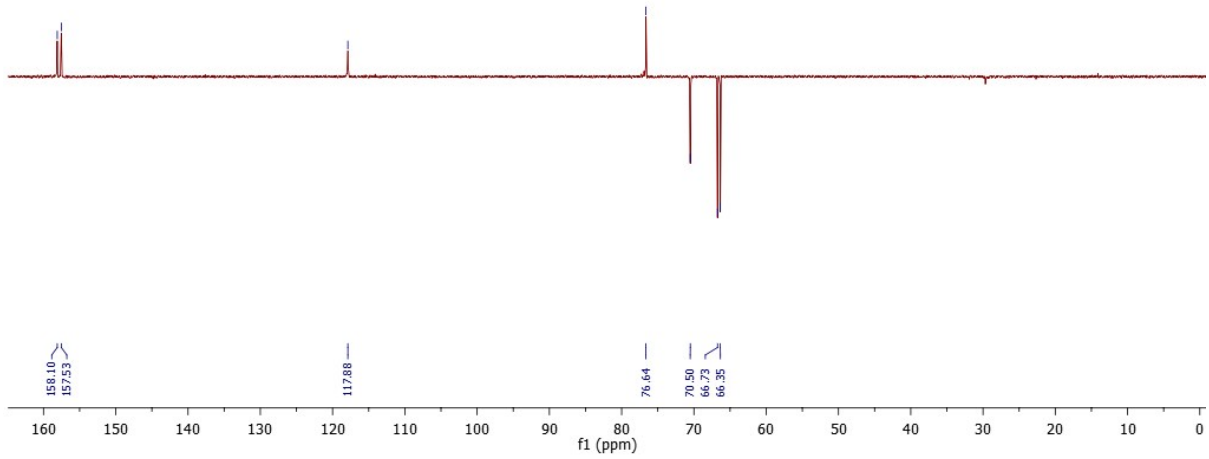
**$^{1}$H NMR of 4-(1,4-dioxan-2-yl)pyrimidine (3la)**



**$^{13}$C NMR of 4-(1,4-dioxan-2-yl)pyrimidine (3la)**



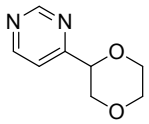

**DEPT NMR of 4-(1,4-dioxan-2-yl)pyrimidine (3la)**



## HRMS of 4-(1,4-dioxan-2-yl)pyrimidine (3la)

### Qualitative Compound Report

| | | | |
|---|---|---|---|
| **Data File** | Py-DO.d | **Sample Name** | Py-DO |
| **Sample Type** | Sample | **Position** | Vial 16 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | vishal_12-01-13.m | **Acquired Time** | 03-02-2015 PM 2:34:15 |
| **IRM Calibration Status** | Success | **DA Method** | daily_report.m |
| **Comment** | | | |



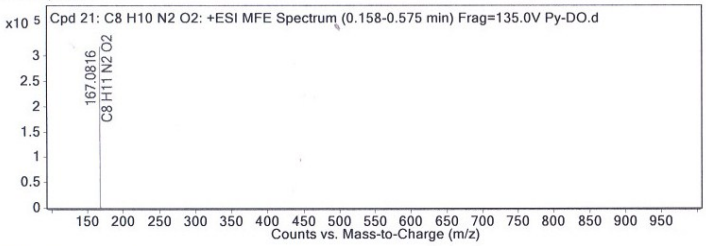
| | |
|---|---|
| **Sample Group** | **Info.** |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) |

**Compound Table**

| Compound Label | RT | Mass | Formula | MFG Formula | MFG Diff (ppm) | DB Formula |
|---|---|---|---|---|---|---|
| Cpd 21: C8 H10 N2 O2 | 0.288 | 166.0743 | C8 H10 N2 O2 | C8 H10 N2 O2 | -0.47 | C8 H10 N2 O2 |

| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 21: C8 H10 N2 O2 | 167.0816 | 0.288 | Find by Molecular Feature | 166.0743 |

MFE MS Spectrum




**MS Spectrum Peak List**

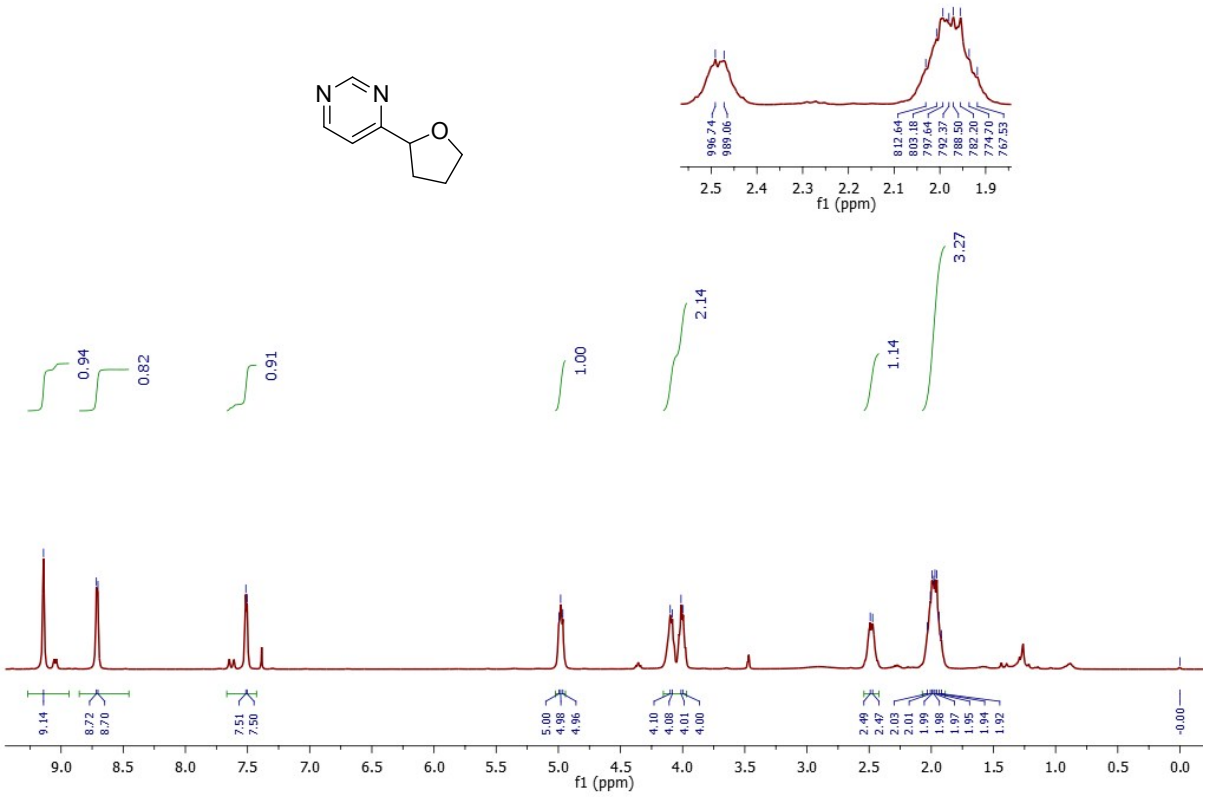
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 167.0816 | 1 | 318772.56 | C8 H11 N2 O2 | (M+H)+ |
| 168.0845 | 1 | 28057.06 | C8 H11 N2 O2 | (M+H)+ |
| 169.0869 | 1 | 2319.13 | C8 H11 N2 O2 | (M+H)+ |

**Predicted Isotope Match Table**

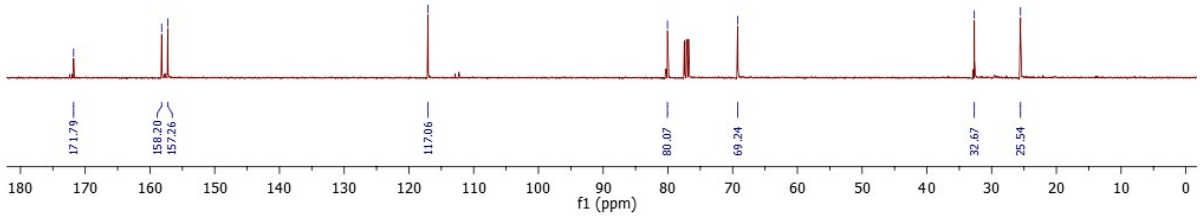
| Isotope | *m/z* | Calc m/z | Diff (ppm) | Abund % | Calc Abund % | Abund Sum % | Calc Abund Sum % |
|---|---|---|---|---|---|---|---|
| 1 | 167.0816 | 167.0815 | -0.43 | 100 | 100 | 91.3 | 90.57 |
| 2 | 168.0845 | 168.0844 | -0.73 | 8.8 | 9.59 | 8.04 | 8.68 |
| 3 | 169.0869 | 169.0865 | -2.05 | 0.73 | 0.82 | 0.66 | 0.74 |

--- End Of Report ---

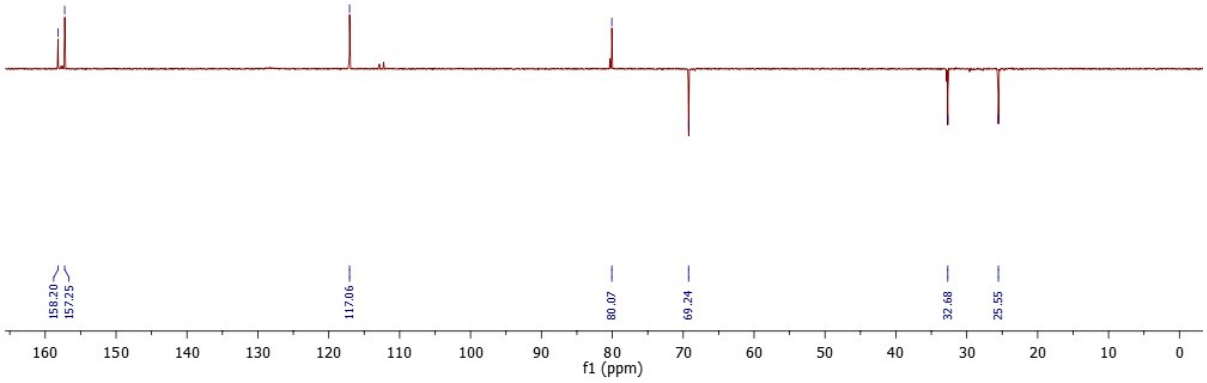
**$^{1}$H NMR of 4-(tetrahydrofuran-2-yl)pyrimidine (3lb)**



**$^{13}$C NMR of 4-(tetrahydrofuran-2-yl)pyrimidine (3lb)**



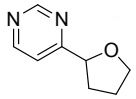

**DEPT NMR of 4-(tetrahydrofuran-2-yl)pyrimidine (3lb)**



## HRMS of 4-(tetrahydrofuran-2-yl)pyrimidine (3lb)

### Qualitative Compound Report

| | | | |
|---|---|---|---|
| **Data File** | PY-THF.d | **Sample Name** | PY-THF |
| **Sample Type** | Sample | **Position** | Vial 26 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | vishal_12-01-13.m | **Acquired Time** | 07-02-2015 PM 1:31:58 |
| **IRM Calibration Status** | Success | **DA Method** | daily_report.m |
| **Comment** | | | |



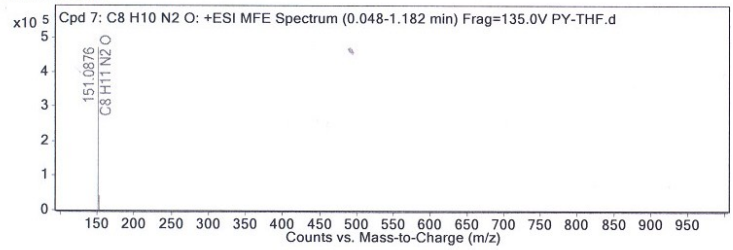
| | |
|---|---|
| **Sample Group** | **Info.** |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) |

**Compound Table**

| Compound Label | RT | Mass | Formula | MFG Formula | MFG Diff (ppm) | DB Formula |
|---|---|---|---|---|---|---|
| Cpd 7: C8 H10 N2 O | 0.278 | 150.0803 | C8 H10 N2 O | C8 H10 N2 O | -6.79 | C8 H10 N2 O |

| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 7: C8 H10 N2 O | 151.0876 | 0.278 | Find by Molecular Feature | 150.0803 |

MFE MS Spectrum




**MS Spectrum Peak List**

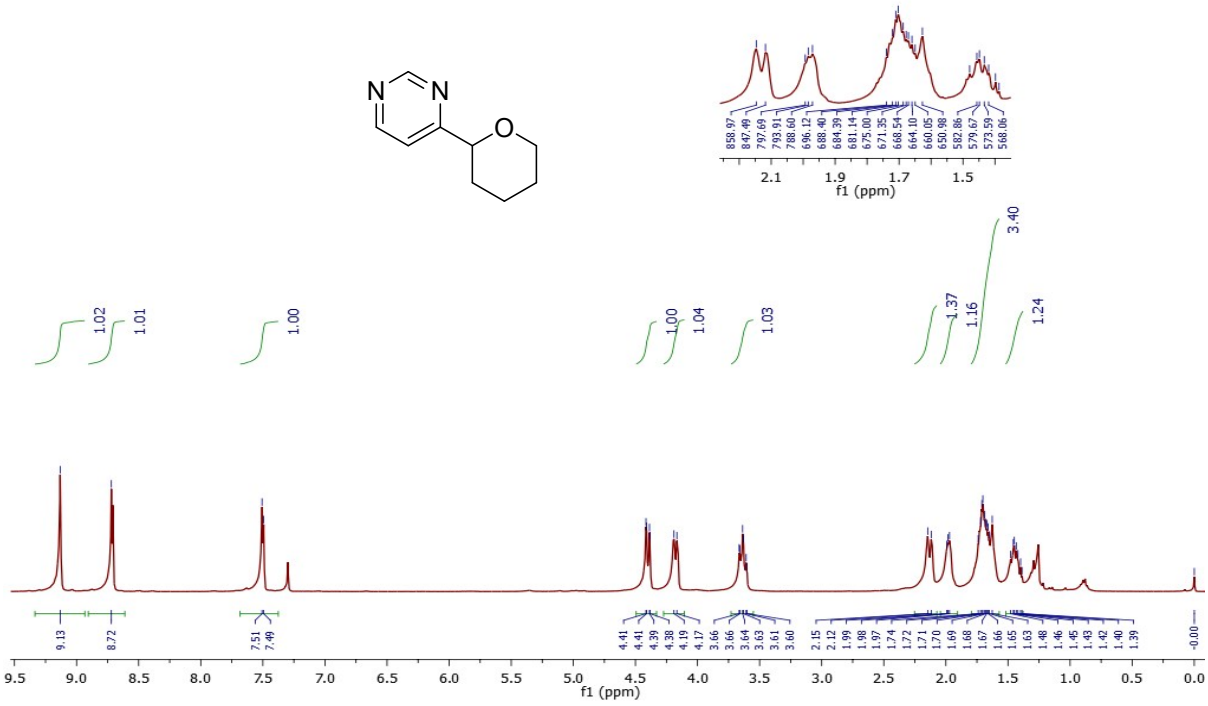
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 151.0876 | 1 | 471692.78 | C8 H11 N2 O | (M+H)+ |
| 152.0904 | 1 | 43206.74 | C8 H11 N2 O | (M+H)+ |
| 153.0939 | 1 | 4047.67 | C8 H11 N2 O | (M+H)+ |

**Predicted Isotope Match Table**

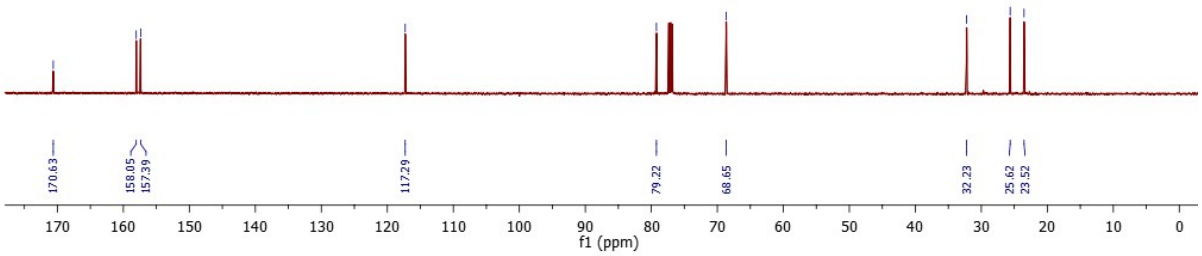
| Isotope | *m/z* | Calc m/z | Diff (ppm) | Abund % | Calc Abund % | Abund Sum % | Calc Abund Sum % |
|---|---|---|---|---|---|---|---|
| 1 | 151.0876 | 151.0866 | -6.74 | 100 | 100 | 90.89 | 90.78 |
| 2 | 152.0904 | 152.0895 | -6.1 | 9.16 | 9.55 | 8.33 | 8.67 |
| 3 | 153.0939 | 153.0918 | -13.66 | 0.86 | 0.61 | 0.78 | 0.56 |

--- End Of Report ---

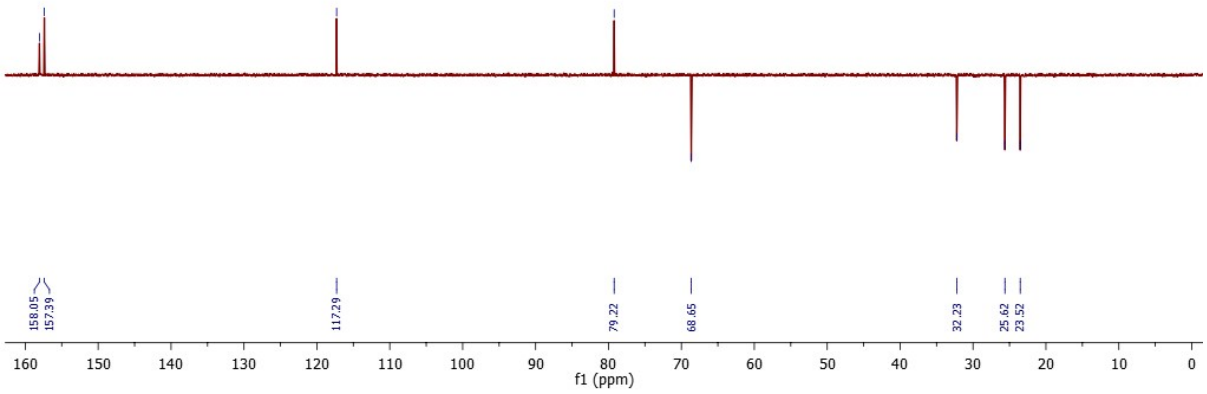
**$^1$H NMR of 4-(tetrahydro-2*H*-pyran-2-yl)pyrimidine (3lc)**



**$^{13}$C NMR of 4-(tetrahydro-2*H*-pyran-2-yl)pyrimidine (3lc)**



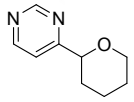

**DEPT NMR of 4-(tetrahydro-2*H*-pyran-2-yl)pyrimidine (3lc)**



**HRMS of 4-(tetrahydro-2H-pyran-2-yl)pyrimidine (3lc)**

## Qualitative Compound Report

| | | | |
|---|---|---|---|
| **Data File** | Py-THP.d | **Sample Name** | Py-THP |
| **Sample Type** | Sample | **Position** | Vial 14 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | vishal_12-01-13.m | **Acquired Time** | 03-02-2015 PM 2:25:42 |
| **IRM Calibration Status** | Success | **DA Method** | daily_report.m |
| **Comment** | | | |



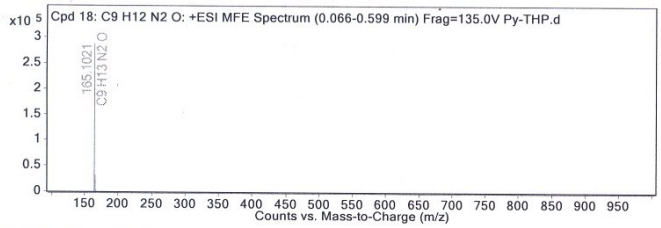
| | |
|---|---|
| **Sample Group** | **Info.** |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) |

**Compound Table**

| Compound Label | RT | Mass | Formula | MFG Formula | MFG Diff (ppm) | DB Formula |
|---|---|---|---|---|---|---|
| Cpd 18: C9 H12 N2 O | 0.289 | 164.0948 | C9 H12 N2 O | C9 H12 N2 O | 1.11 | C9 H12 N2 O |

| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 18: C9 H12 N2 O | 165.1021 | 0.289 | Find by Molecular Feature | 164.0948 |

MFE MS Spectrum




**MS Spectrum Peak List**

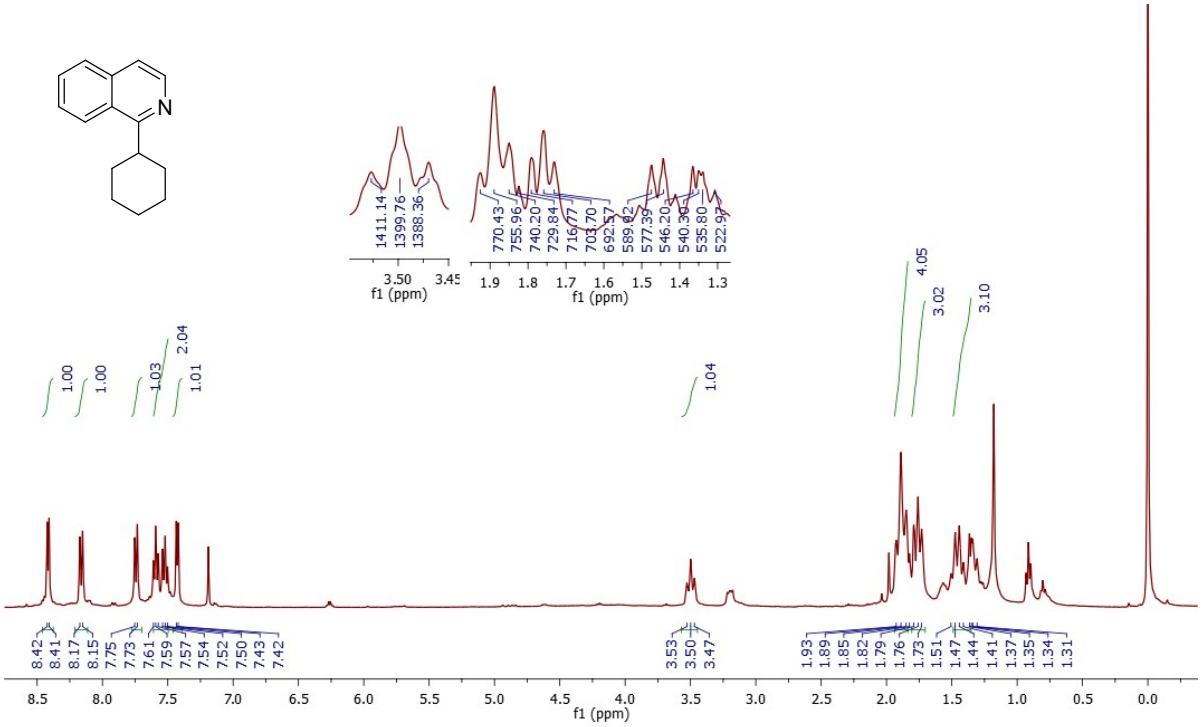
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 165.1021 | 1 | 287070.28 | C9 H13 N2 O | (M+H)+ |
| 166.105 | 1 | 30353.21 | C9 H13 N2 O | (M+H)+ |
| 167.1077 | 1 | 3538.25 | C9 H13 N2 O | (M+H)+ |

**Predicted Isotope Match Table**

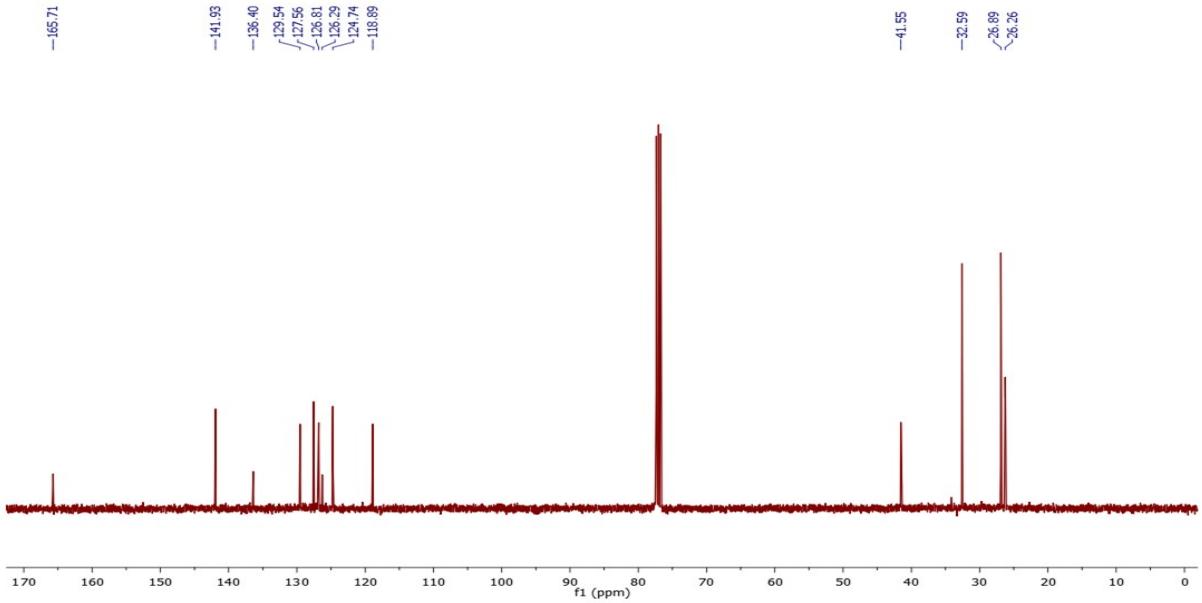
| Isotope | *m/z* | Calc m/z | Diff (ppm) | Abund % | Calc Abund % | Abund Sum % | Calc Abund Sum % |
|---|---|---|---|---|---|---|---|
| 1 | 165.1021 | 165.1022 | 1.11 | 100 | 100 | 89.44 | 89.79 |
| 2 | 166.105 | 166.1052 | 1.22 | 10.57 | 10.65 | 9.46 | 9.56 |
| 3 | 167.1077 | 167.1077 | -0.1 | 1.23 | 0.72 | 1.1 | 0.65 |

--- End Of Report ---

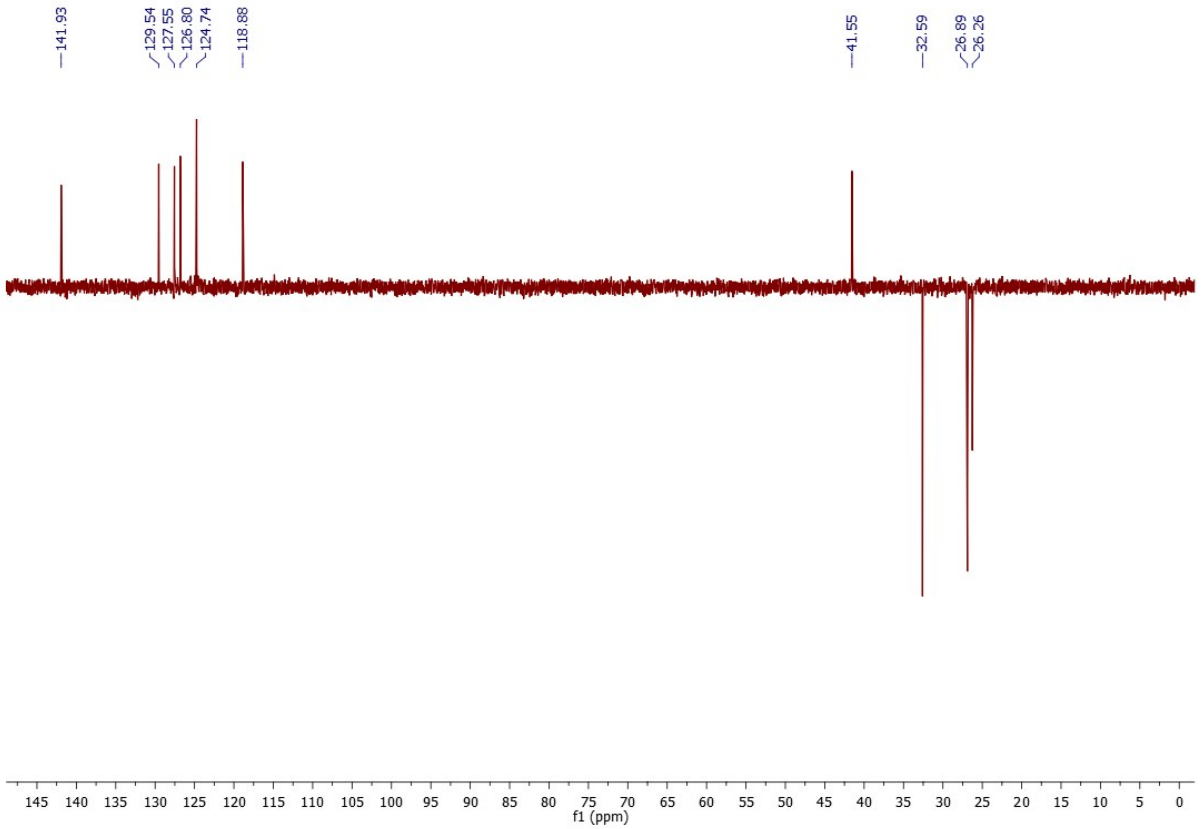
**[1]H NMR of 1-cyclohexyl *iso*-quinoline (3ae)**



## $^{13}$C NMR of 1-cyclohexyl *iso*-quinoline (3ae)



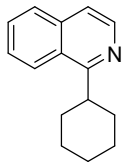

## DEPT of 1-cyclohexyl *iso*-quinoline (3ae)



**HRMS of 1-cyclohexyl *iso*-quinoline (3ae)**

## Qualitative Compound Report

| | | | |
|---|---|---|---|
| **Data File** | F-4.d | **Sample Name** | F-4 |
| **Sample Type** | Sample | **Position** | Vial 22 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | vishal_12-01-13.m | **Acquired Time** | 07-02-2015 PM 1:14:45 |
| **IRM Calibration Status** | Success | **DA Method** | daily_report.m |
| **Comment** | | | |



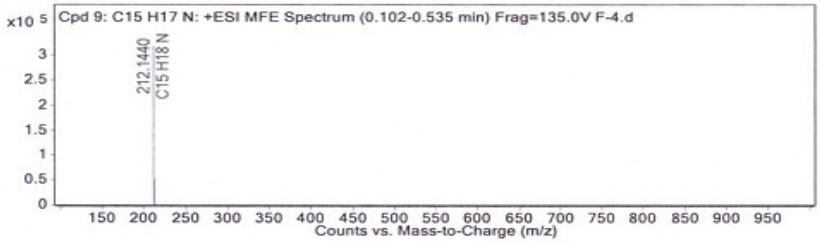

| | |
|---|---|
| **Sample Group** | **Info.** |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) |

**Compound Table**

| Compound Label | RT | Mass | Formula | MFG Formula | MFG Diff (ppm) | DB Formula |
|---|---|---|---|---|---|---|
| Cpd 9: C15 H17 N | 0.276 | 211.1367 | C15 H17 N | C15 H17 N | -2.84 | C15 H17 N |

| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 9: C15 H17 N | 212.144 | 0.276 | Find by Molecular Feature | 211.1367 |

MFE MS Spectrum




**MS Spectrum Peak List**

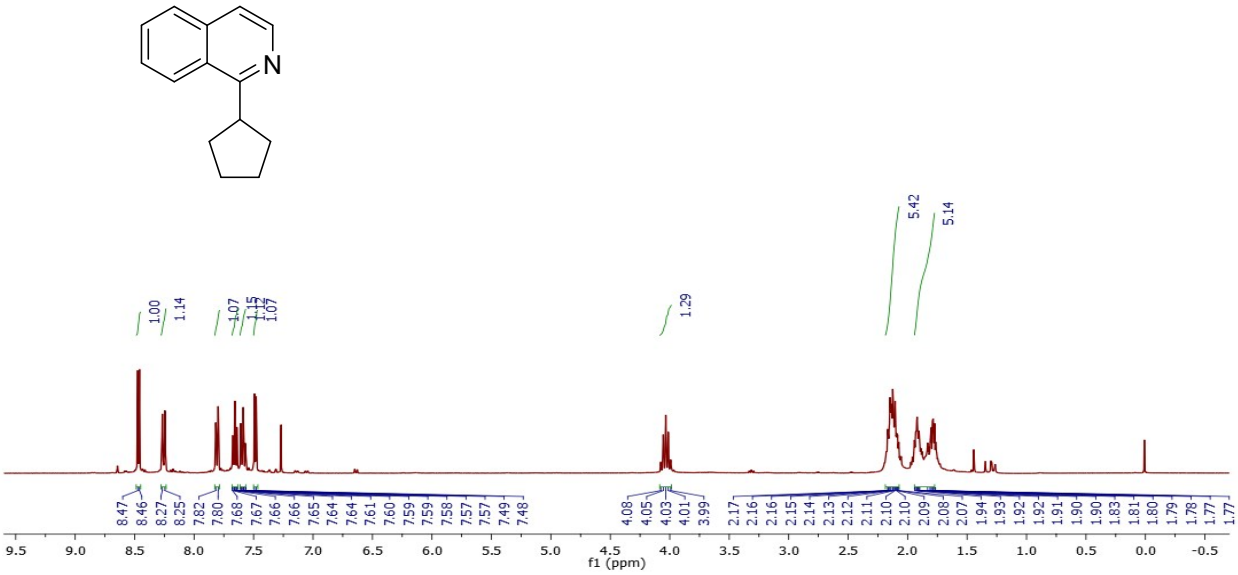
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 212.144 | 1 | 318041.19 | C15 H18 N | (M+H)+ |
| 213.1471 | 1 | 53197.42 | C15 H18 N | (M+H)+ |
| 214.1499 | 1 | 4387.23 | C15 H18 N | (M+H)+ |
| 215.1504 | 1 | 807.73 | C15 H18 N | (M+H)+ |

**Predicted Isotope Match Table**

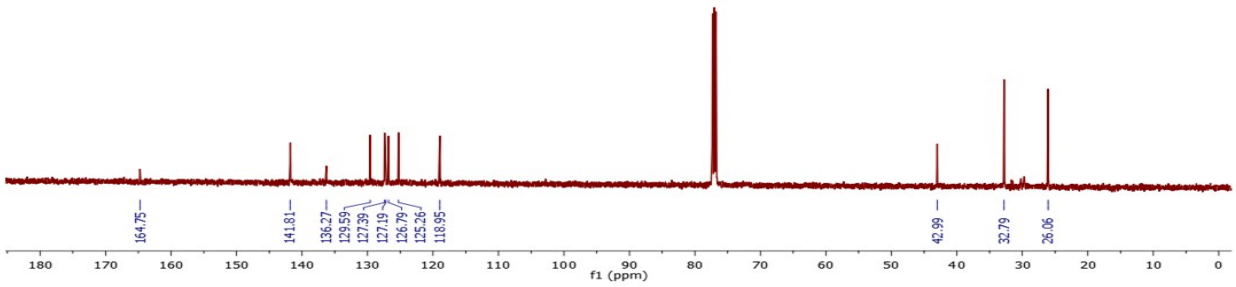
| Isotope | *m/z* | Calc m/z | Diff (ppm) | Abund % | Calc Abund % | Abund Sum % | Calc Abund Sum % |
|---|---|---|---|---|---|---|---|
| 1 | 212.144 | 212.1434 | -2.98 | 100 | 100 | 84.49 | 84.61 |
| 2 | 213.1471 | 213.1466 | -2.33 | 16.73 | 16.8 | 14.13 | 14.21 |
| 3 | 214.1499 | 214.1499 | -0.07 | 1.38 | 1.32 | 1.17 | 1.12 |
| 4 | 215.1504 | 215.1531 | 12.41 | 0.25 | 0.06 | 0.21 | 0.05 |

--- End Of Report ---

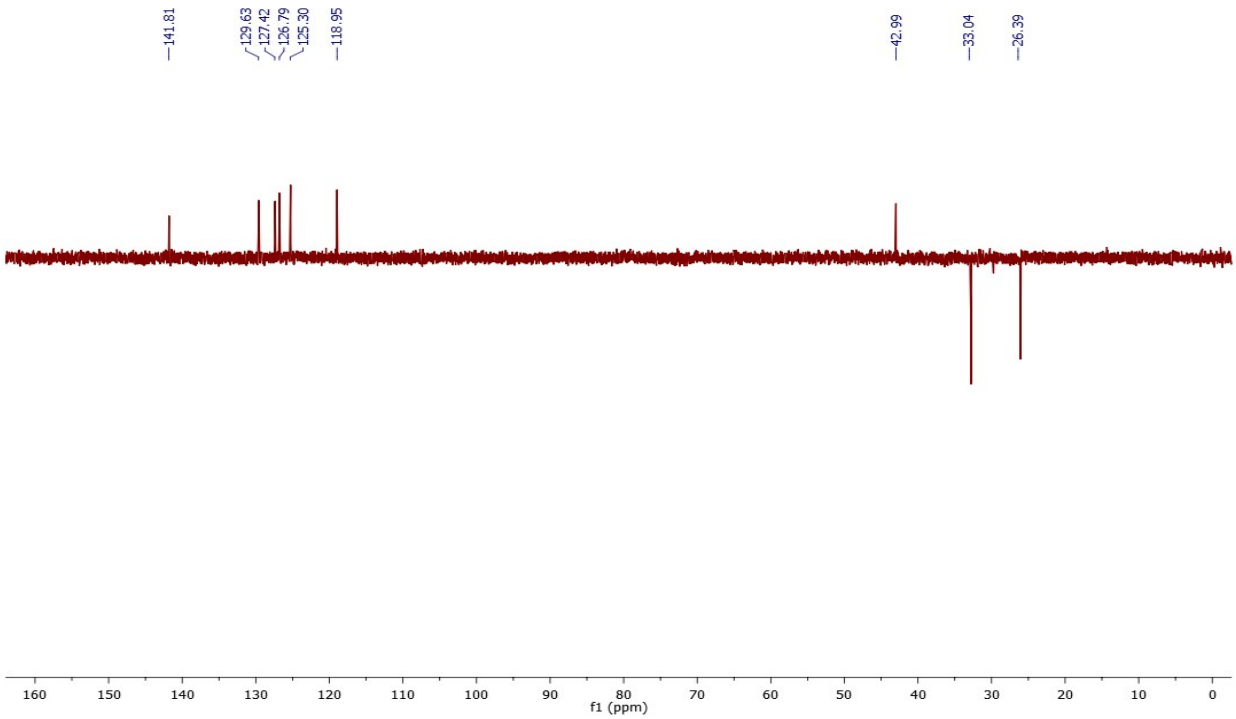
**$^{1}$H NMR of 1-cyclopentyl*iso*-quinoline (3af)**



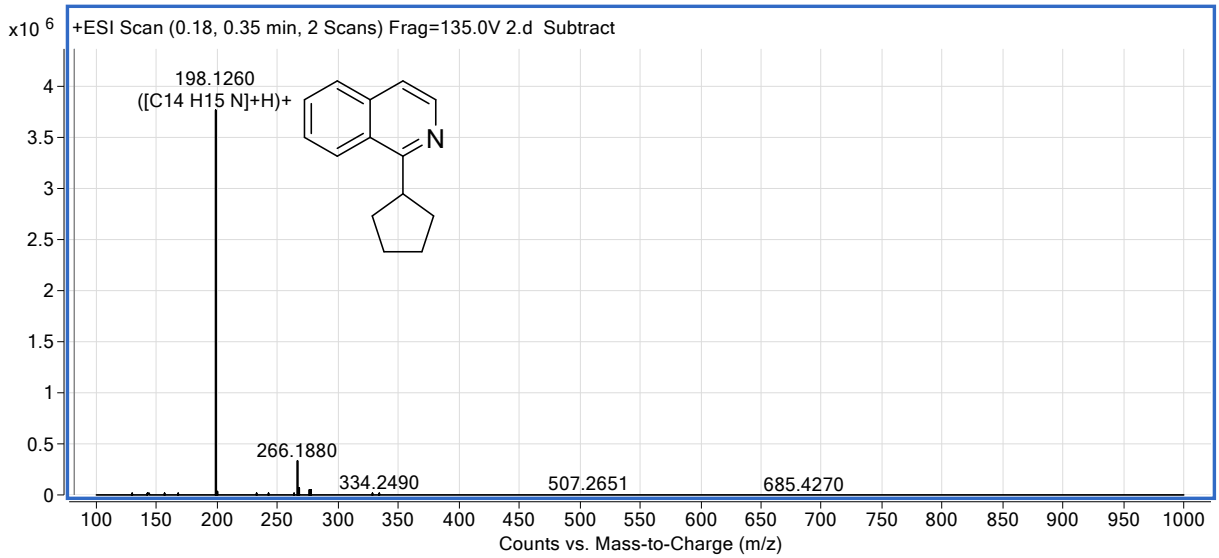
**$^{13}$C NMR of 1-cyclopentyl*iso*-quinoline (3af)**



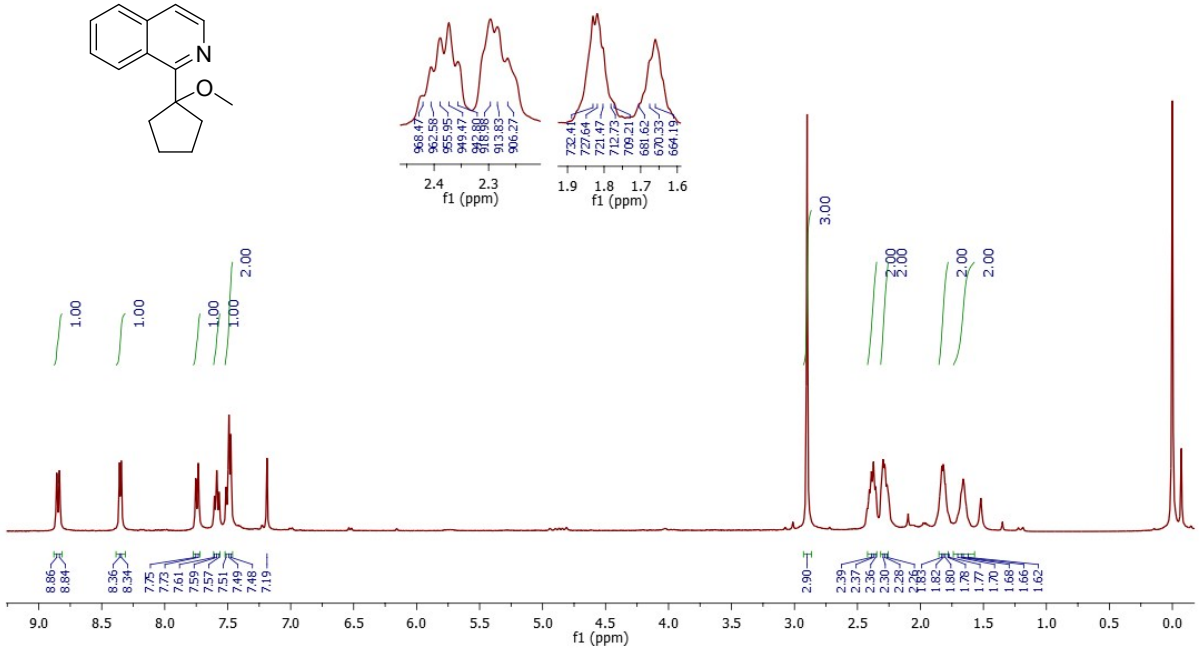

**DEPT of 1-cyclopentyl*iso*-quinoline (3af)**



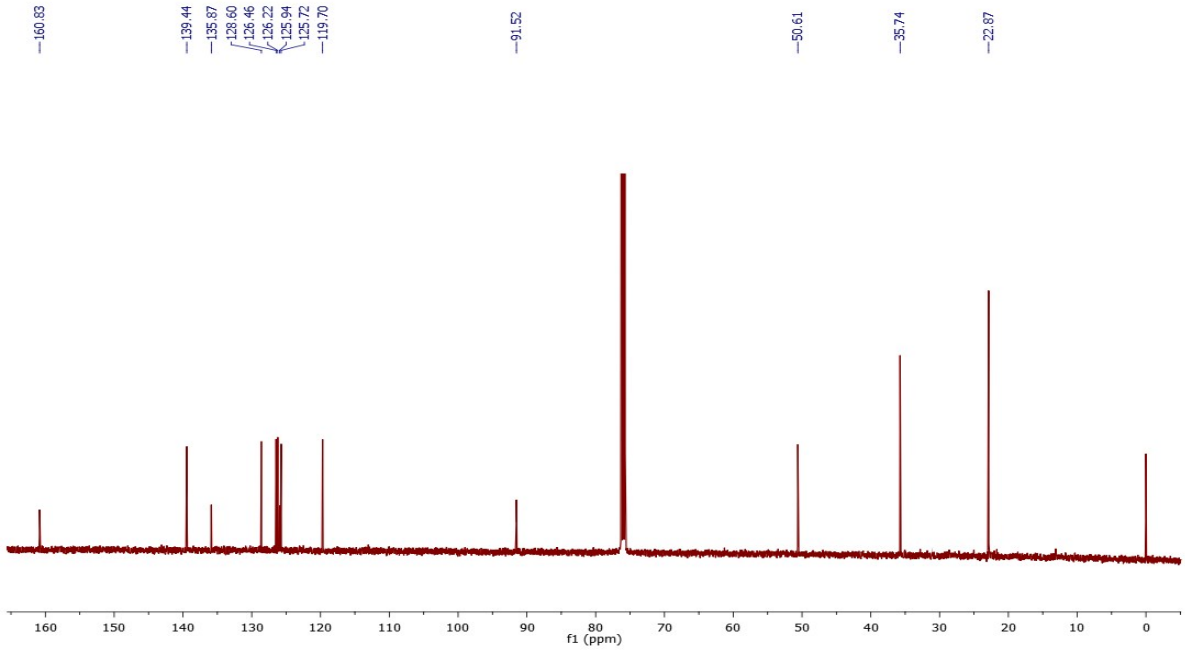
## LC-MS of 1-cyclopentyl*iso*-quinoline (3af)



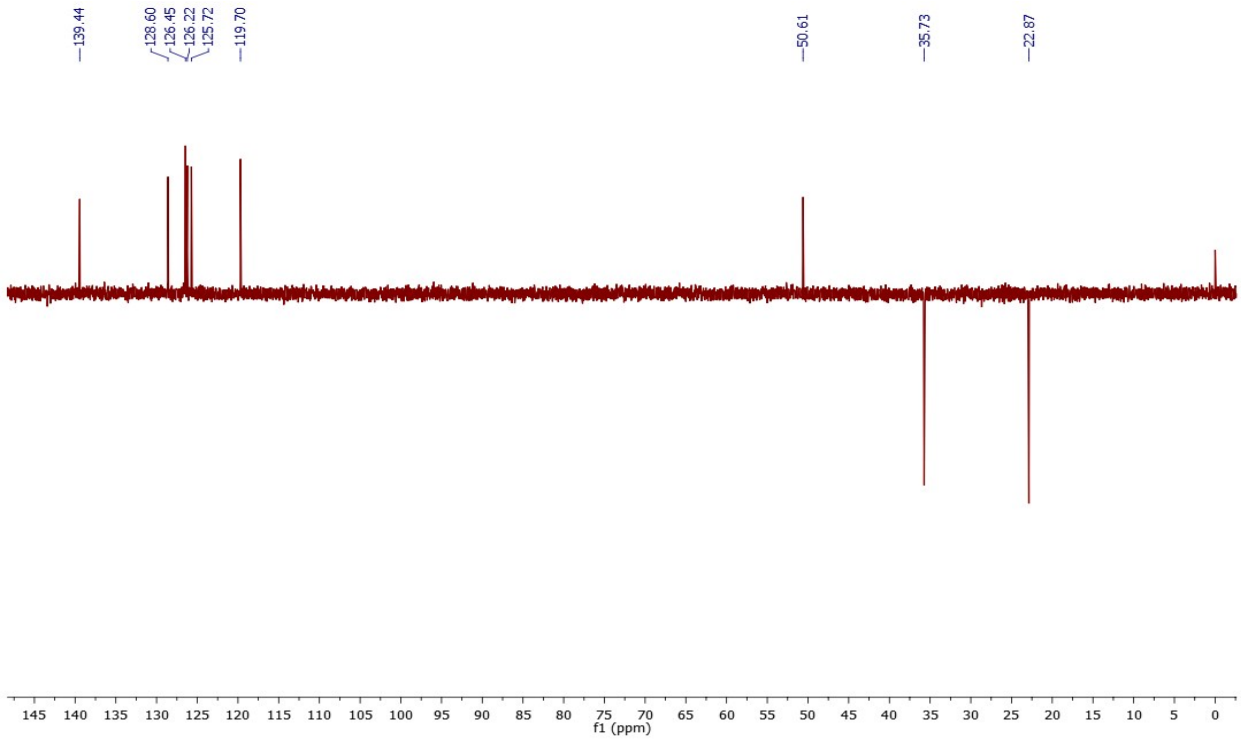

## $^{1}$H NMR of 1-(1-methoxycyclopentyl)*iso*-quinoline (3ag)



**$^{13}$C NMR of 1-(1-methoxycyclopentyl)*iso*-quinoline (3ag)**




**DEPT of 1-(1-methoxycyclopentyl)*iso*-quinoline (3ag)**

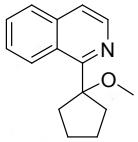


**HRMS of 1-(1-methoxycyclopentyl)*iso*-quinoline (3ag)**

## Qualitative Compound Report

| | | | |
|---|---|---|---|
| **Data File** | E-99(1).d | **Sample Name** | E-99(1) |
| **Sample Type** | Sample | **Position** | Vial 3 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | vishal_12-01-13.m | **Acquired Time** | 10-02-2015 PM 12:01:45 |
| **IRM Calibration Status** | Success | **DA Method** | daily_report.m |
| **Comment** | | | |

**Sample Group** **Info.**
**Acquisition SW Version** 6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

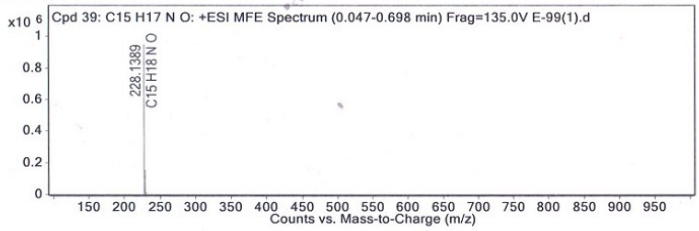



**Compound Table**

| Compound Label | RT | Mass | Formula | MFG Formula | MFG Diff (ppm) | DB Formula |
|---|---|---|---|---|---|---|
| Cpd 39: C15 H17 N O | 0.278 | 227.1317 | C15 H17 N O | C15 H17 N O | -3.12 | C15 H17 N O |

| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 39: C15 H17 N O | 228.1389 | 0.278 | Find by Molecular Feature | 227.1317 |

MFE MS Spectrum




**MS Spectrum Peak List**

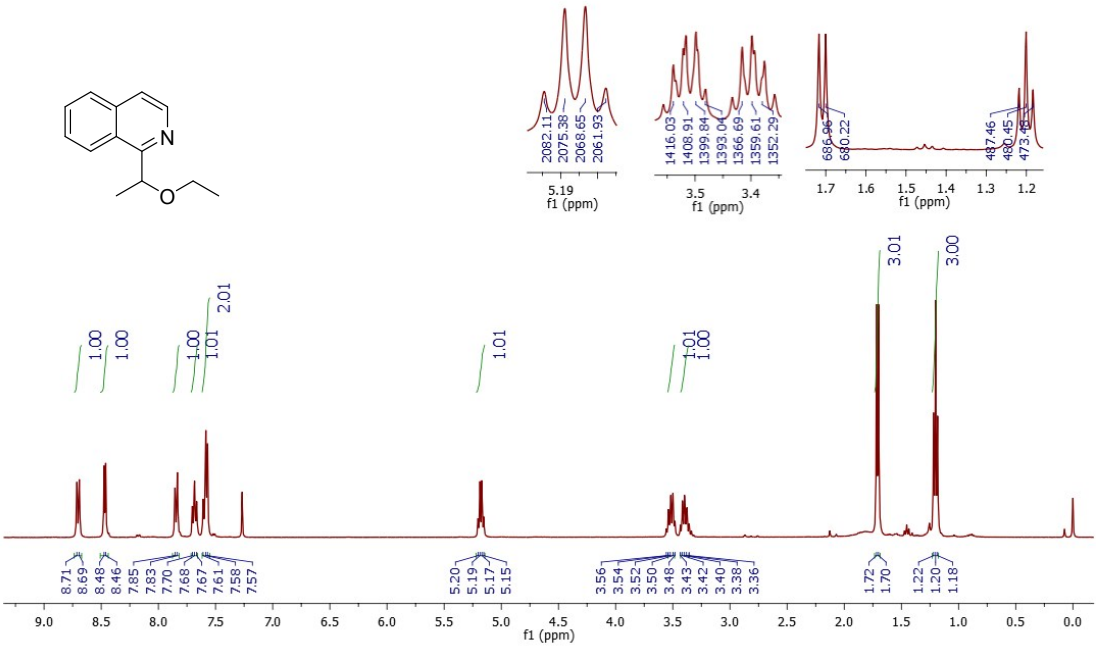
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 228.1389 | 1 | 946992.75 | C15 H18 N O | (M+H)+ |
| 229.1426 | 1 | 155516.95 | C15 H18 N O | (M+H)+ |
| 230.1454 | 1 | 13431.65 | C15 H18 N O | (M+H)+ |
| 231.148 | 1 | 1747.51 | C15 H18 N O | (M+H)+ |

**Predicted Isotope Match Table**

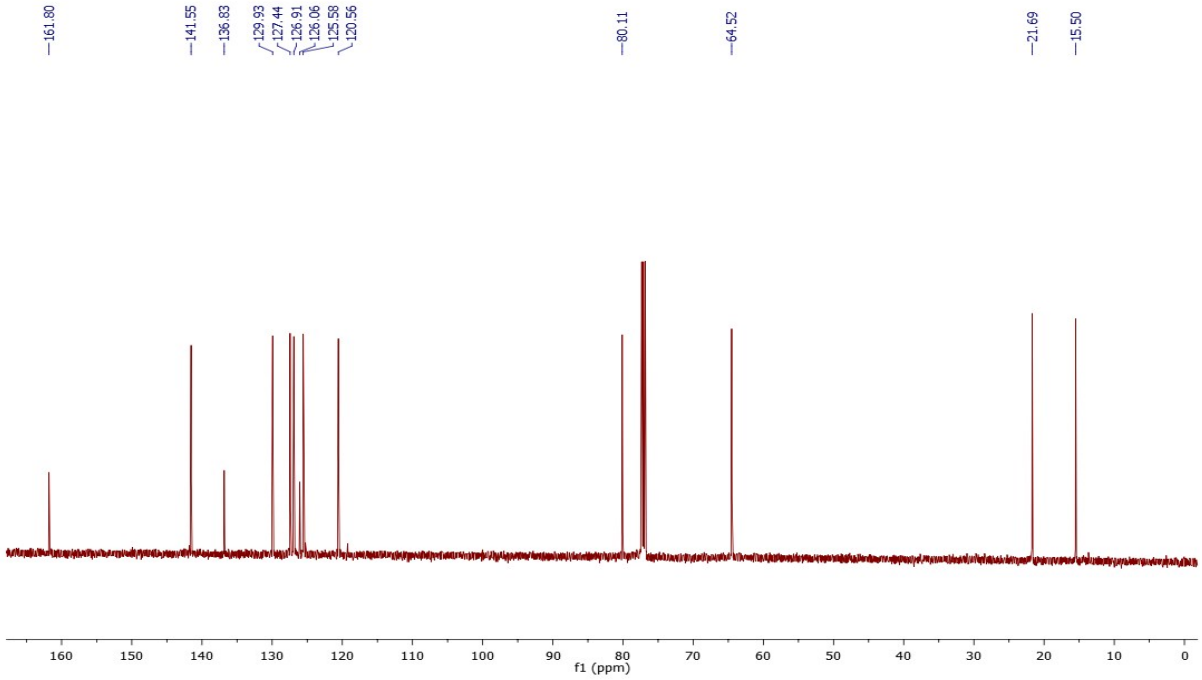
| Isotope | *m/z* | Calc m/z | Diff (ppm) | Abund % | Calc Abund % | Abund Sum % | Calc Abund Sum % |
|---|---|---|---|---|---|---|---|
| 1 | 228.1389 | 228.1383 | -2.84 | 100 | 100 | 84.73 | 84.41 |
| 2 | 229.1426 | 229.1415 | -4.63 | 16.42 | 16.83 | 13.91 | 14.21 |
| 3 | 230.1454 | 230.1445 | -4.1 | 1.42 | 1.53 | 1.2 | 1.29 |
| 4 | 231.148 | 231.1473 | -3.2 | 0.18 | 0.1 | 0.16 | 0.08 |

--- End Of Report ---

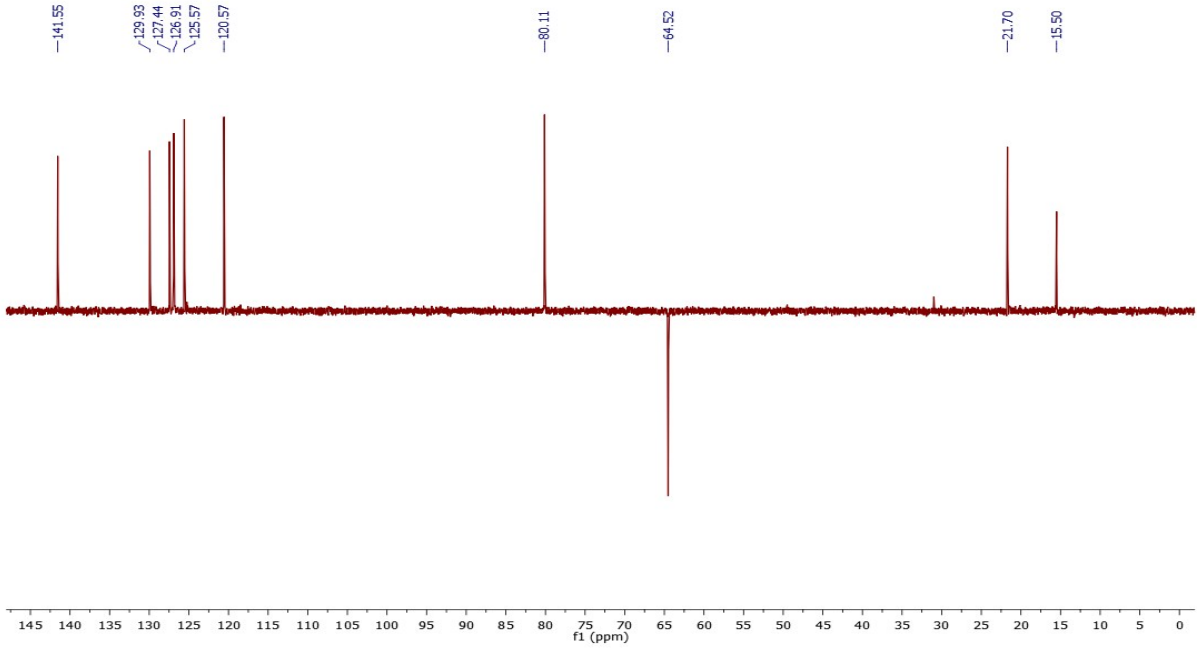
**$^{1}$H NMR of 1-(1-ethoxyethyl)*iso*-quinoline (3ah)**



**$^{13}$C NMR of 1-(1-ethoxyethyl)*iso*-quinoline (3ah)**



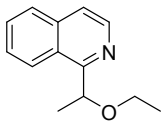

**DEPT of 1-(1-ethoxyethyl)*iso*-quinoline (3ah)**



**HRMS of 1-(1-ethoxyethyl)*iso*-quinoline (3ah)**

## Qualitative Compound Report

| | | | |
|---|---|---|---|
| **Data File** | E-153.d | **Sample Name** | E-153 |
| **Sample Type** | Sample | **Position** | Vial 16 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | vishal_12-01-13.m | **Acquired Time** | 07-02-2015 PM 12:40:05 |
| **IRM Calibration Status** | Success | **DA Method** | daily_report.m |
| **Comment** | | | |



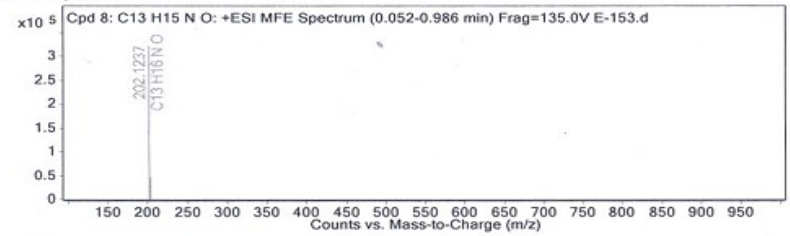

| | |
|---|---|
| **Sample Group** | **Info.** |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) |

**Compound Table**

| Compound Label | RT | Mass | Formula | MFG Formula | MFG Diff (ppm) | DB Formula |
|---|---|---|---|---|---|---|
| Cpd 8: C13 H15 N O | 0.277 | 201.1164 | C13 H15 N O | C13 H15 N O | -4.92 | C13 H15 N O |

| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 8: C13 H15 N O | 202.1237 | 0.277 | Find by Molecular Feature | 201.1164 |

MFE MS Spectrum




**MS Spectrum Peak List**

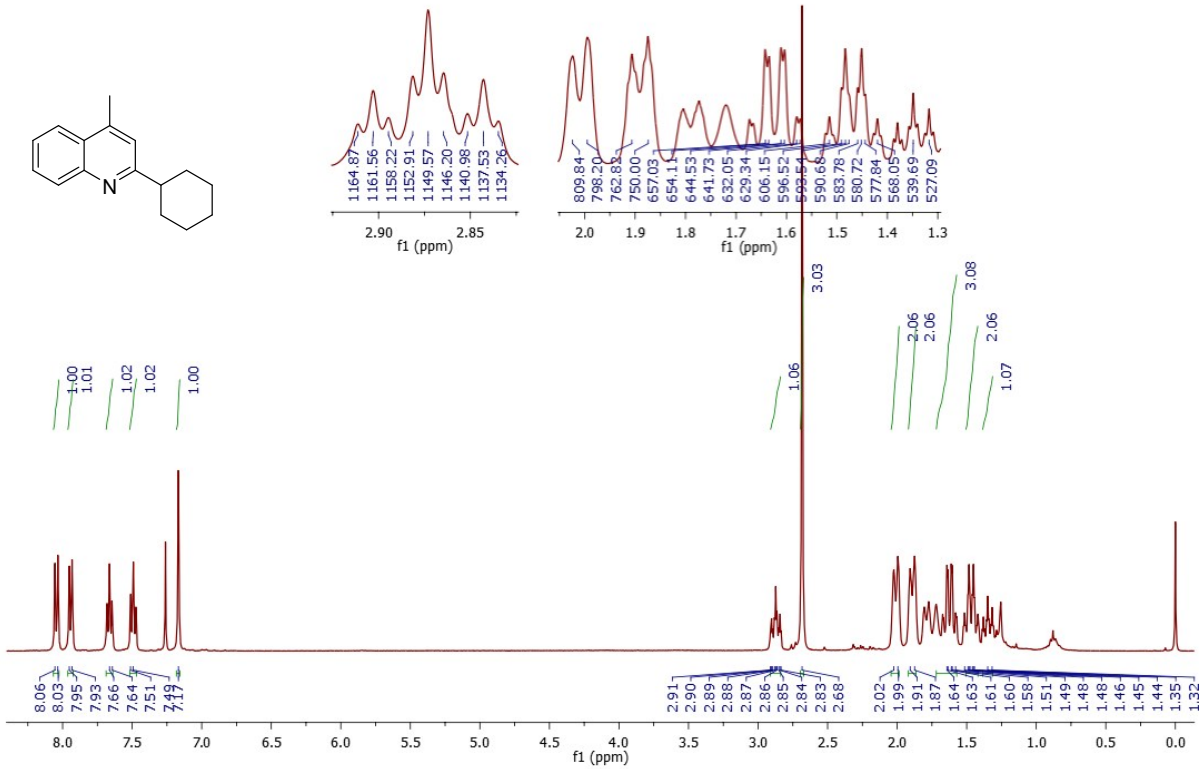
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 202.1237 | 1 | 322737.5 | C13 H16 N O | (M+H)+ |
| 203.1266 | 1 | 46865.66 | C13 H16 N O | (M+H)+ |
| 204.1298 | 1 | 4533.82 | C13 H16 N O | (M+H)+ |

**Predicted Isotope Match Table**

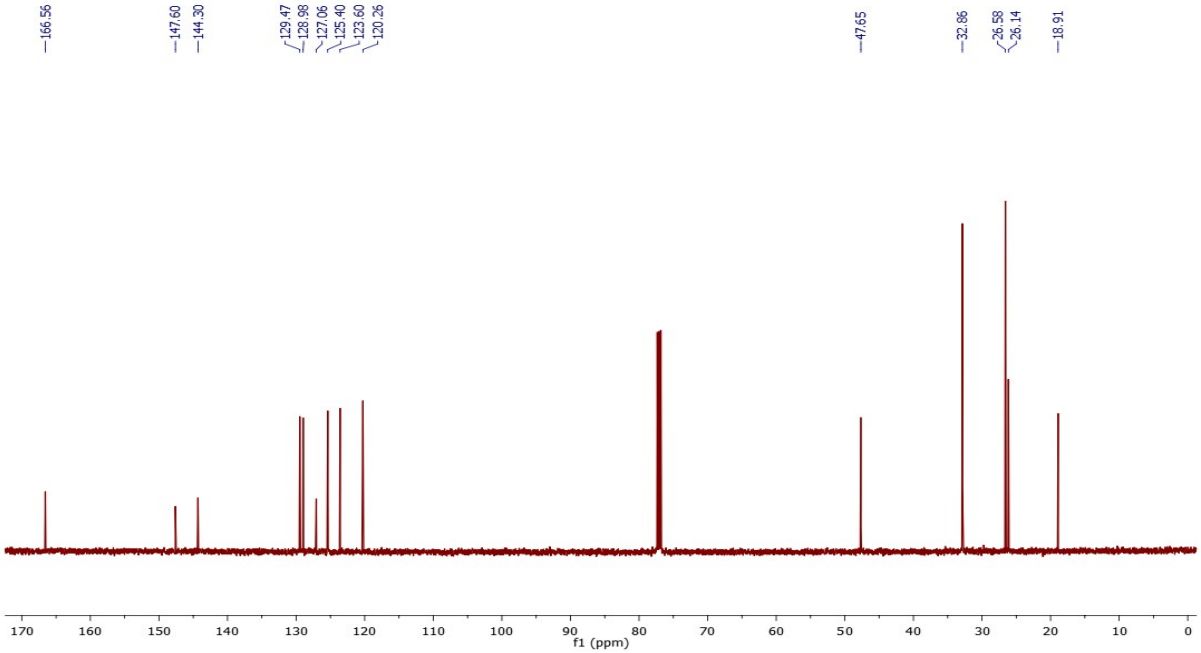
| Isotope | *m/z* | Calc m/z | Diff (ppm) | Abund % | Calc Abund % | Abund Sum % | Calc Abund Sum % |
|---|---|---|---|---|---|---|---|
| 1 | 202.1237 | 202.1226 | -5.07 | 100 | 100 | 86.26 | 86.32 |
| 2 | 203.1266 | 203.1259 | -3.61 | 14.52 | 14.65 | 12.53 | 12.64 |
| 3 | 204.1298 | 204.1287 | -5.43 | 1.4 | 1.2 | 1.21 | 1.04 |

--- End Of Report ---

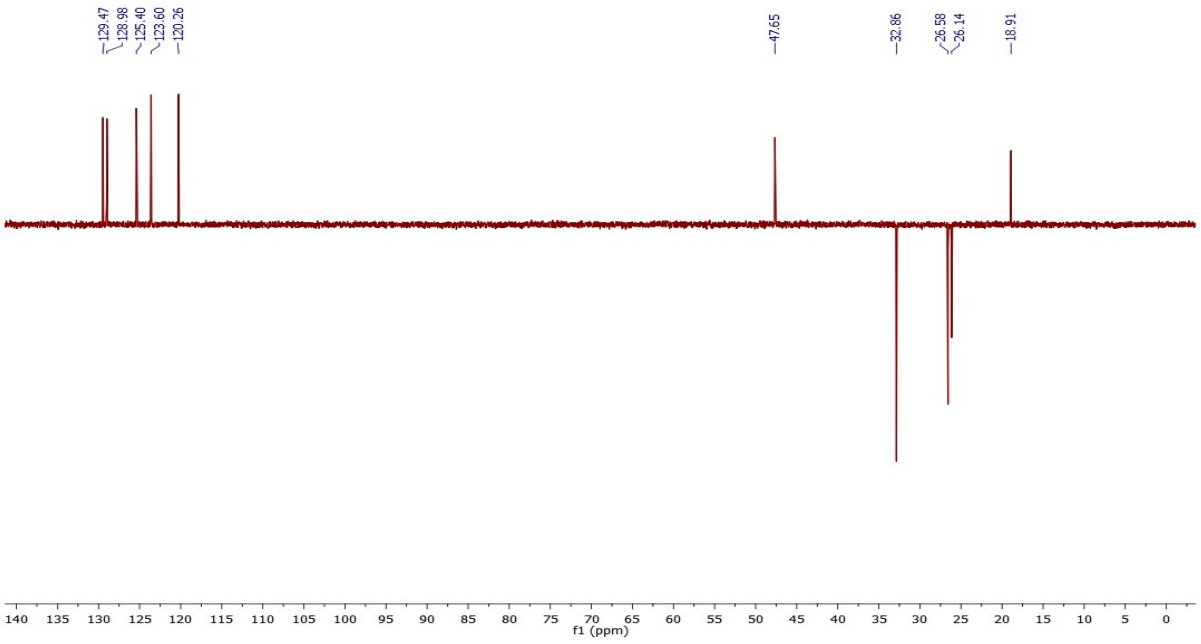
**$^{1}$H NMR of 2-cyclohexyl-4-methylquinoline (3be)**



## $^{13}$C NMR of 2-cyclohexyl-4-methylquinoline (3be)



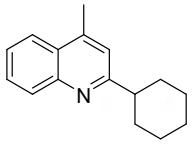

## DEPT of 2-cyclohexyl-4-methylquinoline (3be)



**HRMS of 2-cyclohexyl-4-methylquinoline (3be)**

## Qualitative Compound Report

| | | | |
|---|---|---|---|
| **Data File** | F-23.d | **Sample Name** | F-23 |
| **Sample Type** | Sample | **Position** | Vial 28 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | vishal_12-01-13.m | **Acquired Time** | 07-02-2015 PM 1:44:56 |
| **IRM Calibration Status** | Success | **DA Method** | daily_report.m |
| **Comment** | | | |



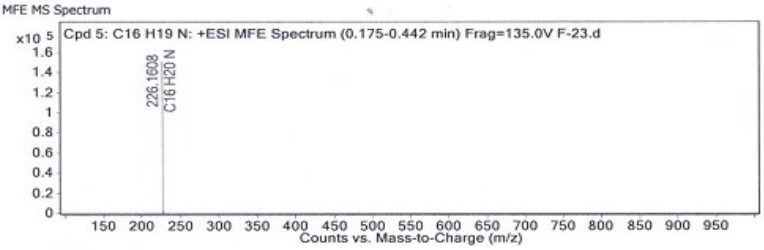

| | |
|---|---|
| **Sample Group** | **Info.** |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) |

**Compound Table**

| Compound Label | RT | Mass | Formula | MFG Formula | MFG Diff (ppm) | DB Formula |
|---|---|---|---|---|---|---|
| Cpd 5: C16 H19 N | 0.27 | 225.1535 | C16 H19 N | C16 H19 N | -7.77 | C16 H19 N |

| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 5: C16 H19 N | 226.1608 | 0.27 | Find by Molecular Feature | 225.1535 |

MFE MS Spectrum




**MS Spectrum Peak List**

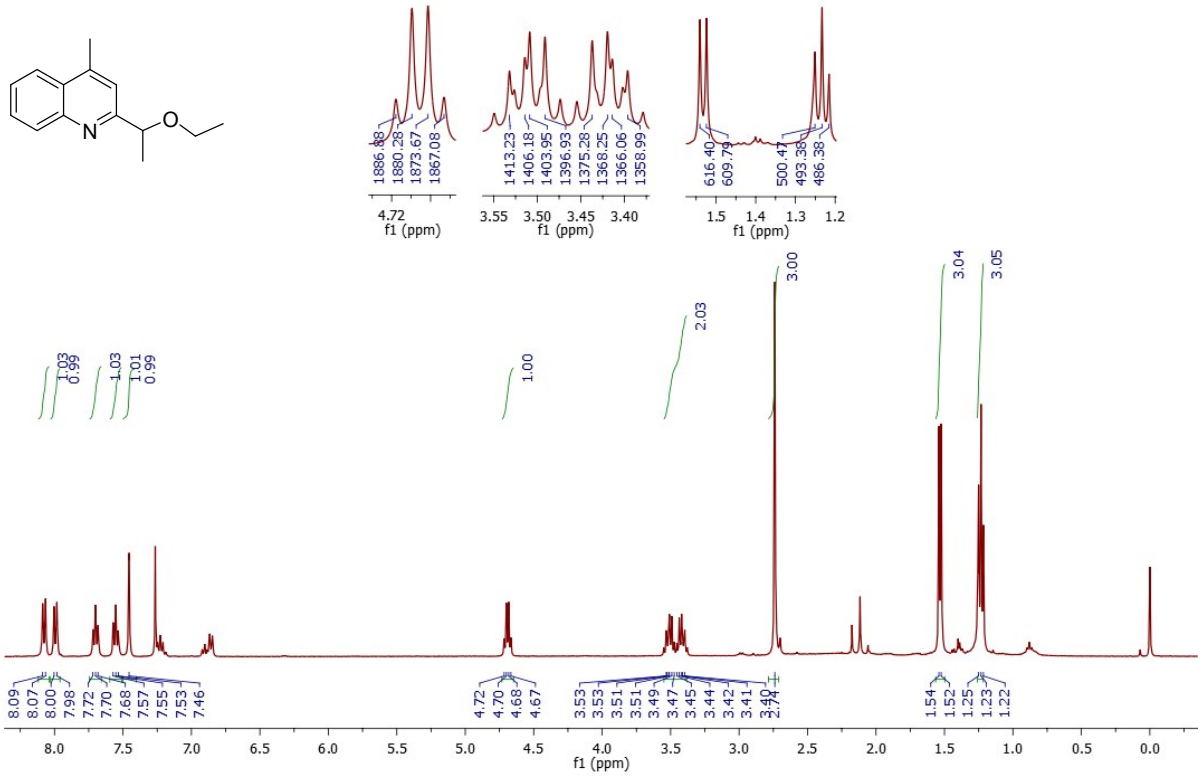
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 226.1608 | 1 | 151306.89 | C16 H20 N | (M+H)+ |
| 227.164 | 1 | 29351.84 | C16 H20 N | (M+H)+ |
| 228.1674 | 1 | 3087.13 | C16 H20 N | (M+H)+ |

**Predicted Isotope Match Table**

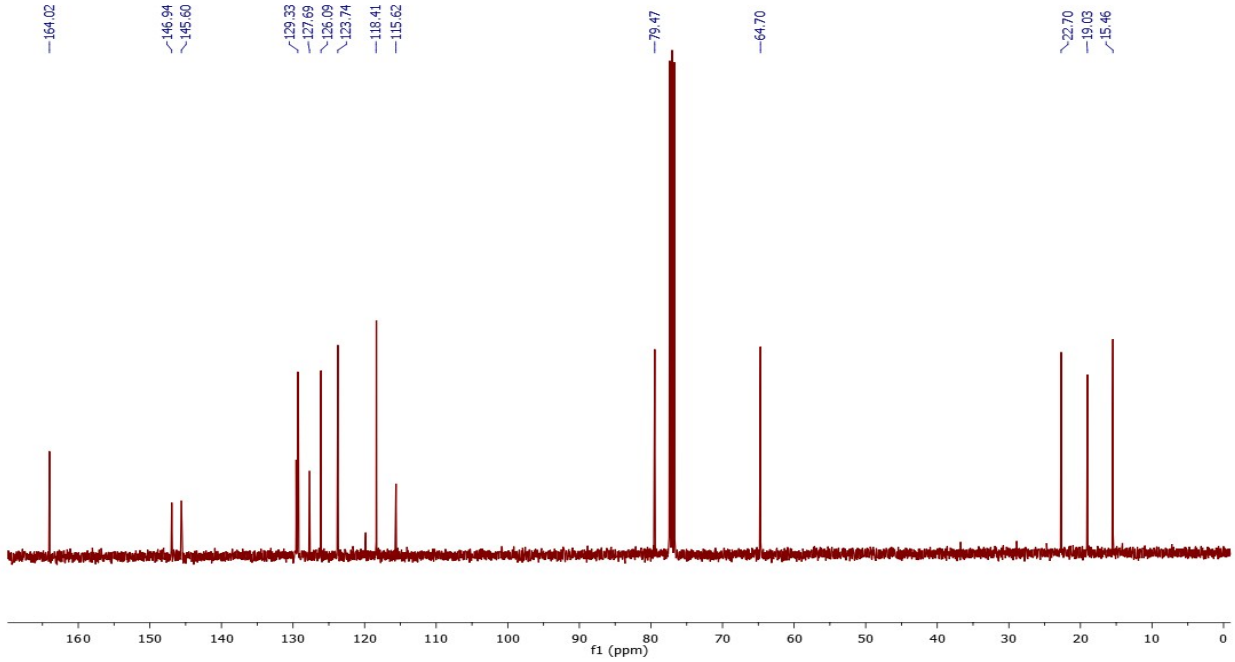
| Isotope | *m/z* | Calc m/z | Diff (ppm) | Abund % | Calc Abund % | Abund Sum % | Calc Abund Sum % |
|---|---|---|---|---|---|---|---|
| 1 | 226.1608 | 226.159 | -7.76 | 100 | 100 | 82.35 | 83.75 |
| 2 | 227.164 | 227.1623 | -7.49 | 19.4 | 17.9 | 15.97 | 14.99 |
| 3 | 228.1674 | 228.1655 | -8.23 | 2.04 | 1.51 | 1.68 | 1.26 |

--- End Of Report ---

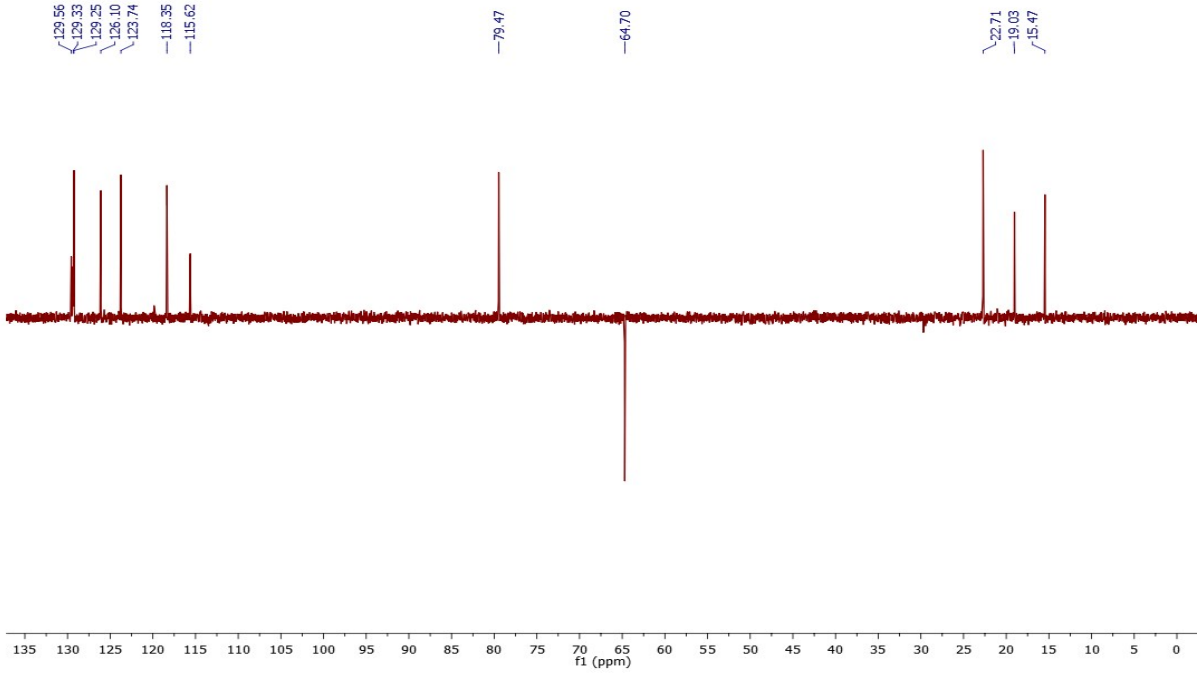
**$^{1}$H NMR of 2-(1-ethoxyethyl)-4-methylquinoline (3bh)**



**$^{13}$C NMR of 2-(1-ethoxyethyl)-4-methylquinoline (3bh)**




**DEPT of 2-(1-ethoxyethyl)-4-methylquinoline (3bh)**

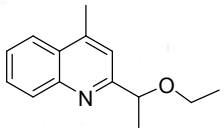


**HRMS of 2-(1-ethoxyethyl)-4-methylquinoline (3bh)**

## Qualitative Compound Report

| | | | |
|---|---|---|---|
| **Data File** | E-179.d | **Sample Name** | E-179 |
| **Sample Type** | Sample | **Position** | Vial 4 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | vishal_12-01-13.m | **Acquired Time** | 18-02-2015 PM 2:55:29 |
| **IRM Calibration Status** | Success | **DA Method** | daily_report.m |
| **Comment** | | | |

| | |
|---|---|
| **Sample Group** | **Info.** |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) |

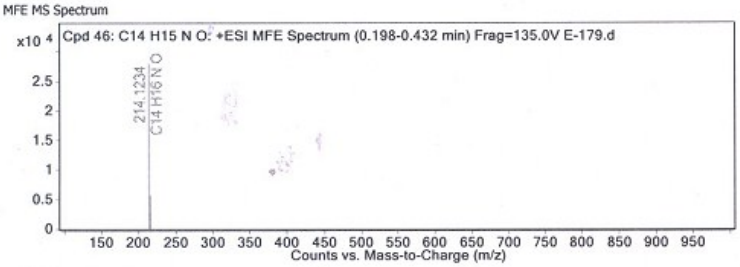



**Compound Table**

| Compound Label | RT | Mass | Formula | MFG Formula | MFG Diff (ppm) | DB Formula |
|---|---|---|---|---|---|---|
| Cpd 46: C14 H15 N O | 0.275 | 213.1164 | C14 H15 N O | C14 H15 N O | -5.01 | C14 H15 N O |

| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 46: C14 H15 N O | 214.1234 | 0.275 | Find by Molecular Feature | 213.1164 |

MFE MS Spectrum




**MS Spectrum Peak List**

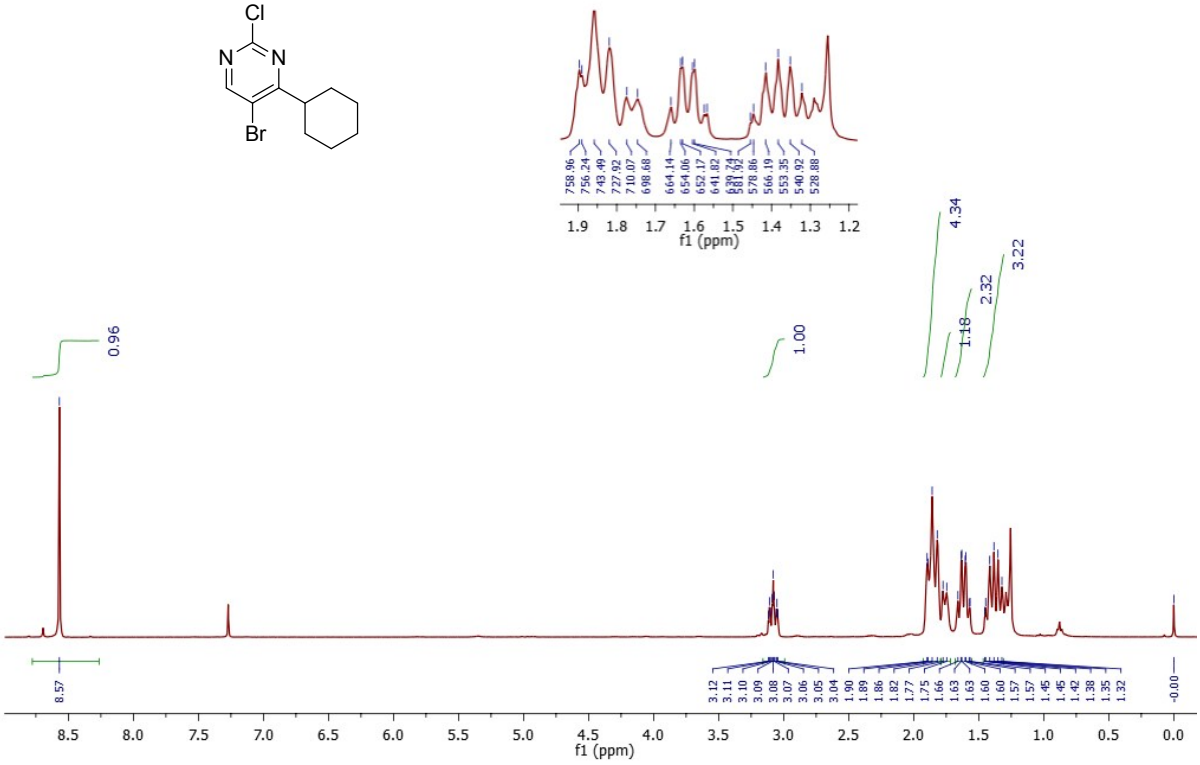
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 214.1234 | 1 | 27941.19 | C14 H16 N O | (M+H)+ |
| 215.1285 | 1 | 5759.62 | C14 H16 N O | (M+H)+ |

**Predicted Isotope Match Table**

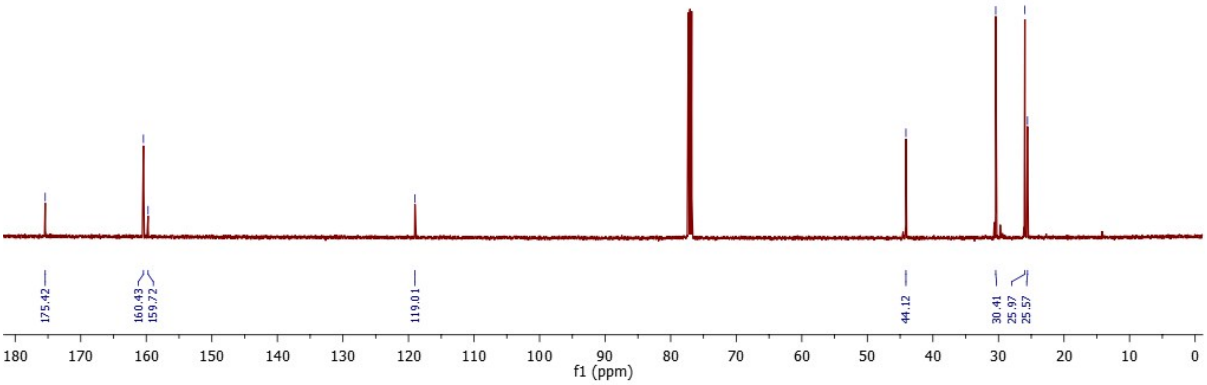
| Isotope | *m/z* | Calc m/z | Diff (ppm) | Abund % | Calc Abund % | Abund Sum % | Calc Abund Sum % |
|---|---|---|---|---|---|---|---|
| 1 | 214.1234 | 214.1226 | -3.52 | 100 | 100 | 82.91 | 86.41 |
| 2 | 215.1285 | 215.1259 | -12.04 | 20.61 | 15.73 | 17.09 | 13.59 |

--- End Of Report ---

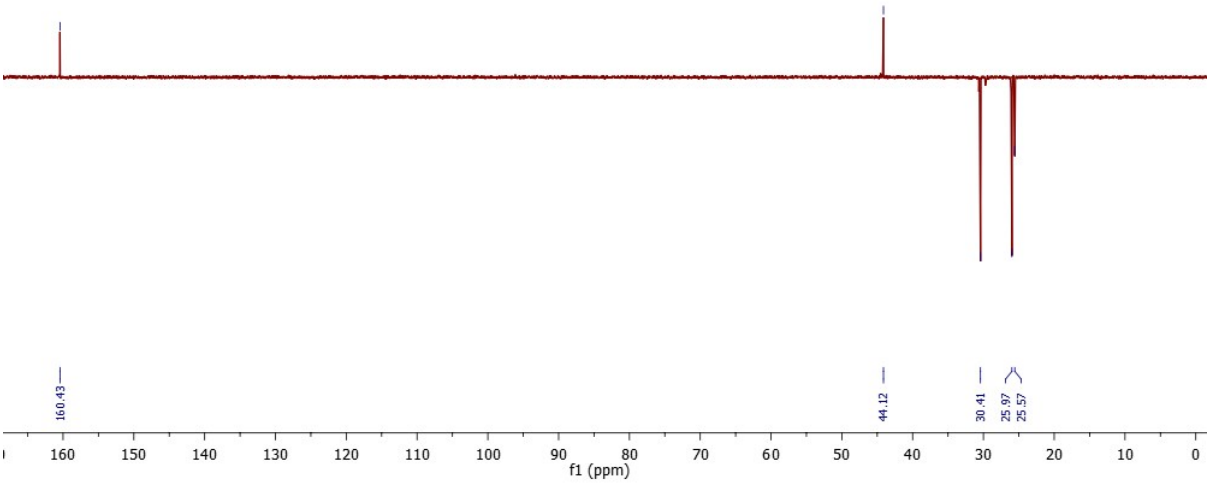
**[1]H NMR of 5-bromo-2-chloro-4-cyclohexylpyrimidine (3je)**



**$^{13}$C NMR of 5-bromo-2-chloro-4-cyclohexylpyrimidine (3je)**



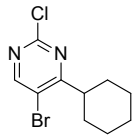

**DEPT NMR of 5-bromo-2-chloro-4-cyclohexylpyrimidine (3je)**



**HRMS spectra of 5-bromo-2-chloro-4-cyclohexylpyrimidine (3je)**

## Qualitative Compound Report

| | | | |
|---|---|---|---|
| **Data File** | 2clbr-ch.d | **Sample Name** | 2clbr-ch |
| **Sample Type** | Sample | **Position** | Vial 7 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | vishal_12-01-13.m | **Acquired Time** | 09-02-2015 PM 12:24:46 |
| **IRM Calibration Status** | Success | **DA Method** | daily_report.m |
| **Comment** | | | |



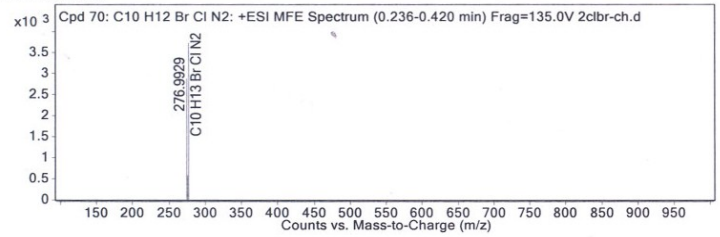

| | |
|---|---|
| **Sample Group** | **Info.** |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) |

**Compound Table**

| Compound Label | RT | Mass | Formula | MFG Formula | MFG Diff (ppm) | DB Formula |
|---|---|---|---|---|---|---|
| Cpd 70: C10 H12 Br Cl N2 | 0.288 | 273.9882 | C10 H12 Br Cl N2 | C10 H12 Br Cl N2 | -3.55 | C10 H12 Br Cl N2 |

| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 70: C10 H12 Br Cl N2 | 274.9958 | 0.288 | Find by Molecular Feature | 273.9882 |

MFE MS Spectrum




**MS Spectrum Peak List**

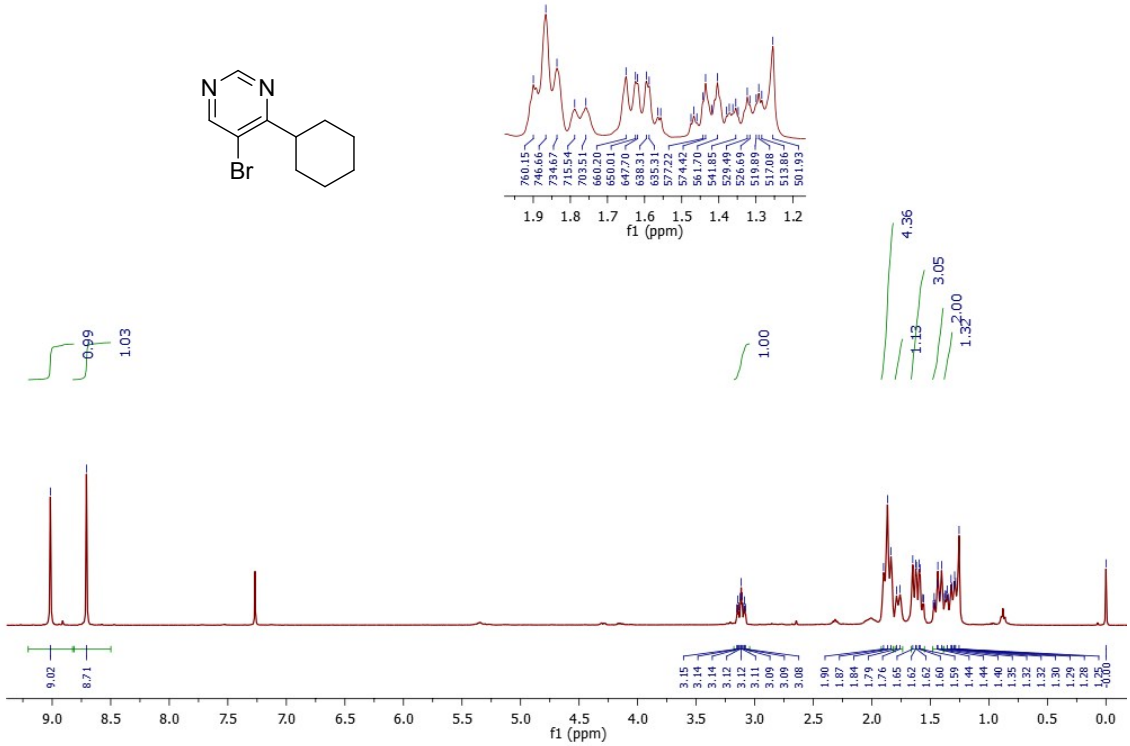
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 274.9958 | 1 | 2869.49 | C10 H13 Br Cl N2 | (M+H)+ |
| 275.9958 | 1 | 577.27 | C10 H13 Br Cl N2 | (M+H)+ |
| 276.9929 | 1 | 3716.29 | C10 H13 Br Cl N2 | (M+H)+ |
| 277.9989 | 1 | 804.33 | C10 H13 Br Cl N2 | (M+H)+ |

**Predicted Isotope Match Table**

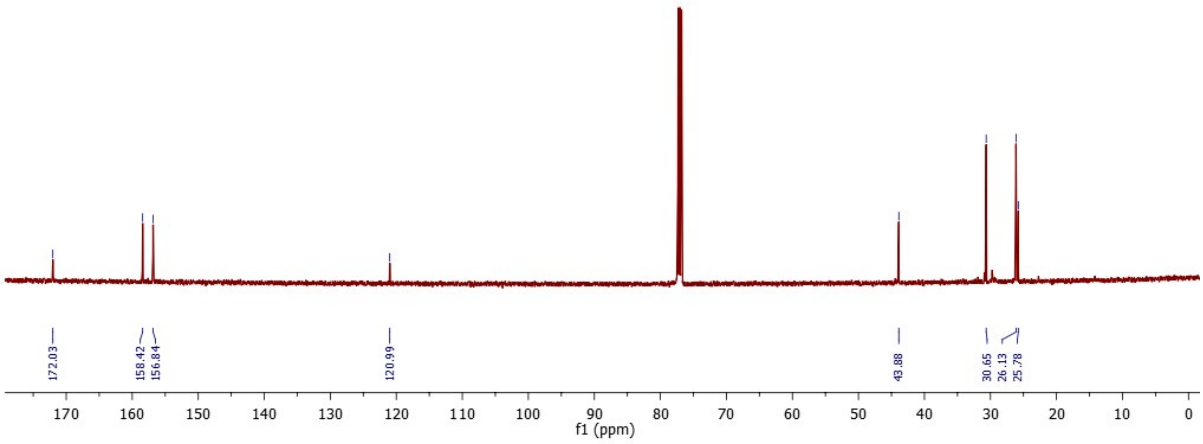
| Isotope | *m/z* | Calc m/z | Diff (ppm) | Abund % | Calc Abund % | Abund Sum % | Calc Abund Sum % |
|---|---|---|---|---|---|---|---|
| 1 | 274.9958 | 274.9945 | -4.5 | 77.21 | 76.98 | 36.02 | 38.95 |
| 2 | 275.9958 | 275.9975 | 6.17 | 15.53 | 9 | 7.25 | 4.56 |
| 3 | 276.9929 | 276.9923 | -2.15 | 100 | 100 | 46.64 | 50.6 |
| 4 | 277.9989 | 277.9953 | -13.24 | 21.64 | 11.66 | 10.1 | 5.9 |

--- End Of Report ---

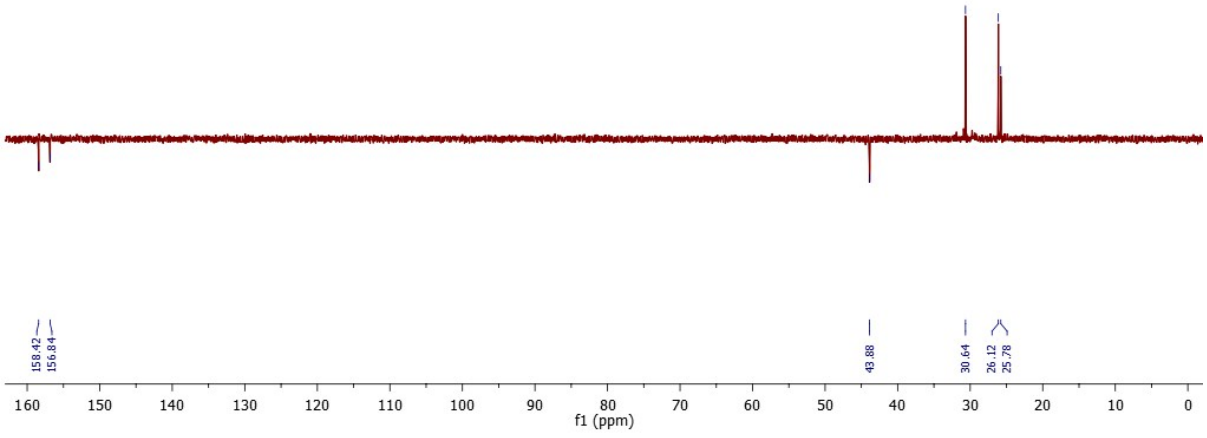
**$^{1}$H NMR of 5-bromo-4-cyclohexylpyrimidine (3ke)**



**$^{13}$C NMRof 5-bromo-4-cyclohexylpyrimidine (3ke)**




**DEPT NMR of 5-bromo-4-cyclohexylpyrimidine (3ke)**

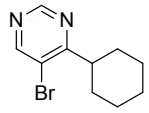


**HRMS of 5-bromo-4-cyclohexylpyrimidine (3ke)**

## Qualitative Compound Report

| | | | |
|---|---|---|---|
| **Data File** | 5BrPy-CH.d | **Sample Name** | 5BrPy-CH |
| **Sample Type** | Sample | **Position** | Vial 15 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | vishal_12-01-13.m | **Acquired Time** | 03-02-2015 PM 2:30:00 |
| **IRM Calibration Status** | Success | **DA Method** | daily_report.m |
| **Comment** | | | |

| | |
|---|---|
| **Sample Group** | **Info.** |
| **Acquisition SW Version** | 6200 series TOF/6500 series Q-TOF B.05.01 (B5125) |

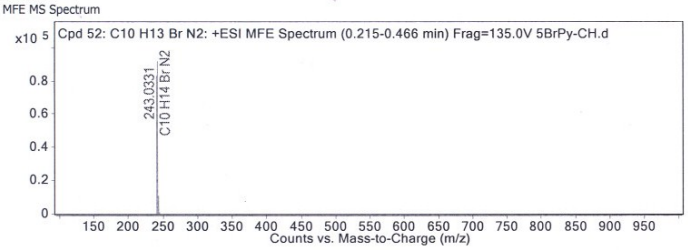



**Compound Table**

| Compound Label | RT | Mass | Formula | MFG Formula | MFG Diff (ppm) | DB Formula |
|---|---|---|---|---|---|---|
| Cpd 52: C10 H13 Br N2 | 0.291 | 240.0279 | C10 H13 Br N2 | C10 H13 Br N2 | -7.22 | C10 H13 Br N2 |

| Compound Label | *m/z* | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 52: C10 H13 Br N2 | 241.0352 | 0.291 | Find by Molecular Feature | 240.0279 |

MFE MS Spectrum




**MS Spectrum Peak List**

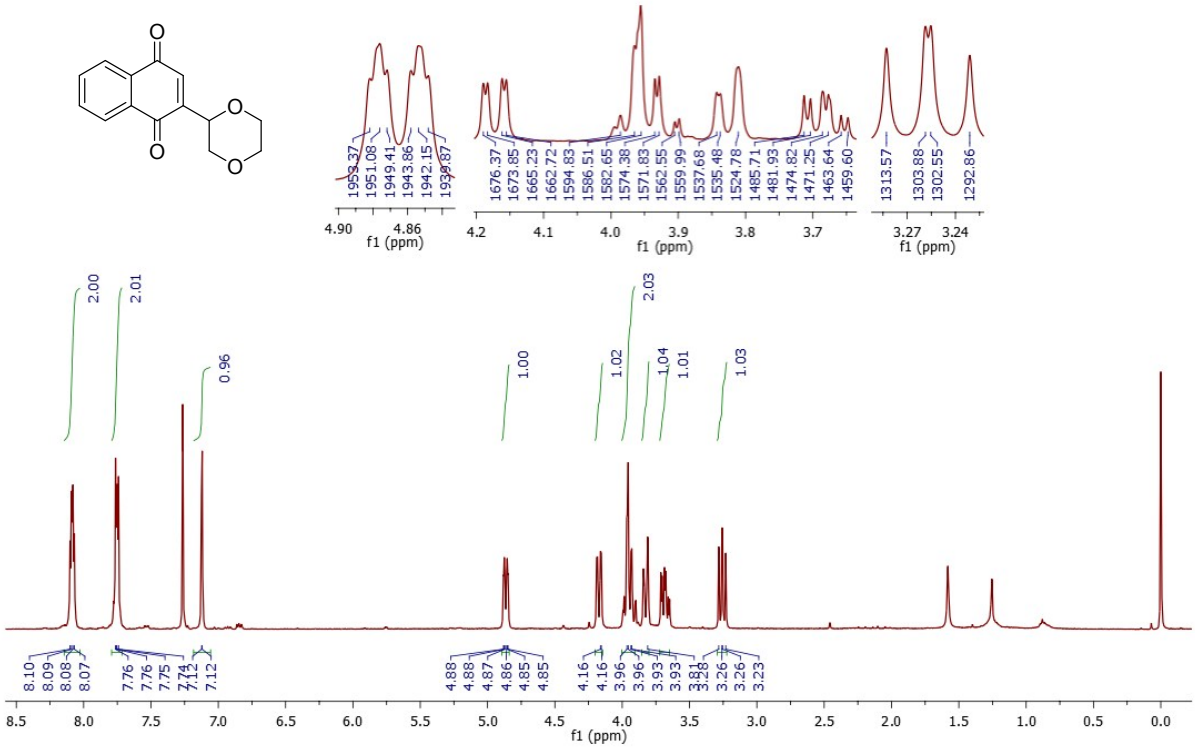
| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 241.0352 | 1 | 82961.88 | C10 H14 Br N2 | (M+H)+ |
| 242.0384 | 1 | 10289.44 | C10 H14 Br N2 | (M+H)+ |
| 243.0331 | 1 | 91797.52 | C10 H14 Br N2 | (M+H)+ |
| 244.0367 | 1 | 10656.15 | C10 H14 Br N2 | (M+H)+ |
| 245.0391 | 1 | 883.72 | C10 H14 Br N2 | (M+H)+ |

**Predicted Isotope Match Table**

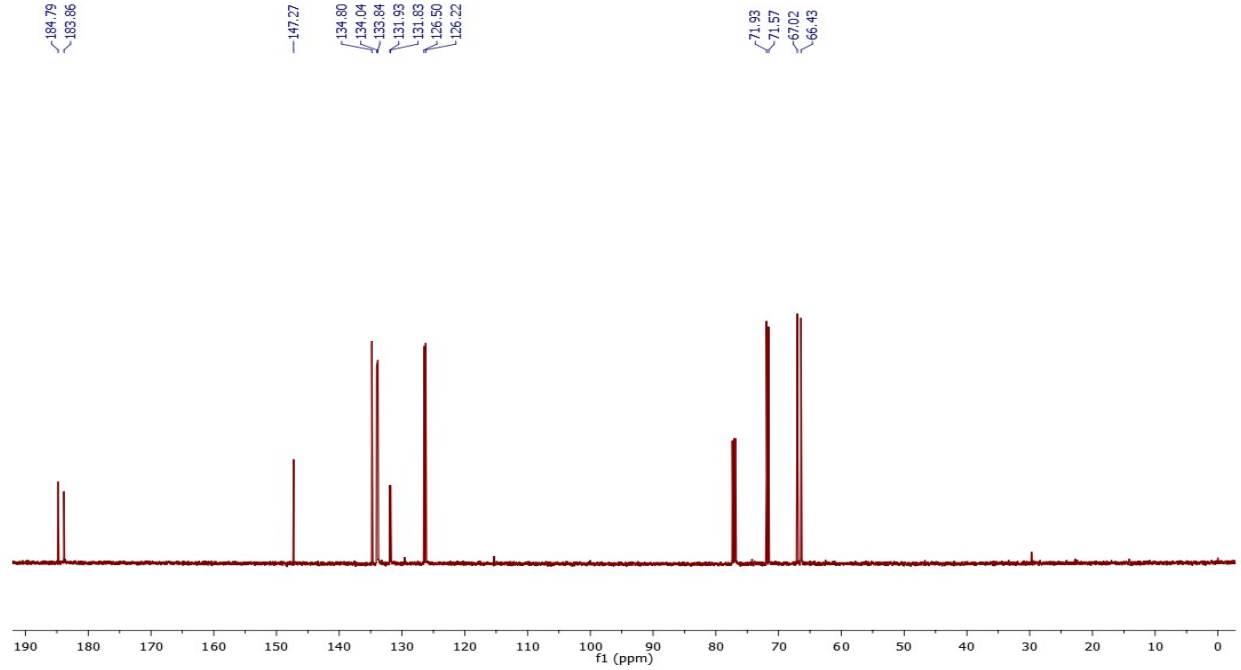
| Isotope | *m/z* | Calc m/z | Diff (ppm) | Abund % | Calc Abund % | Abund Sum % | Calc Abund Sum % |
|---|---|---|---|---|---|---|---|
| 1 | 241.0352 | 241.0335 | -7.17 | 90.37 | 100 | 42.2 | 45.12 |
| 2 | 242.0384 | 242.0365 | -7.88 | 11.21 | 11.71 | 5.23 | 5.28 |
| 3 | 243.0331 | 243.0315 | -6.82 | 100 | 97.9 | 46.7 | 44.17 |
| 4 | 244.0367 | 244.0345 | -9.23 | 11.61 | 11.41 | 5.42 | 5.15 |
| 5 | 245.0391 | 245.0374 | -7.11 | 0.96 | 0.61 | 0.45 | 0.27 |

--- End Of Report ---

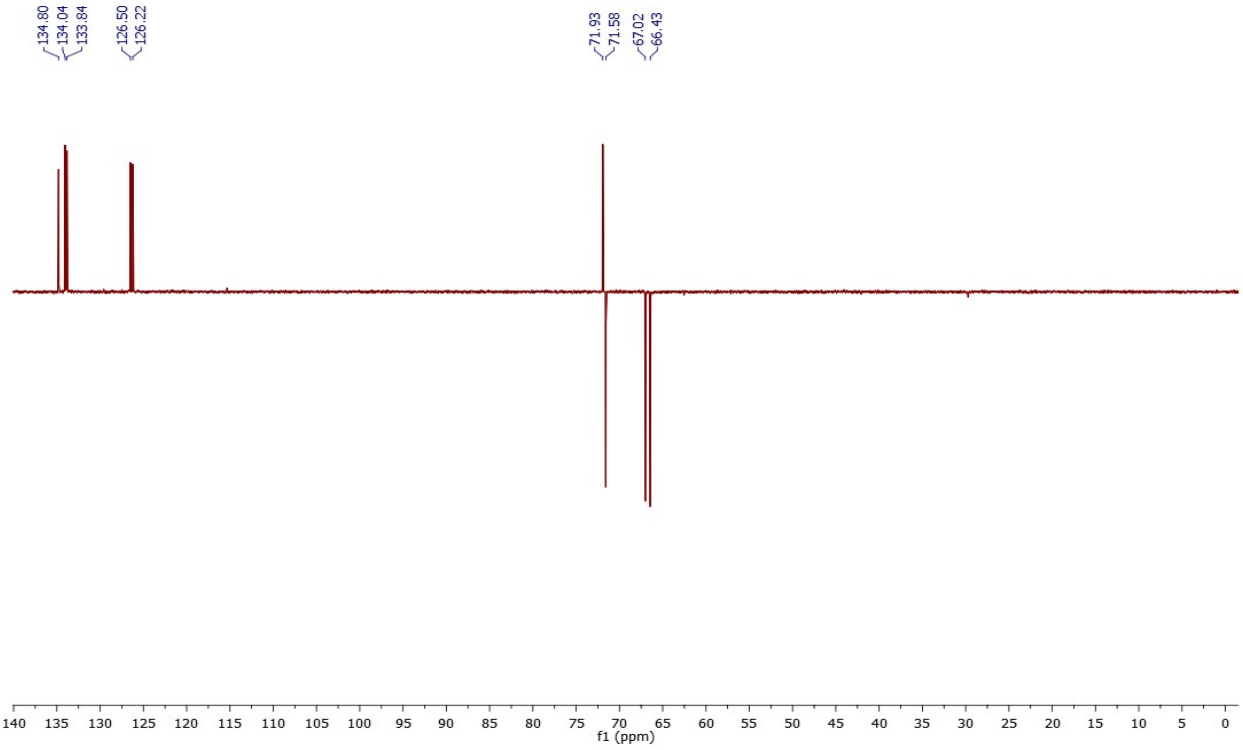
**$^{1}$H NMR of 2-(1,4-dioxan-2-yl)naphthalene-1,4-dione (5aa)**



**$^{13}$C NMR of 2-(1,4-dioxan-2-yl)naphthalene-1,4-dione (5aa)**




**DEPT of 2-(1,4-dioxan-2-yl)naphthalene-1,4-dione (5aa)**



**GC-MS of 2-(1,4-dioxan-2-yl)naphthalene-1,4-dione (5aa)**