

## Supporting Information

### Synthesis of C2-tetrasubstituted indolin-3-ones via Cu-catalyzed oxidative dimerization of 2-aryl indoles and cross-addition of indoles

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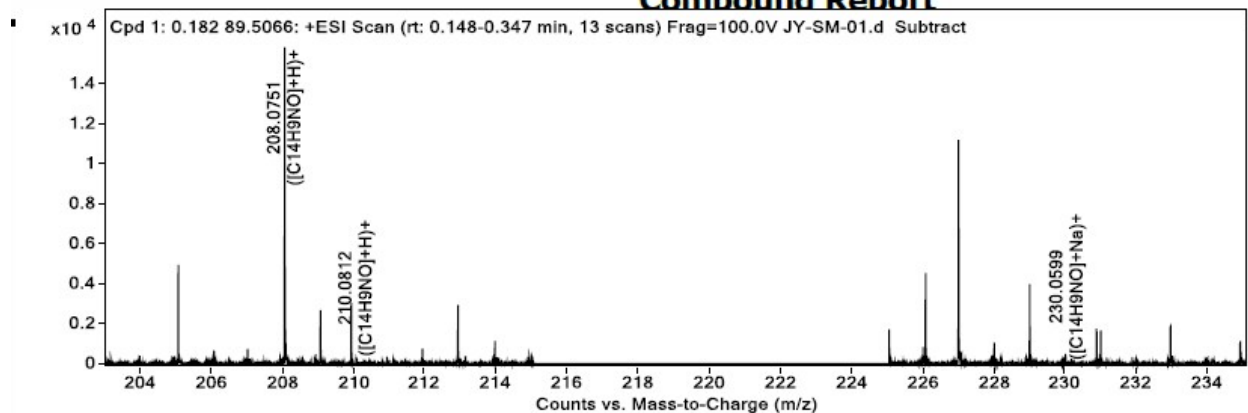
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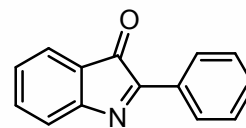
## HRMS Facility, BITS Pilani, Pilani Campus

### Compound Report



MS Spectrum Peak List

| m/z      | Calc m/z | Diff(ppm) | z | Abund    | Formula                           | Ion                 |
|----------|----------|-----------|---|----------|-----------------------------------|---------------------|
| 208.0751 | 208.0757 | 2.63      | 1 | 16179.21 | C <sub>14</sub> H <sub>9</sub> NO | (M+H) <sup>+</sup>  |
| 209.0794 | 209.0789 | -2.3      | 1 | 2670.21  | C <sub>14</sub> H <sub>9</sub> NO | (M+H) <sup>+</sup>  |
| 210.0812 | 210.0818 | 3.01      | 1 | 238.68   | C <sub>14</sub> H <sub>9</sub> NO | (M+H) <sup>+</sup>  |
| 230.0599 | 230.0576 | -9.85     | 1 | 59.78    | C <sub>14</sub> H <sub>9</sub> NO | (M+Na) <sup>+</sup> |



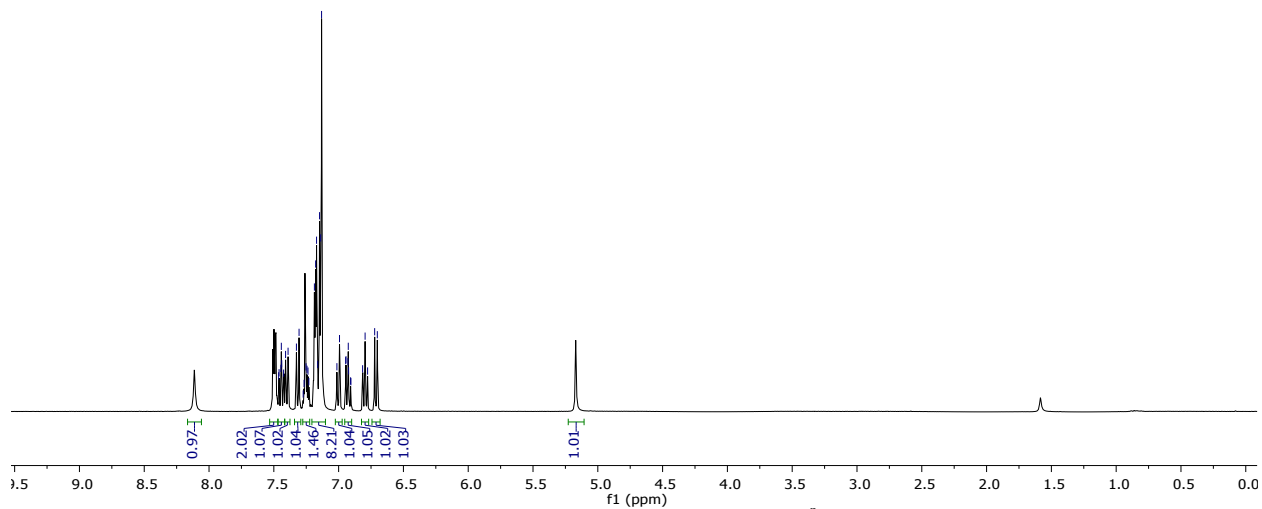
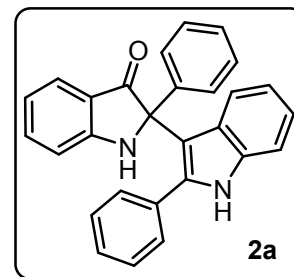
Calcd m/z = 208.0762

Found m/z = 208.0757

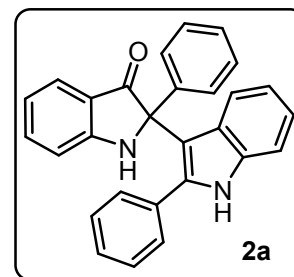
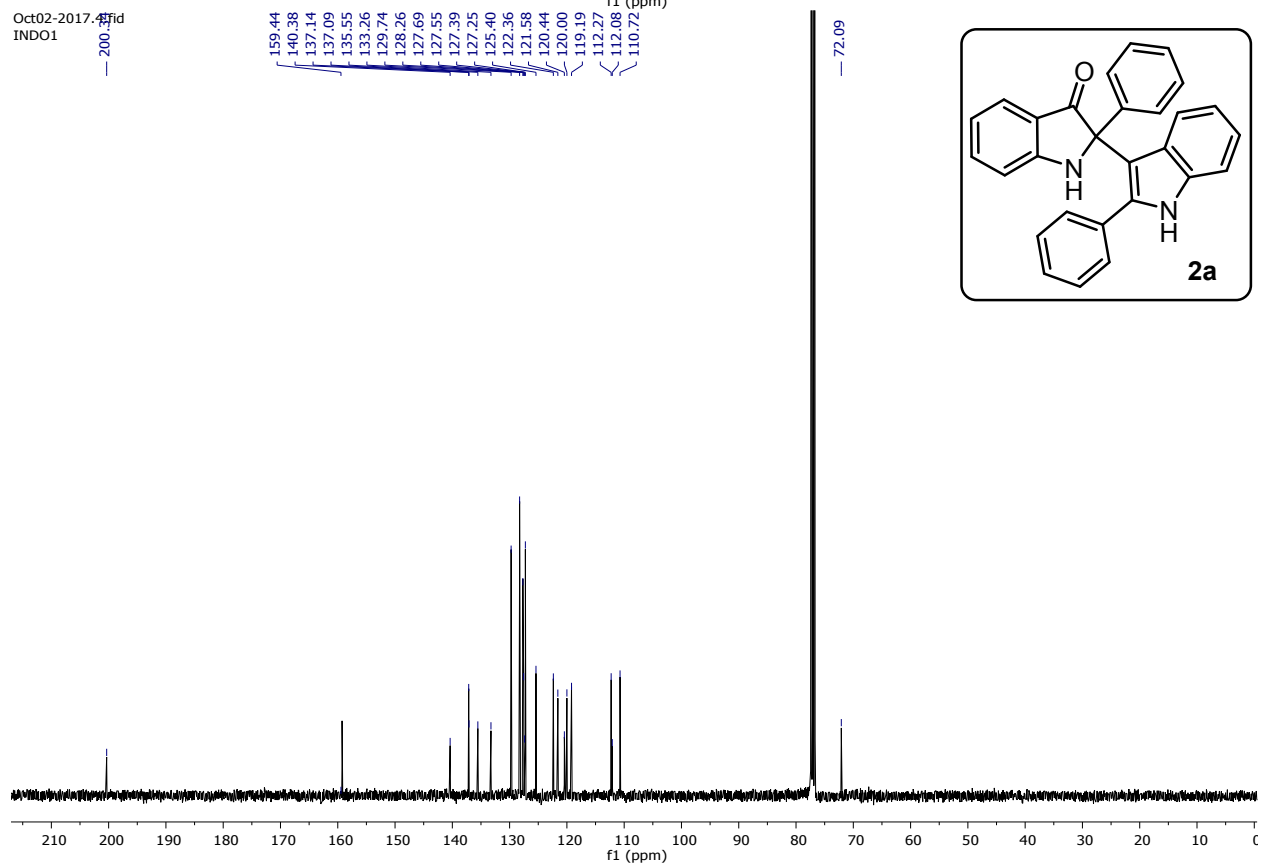
Instrument Info : Agilent Technologies 6545 Q-TOF LC/MS

**Figure S1:** HRMS confirmation of in situ generated 2-phenyl indole-3-one

Oct02-2017-47f1  
INDO1



Oct02-2017-47f1  
INDO1



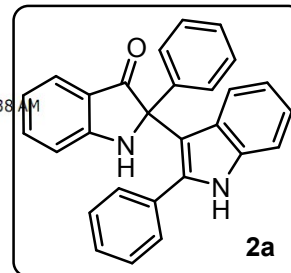
# Qualitative Compound Report

**Data File** IND 01.d  
**Sample Type** Sample  
**Instrument Name** Instrument 1  
**Acq Method** water\_meoh\_grad\_6min\_reg.m  
**IRM Calibration Status** Success  
**Comment**

**Sample Name** IND 01  
**Position** P2-D3  
**User Name**  
**Acquired Time** 1/5/2018 11:05:38 AM  
**DA Method** PROCESSNEW.m

**Sample Group**  
**Stream Name** LC 1

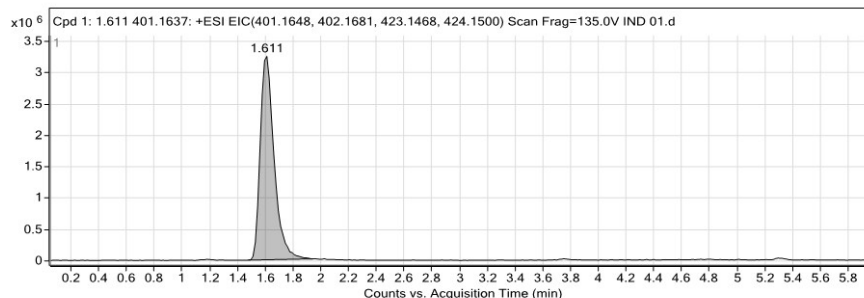
**Info.**  
**Acquisition SW** 6200 series TOF/6500 series  
**Version** Q-TOF B.06.01 (B6172 SP1)



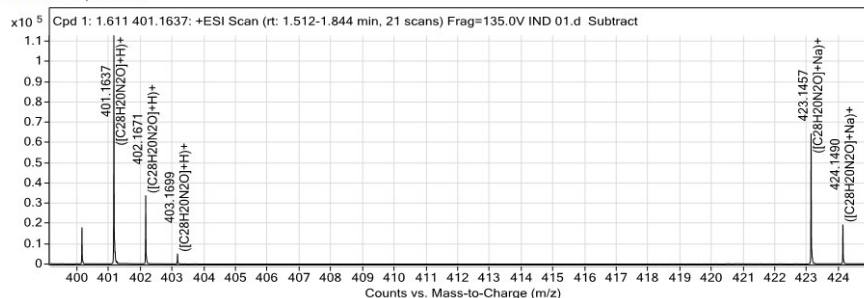
## Compound Table

| Compound Label        | RT    | Mass     | Abund  | Formula      | Tgt Mass | Diff (ppm) |
|-----------------------|-------|----------|--------|--------------|----------|------------|
| Cpd 1: 1.611 401.1637 | 1.611 | 400.1565 | 112812 | C28 H20 N2 O | 400.1576 | -2.73      |

| Compound Label        | m/z      | RT    | Algorithm       | Mass     |
|-----------------------|----------|-------|-----------------|----------|
| Cpd 1: 1.611 401.1637 | 401.1637 | 1.611 | Find By Formula | 400.1565 |



## MS Zoomed Spectrum

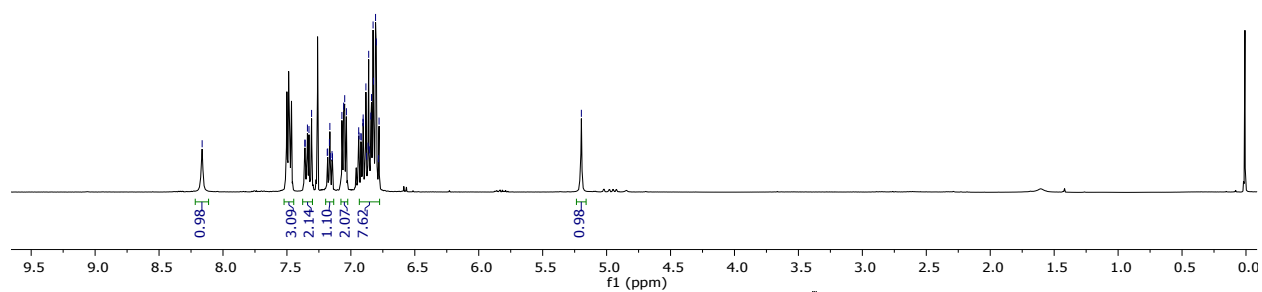


## MS Spectrum Peak List

| m/z      | Calc m/z | Diff(ppm) | z | Abund     | Formula   | Ion    |
|----------|----------|-----------|---|-----------|-----------|--------|
| 401.1637 | 401.1648 | 2.91      | 1 | 112812.26 | C28H20N2O | (M+H)+ |
| 402.1671 | 402.1681 | 2.42      | 1 | 33913.1   | C28H20N2O | (M+H)+ |

A number line from -8.16 to 5.20 with tick marks every 0.01. The line is divided into three sections by brackets: the first section from -8.16 to -7.18 is labeled 'a', the second section from -7.18 to 0.00 is labeled 'b', and the third section from 0.00 to 5.20 is labeled 'c'. The tick marks are labeled with their respective decimal values.

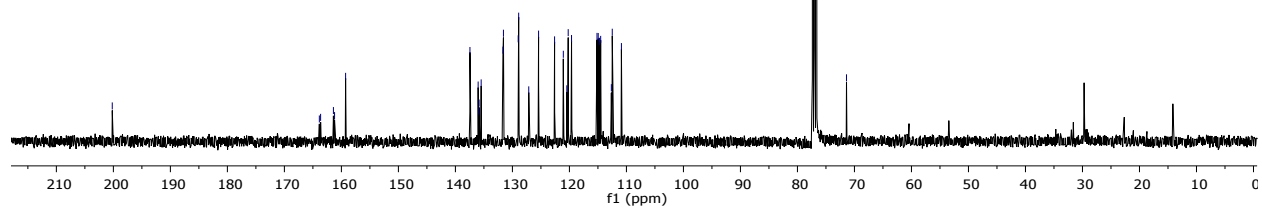
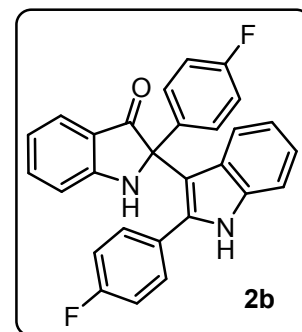
| Section | Value |
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| a       | -8.16 |
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|         | -8.14 |
|         | -8.13 |
|         | -8.12 |
|         | -8.11 |
|         | -8.10 |
|         | -8.09 |
|         | -8.08 |
|         | -8.07 |
| b       | -8.06 |
|         | -8.05 |
|         | -8.04 |
|         | -8.03 |
|         | -8.02 |
|         | -8.01 |
|         | -8.00 |
|         | -7.99 |
|         | -7.98 |
|         | -7.97 |
| c       | -7.96 |
|         | -7.95 |
|         | -7.94 |
|         | -7.93 |
|         | -7.92 |
|         | -7.91 |
|         | -7.90 |
|         | -7.89 |
|         | -7.88 |
|         | -7.87 |
|         | -7.86 |
|         | -7.85 |
|         | -7.84 |
|         | -7.83 |
|         | -7.82 |
|         | -7.81 |
|         | -7.80 |
|         | -7.79 |
|         | -7.78 |
|         | -7.77 |
|         | -7.76 |
|         | -7.75 |
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| -7.73   |       |
| -7.72   |       |
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| -7.70   |       |
| -7.69   |       |
| -7.68   |       |
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80.0d

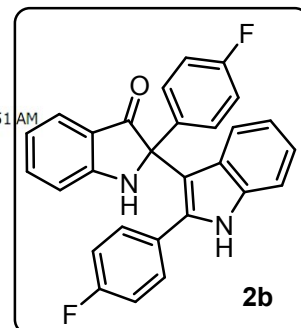
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110.88

71.39



## Qualitative Compound Report

|                               |                            |                      |                      |
|-------------------------------|----------------------------|----------------------|----------------------|
| <b>Data File</b>              | IND 03.d                   | <b>Sample Name</b>   | IND 03               |
| <b>Sample Type</b>            | Sample                     | <b>Position</b>      | P2-D5                |
| <b>Instrument Name</b>        | Instrument 1               | <b>User Name</b>     |                      |
| <b>Acq Method</b>             | water_meoh_grad_6min_reg.m | <b>Acquired Time</b> | 1/5/2018 11:33:51 AM |
| <b>IRM Calibration Status</b> | Success                    | <b>DA Method</b>     | PROCESSNEW.m         |
| <b>Comment</b>                |                            |                      |                      |

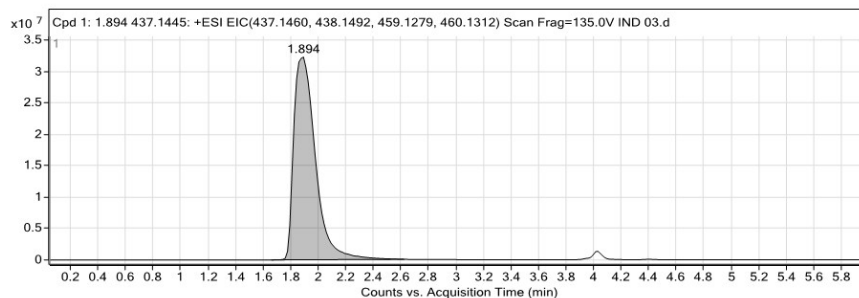


|                     |      |                               |                                                       |
|---------------------|------|-------------------------------|-------------------------------------------------------|
| <b>Sample Group</b> | LC 1 | <b>Info.</b>                  |                                                       |
| <b>Stream Name</b>  | LC 1 | <b>Acquisition SW Version</b> | 6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1) |

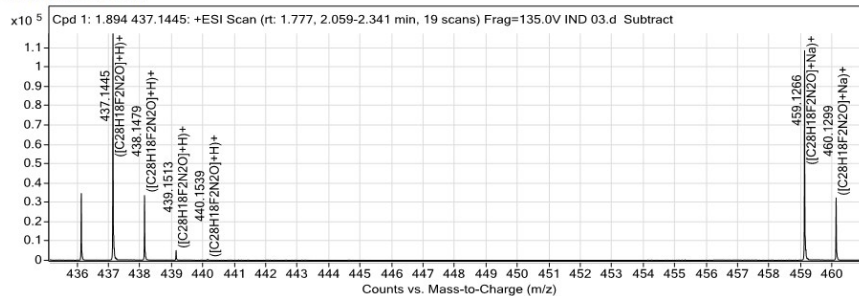
### Compound Table

| Compound Label        | RT    | Mass     | Abund  | Formula                                                         | Tgt Mass | Diff (ppm) |
|-----------------------|-------|----------|--------|-----------------------------------------------------------------|----------|------------|
| Cpd 1: 1.894 437.1445 | 1.894 | 436.1373 | 108534 | C <sub>28</sub> H <sub>18</sub> F <sub>2</sub> N <sub>2</sub> O | 436.1387 | -3.2       |

| Compound Label        | m/z      | RT    | Algorithm       | Mass     |
|-----------------------|----------|-------|-----------------|----------|
| Cpd 1: 1.894 437.1445 | 459.1266 | 1.894 | Find By Formula | 436.1373 |



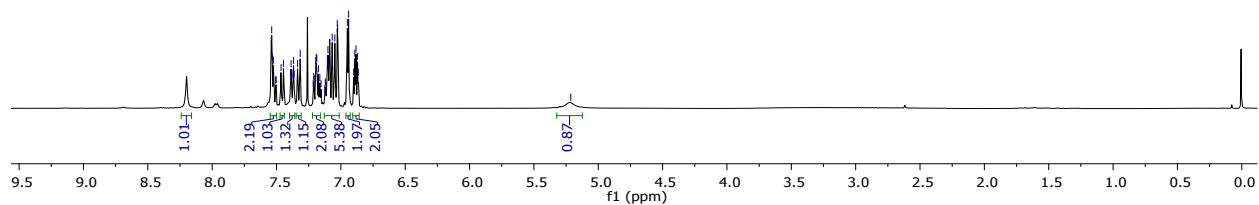
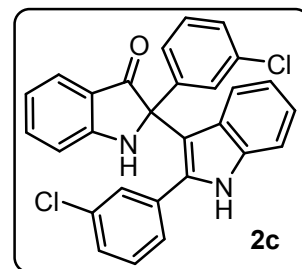
### MS Zoomed Spectrum



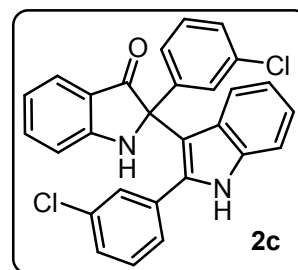
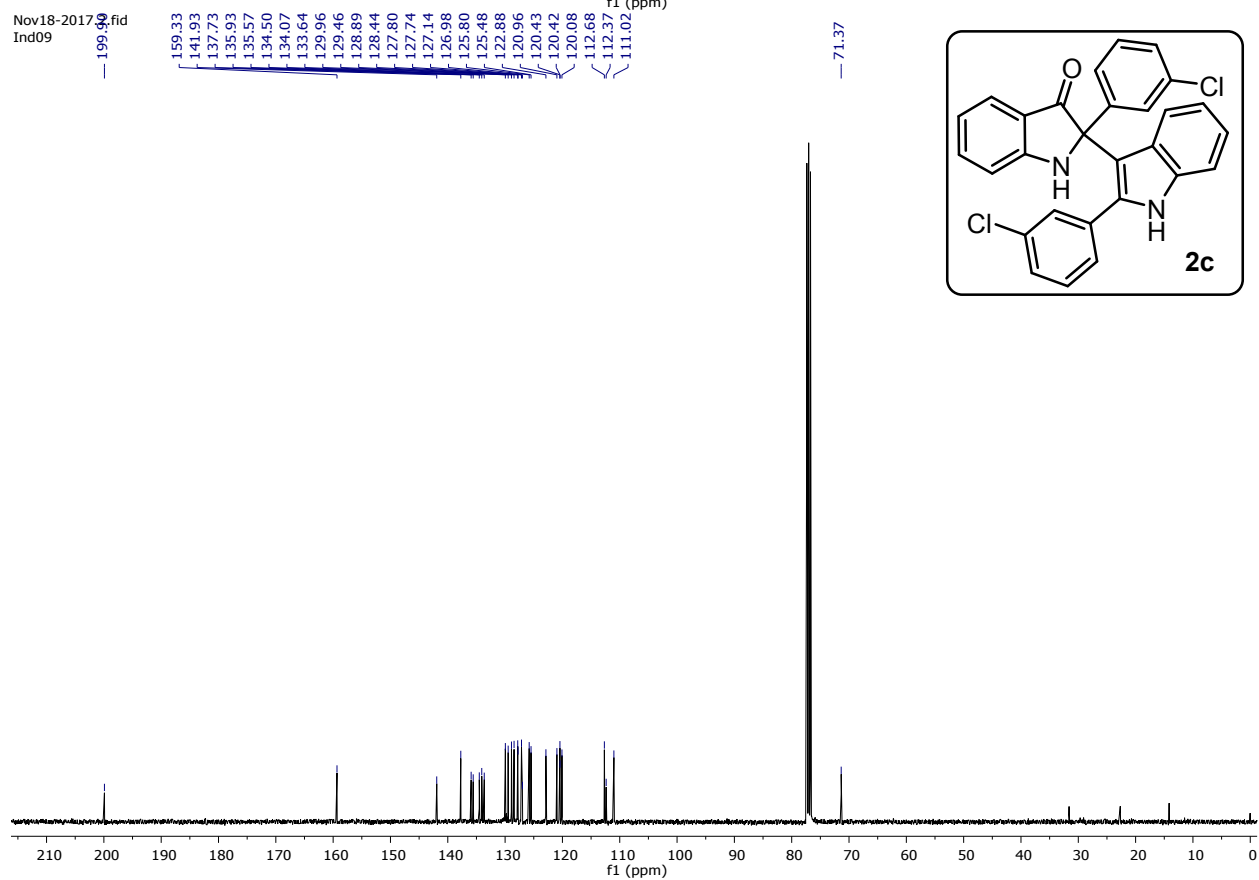
### MS Spectrum Peak List

| m/z      | Calc m/z | Diff(ppm) | z | Abund     | Formula                                                         | Ion                |
|----------|----------|-----------|---|-----------|-----------------------------------------------------------------|--------------------|
| 437.1445 | 437.146  | 3.47      | 1 | 118437.31 | C <sub>28</sub> H <sub>18</sub> F <sub>2</sub> N <sub>2</sub> O | (M+H) <sup>+</sup> |
| 438.1479 | 438.1492 | 3.1       | 1 | 34135.9   | C <sub>28</sub> H <sub>18</sub> F <sub>2</sub> N <sub>2</sub> O | (M+H) <sup>+</sup> |

Nov18-2017  
Ind09

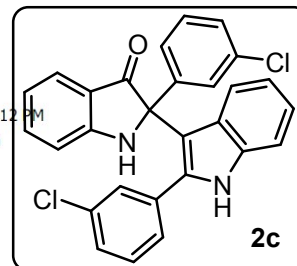


Nov18-2017  
Ind09



## Qualitative Compound Report

|                               |                            |                      |                      |
|-------------------------------|----------------------------|----------------------|----------------------|
| <b>Data File</b>              | IND 09.d                   | <b>Sample Name</b>   | IND 09               |
| <b>Sample Type</b>            | Sample                     | <b>Position</b>      | P2-D8                |
| <b>Instrument Name</b>        | Instrument 1               | <b>User Name</b>     |                      |
| <b>Acq Method</b>             | water_meoh_grad_6min_reg.m | <b>Acquired Time</b> | 1/5/2018 12:16:12 PM |
| <b>IRM Calibration Status</b> | Success                    | <b>DA Method</b>     | PROCESSNEW.m         |
| <b>Comment</b>                |                            |                      |                      |

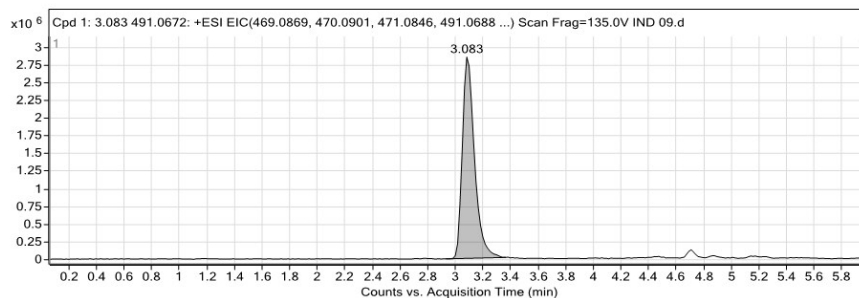


|                     |      |                               |                                                       |
|---------------------|------|-------------------------------|-------------------------------------------------------|
| <b>Sample Group</b> | LC 1 | <b>Info.</b>                  |                                                       |
| <b>Stream Name</b>  |      | <b>Acquisition SW Version</b> | 6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1) |

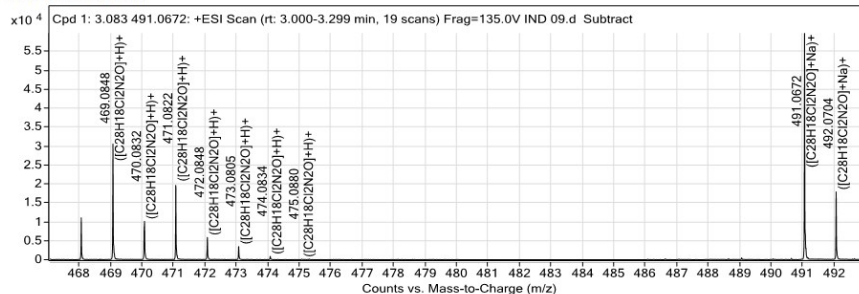
### Compound Table

| Compound Label        | RT    | Mass     | Abund | Formula          | Tgt Mass | Diff (ppm) |
|-----------------------|-------|----------|-------|------------------|----------|------------|
| Cpd 1: 3.083 491.0672 | 3.083 | 468.0774 | 59963 | C28 H18 Cl2 N2 O | 468.0796 | -4.7       |

| Compound Label        | m/z      | RT    | Algorithm       | Mass     |
|-----------------------|----------|-------|-----------------|----------|
| Cpd 1: 3.083 491.0672 | 491.0672 | 3.083 | Find By Formula | 468.0774 |



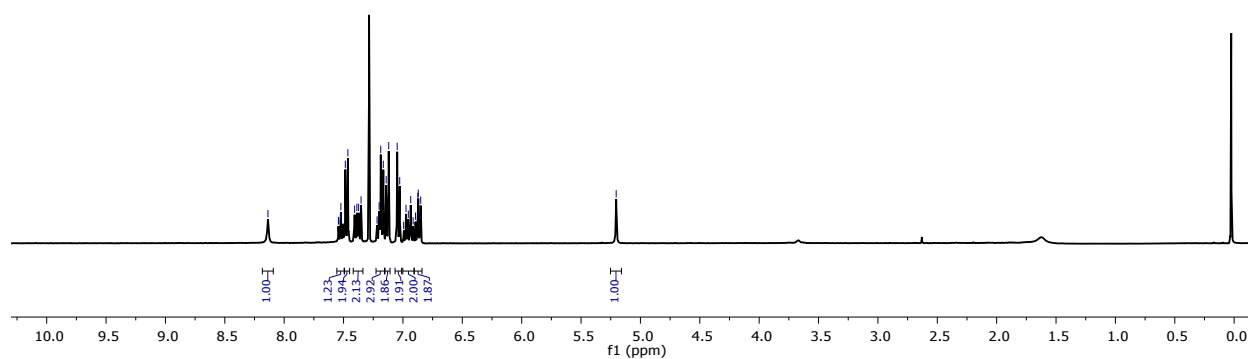
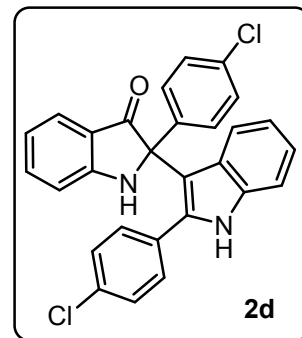
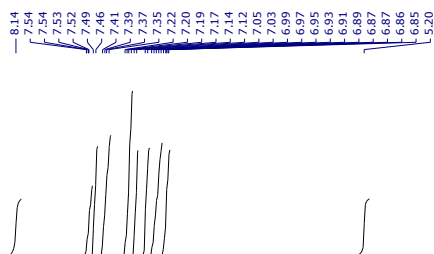
### MS Zoomed Spectrum



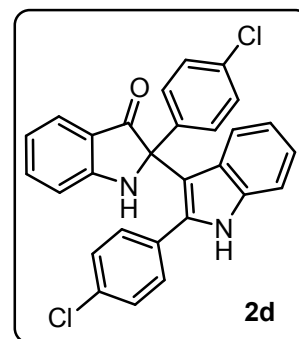
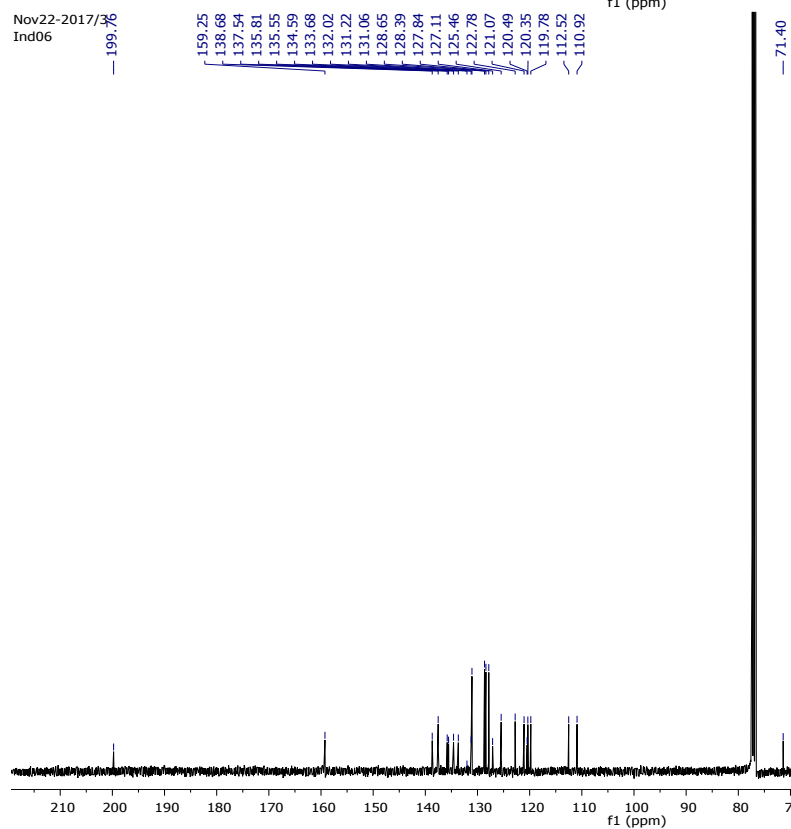
### MS Spectrum Peak List

| m/z      | Calc m/z | Diff(ppm) | z | Abund    | Formula      | Ion    |
|----------|----------|-----------|---|----------|--------------|--------|
| 469.0848 | 469.0869 | 4.46      | 1 | 30947.37 | C28H18Cl2N2O | (M+H)+ |
| 470.0832 | 470.0901 | 14.75     | 1 | 10161.32 | C28H18Cl2N2O | (M+H)+ |

Nov22-2017/1  
Ind06



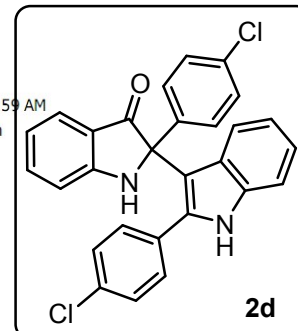
Nov22-2017/36  
Ind06



## Qualitative Compound Report

|                               |                            |                      |                      |
|-------------------------------|----------------------------|----------------------|----------------------|
| <b>Data File</b>              | IND 06.d                   | <b>Sample Name</b>   | IND 06               |
| <b>Sample Type</b>            | Sample                     | <b>Position</b>      | P2-D6                |
| <b>Instrument Name</b>        | Instrument 1               | <b>User Name</b>     |                      |
| <b>Acq Method</b>             | water_meoh_grad_6min_reg.m | <b>Acquired Time</b> | 1/5/2018 11:47:59 AM |
| <b>IRM Calibration Status</b> | Success                    | <b>DA Method</b>     | PROCESSNEW.m         |
| <b>Comment</b>                |                            |                      |                      |

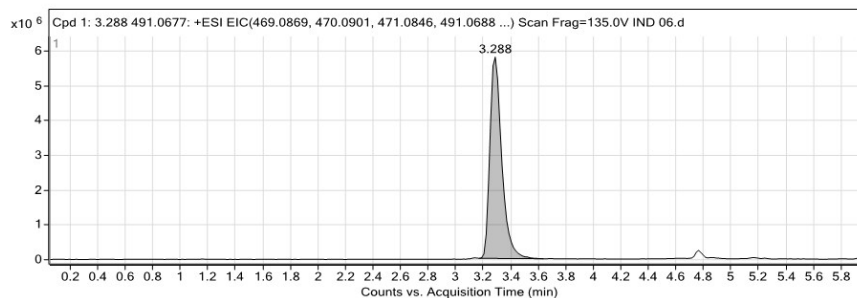
|                     |      |                               |                                                       |
|---------------------|------|-------------------------------|-------------------------------------------------------|
| <b>Sample Group</b> | LC 1 | <b>Info.</b>                  |                                                       |
| <b>Stream Name</b>  |      | <b>Acquisition SW Version</b> | 6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1) |



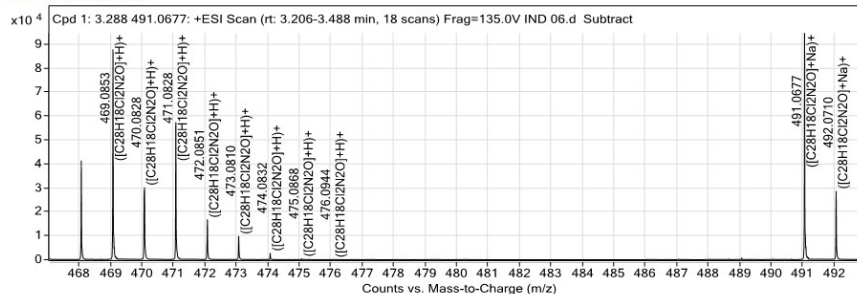
### Compound Table

| Compound Label        | RT    | Mass     | Abund | Formula          | Tgt Mass | Diff (ppm) |
|-----------------------|-------|----------|-------|------------------|----------|------------|
| Cpd 1: 3.288 491.0677 | 3.288 | 468.0777 | 95804 | C28 H18 Cl2 N2 O | 468.0796 | -4.02      |

| Compound Label        | m/z      | RT    | Algorithm       | Mass     |
|-----------------------|----------|-------|-----------------|----------|
| Cpd 1: 3.288 491.0677 | 491.0677 | 3.288 | Find By Formula | 468.0777 |



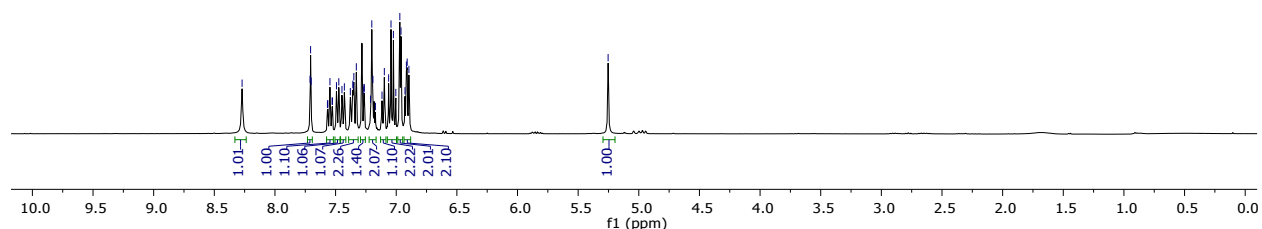
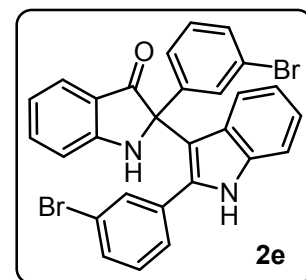
### MS Zoomed Spectrum



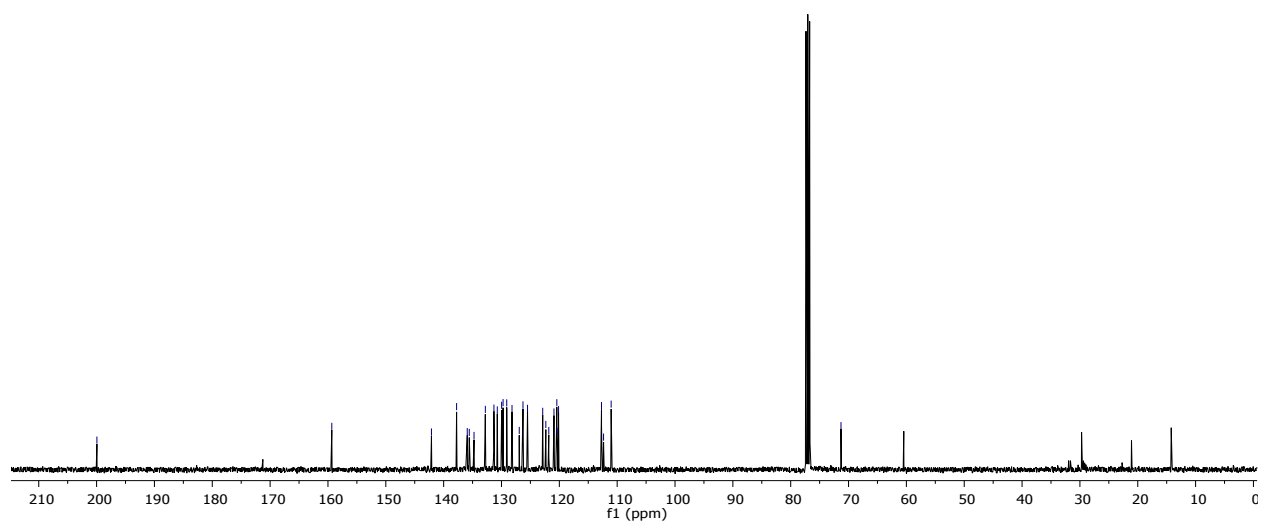
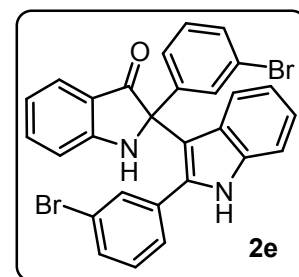
### MS Spectrum Peak List

| m/z      | Calc m/z | Diff(ppm) | z | Abund    | Formula      | Ion    |
|----------|----------|-----------|---|----------|--------------|--------|
| 469.0853 | 469.0869 | 3.31      | 1 | 90402.71 | C28H18Cl2N2O | (M+H)+ |
| 470.0828 | 470.0901 | 15.59     | 1 | 30174.06 | C28H18Cl2N2O | (M+H)+ |

Oct02-2017.5.fid  
INDO2

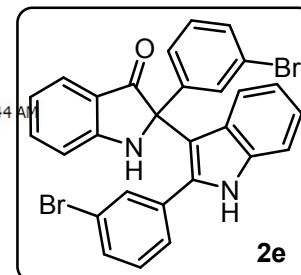


Oct02-2017.5.fid  
INDO2



## Qualitative Compound Report

|                               |                            |                      |                      |
|-------------------------------|----------------------------|----------------------|----------------------|
| <b>Data File</b>              | IND 02.d                   | <b>Sample Name</b>   | IND 02               |
| <b>Sample Type</b>            | Sample                     | <b>Position</b>      | P2-D4                |
| <b>Instrument Name</b>        | Instrument 1               | <b>User Name</b>     |                      |
| <b>Acq Method</b>             | water_meoh_grad_6min_reg.m | <b>Acquired Time</b> | 1/5/2018 11:19:44 AM |
| <b>IRM Calibration Status</b> | Success                    | <b>DA Method</b>     | PROCESSNEW.m         |
| <b>Comment</b>                |                            |                      |                      |

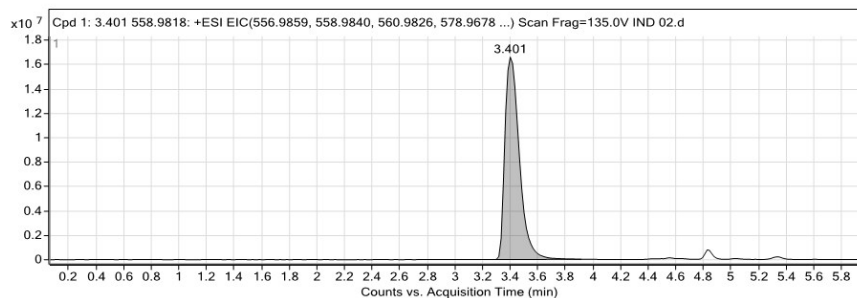


|                     |      |                               |                                                       |
|---------------------|------|-------------------------------|-------------------------------------------------------|
| <b>Sample Group</b> | LC 1 | <b>Info.</b>                  |                                                       |
| <b>Stream Name</b>  |      | <b>Acquisition SW Version</b> | 6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1) |

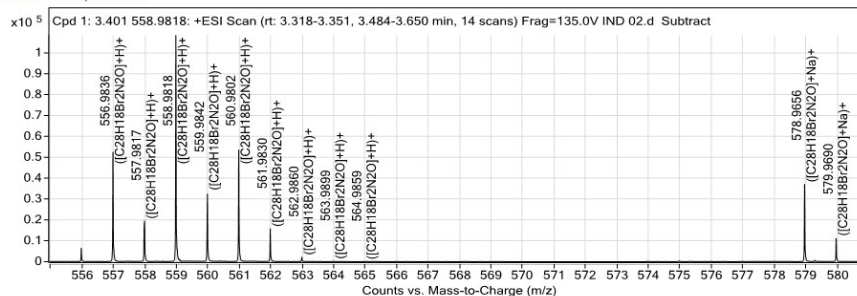
### Compound Table

| Compound Label        | RT    | Mass     | Abund | Formula          | Tgt Mass | Diff (ppm) |
|-----------------------|-------|----------|-------|------------------|----------|------------|
| Cpd 1: 3.401 558.9818 | 3.401 | 555.9761 | 74707 | C28 H18 Br2 N2 O | 555.9786 | -4.52      |

| Compound Label        | m/z      | RT    | Algorithm       | Mass     |
|-----------------------|----------|-------|-----------------|----------|
| Cpd 1: 3.401 558.9818 | 580.9638 | 3.401 | Find By Formula | 555.9761 |

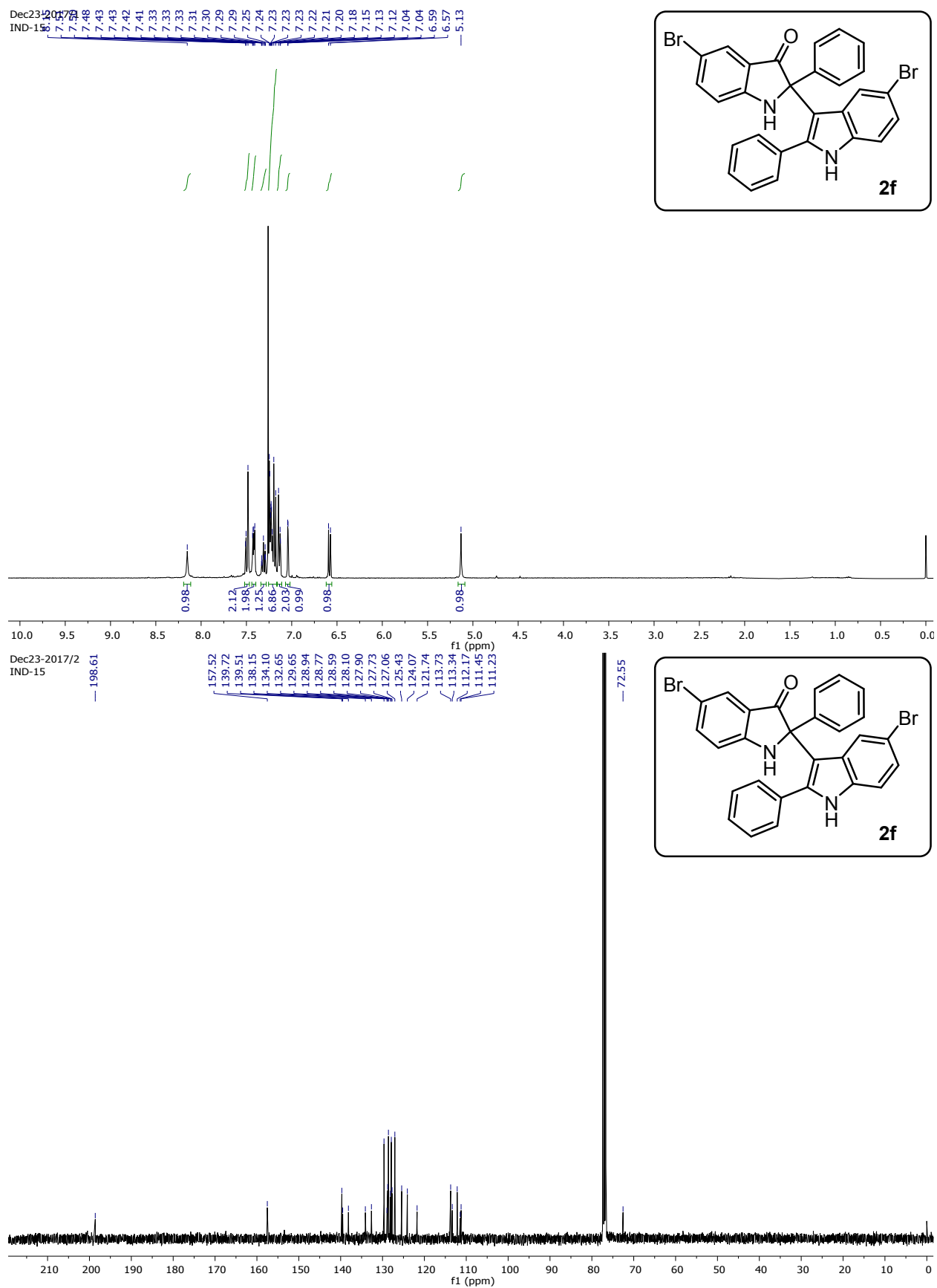


### MS Zoomed Spectrum



### MS Spectrum Peak List

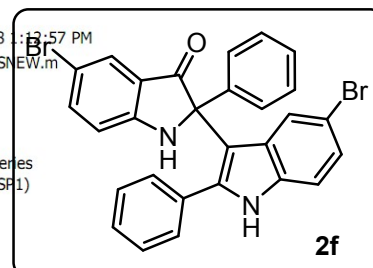
| m/z      | Calc m/z | Diff(ppm) | z | Abund    | Formula      | Ion    |
|----------|----------|-----------|---|----------|--------------|--------|
| 556.9836 | 556.9859 | 3.98      | 1 | 53488.55 | C28H18Br2N2O | (M+H)+ |
| 557.9817 | 557.9891 | 13.22     | 1 | 19551.57 | C28H18Br2N2O | (M+H)+ |



# Qualitative Compound Report

**Data File** IND 15.d  
**Sample Type** Sample  
**Instrument Name** Instrument 1  
**Acq Method** water\_meoh\_grad\_6min\_reg.m  
**IRM Calibration Status** Success  
**Comment**  
**Sample Name** IND 15  
**Position** P2-E1  
**User Name**  
**Acquired Time** 1/5/2018 1:13:57 PM  
**DA Method** PROCESSNEW.m

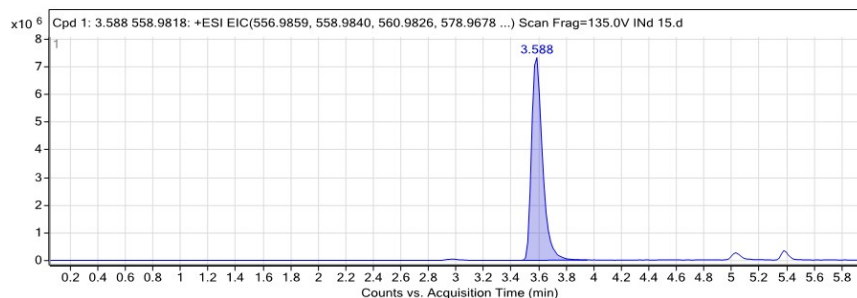
**Sample Group**  
**Stream Name** LC 1  
**Info.**  
**Acquisition SW** 6200 series TOF/6500 series  
**Version** Q-TOF B.06.01 (B6172 SP1)



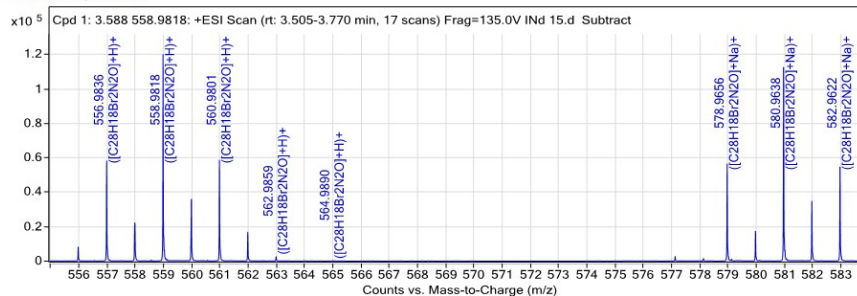
## Compound Table

| Compound Label        | RT    | Mass     | Abund  | Formula          | Tgt Mass | Diff (ppm) |
|-----------------------|-------|----------|--------|------------------|----------|------------|
| Cpd 1: 3.588 558.9818 | 3.588 | 555.9761 | 114294 | C28 H18 Br2 N2 O | 555.9786 | -4.51      |

| Compound Label        | m/z      | RT    | Algorithm       | Mass     |
|-----------------------|----------|-------|-----------------|----------|
| Cpd 1: 3.588 558.9818 | 580.9638 | 3.588 | Find By Formula | 555.9761 |



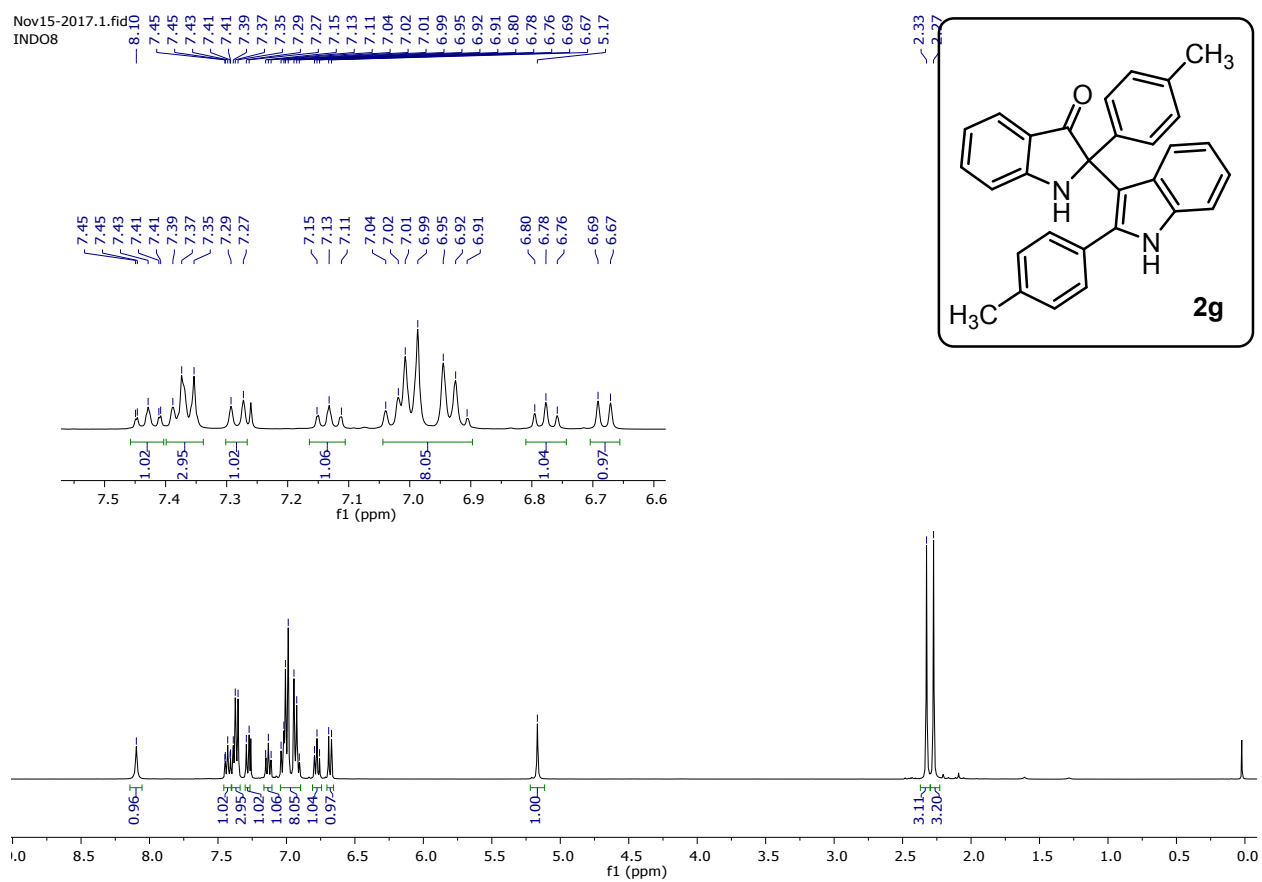
## MS Zoomed Spectrum



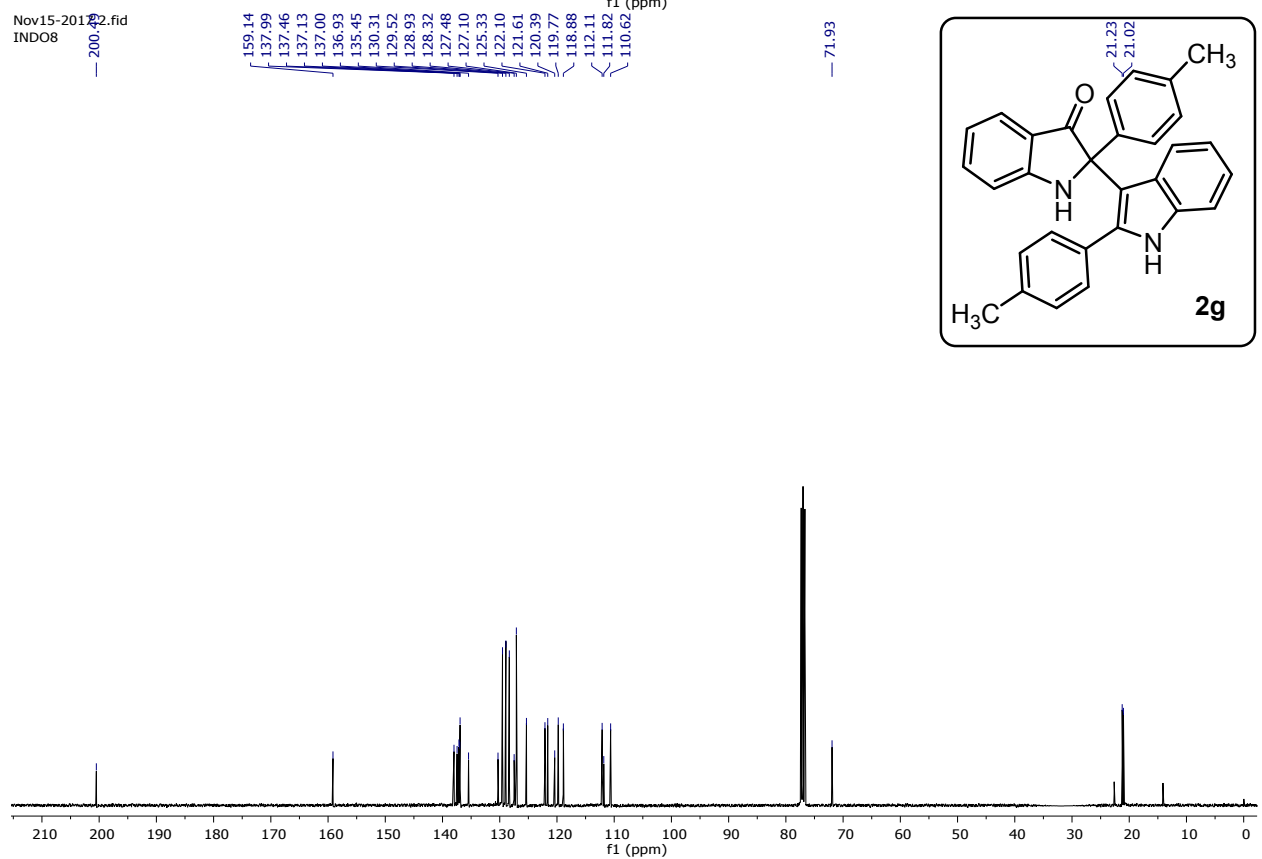
## MS Spectrum Peak List

| m/z      | Calc m/z | Diff(ppm) | z | Abund    | Formula      | Ion    |
|----------|----------|-----------|---|----------|--------------|--------|
| 556.9836 | 556.9859 | 4.07      | 1 | 59351.38 | C28H18Br2N2O | (M+H)+ |
| 557.9813 | 557.9891 | 14.05     | 1 | 22361.84 | C28H18Br2N2O | (M+H)+ |

Nov15-2017.1.fid  
IND08



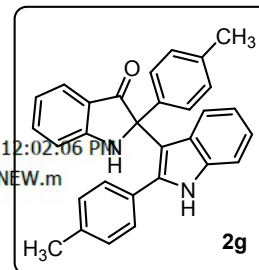
Nov15-2017.2.fid  
IND08



# Qualitative Compound Report

Data File IND 08.d  
 Sample Type Sample  
 Instrument Name Instrument 1  
 Acq Method water\_meoh\_grad\_6min\_reg.m  
 IRM Calibration Status Success  
 Comment

Sample Name IND 08  
 Position P2-D7  
 User Name  
 Acquired Time 1/5/2018 12:02:06 PM  
 DA Method PROCESSNEW.m



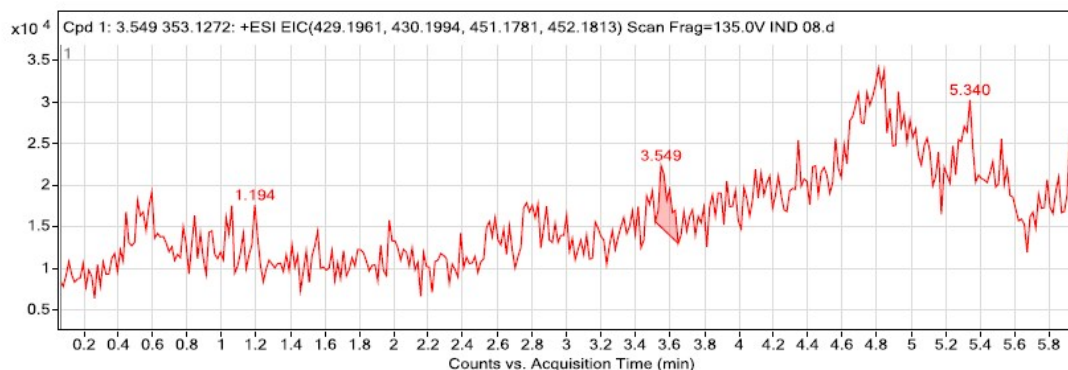
Sample Group  
 Stream Name LC 1

Info.  
 Acquisition SW 6200 series TOF/6500 series  
 Version Q-TOF B.06.01 (B6172 SP1)

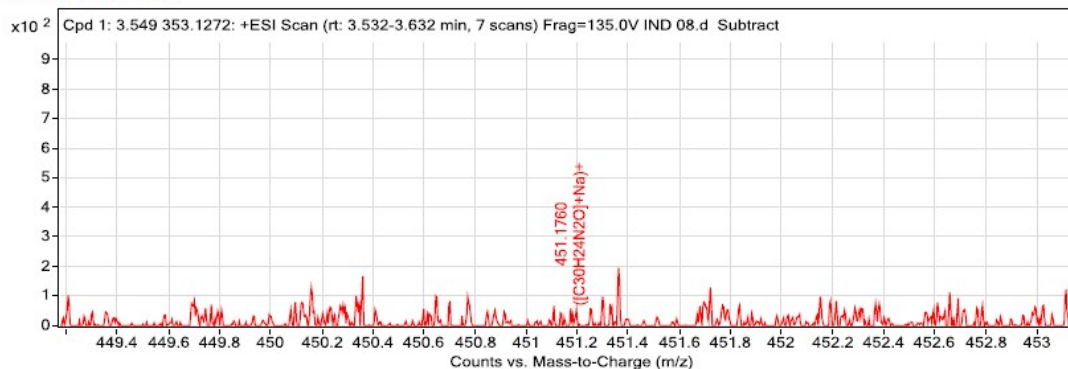
## Compound Table

| Compound Label        | RT    | Mass     | Abund | Formula      | Tgt Mass | Diff (ppm) |
|-----------------------|-------|----------|-------|--------------|----------|------------|
| Cpd 1: 3.549 353.1272 | 3.549 | 428.1868 | 59    | C30 H24 N2 O | 428.1889 | -4.5       |

| Compound Label        | m/z     | RT    | Algorithm       | Mass     |
|-----------------------|---------|-------|-----------------|----------|
| Cpd 1: 3.549 353.1272 | 451.176 | 3.549 | Find By Formula | 428.1868 |



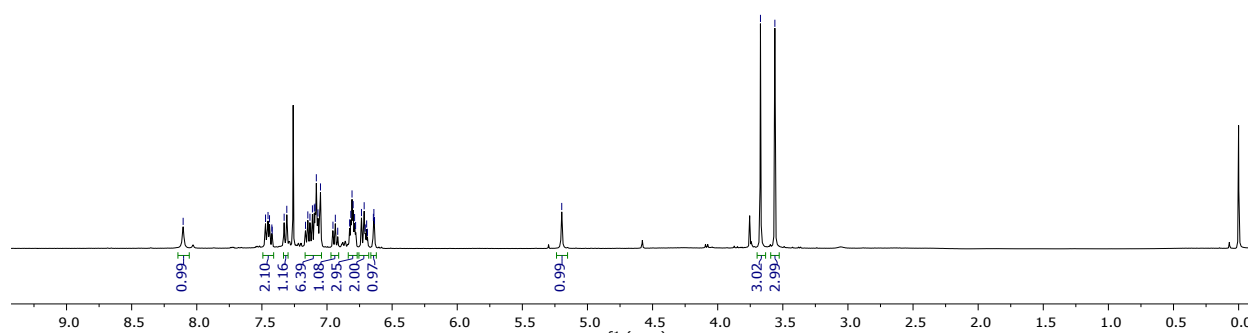
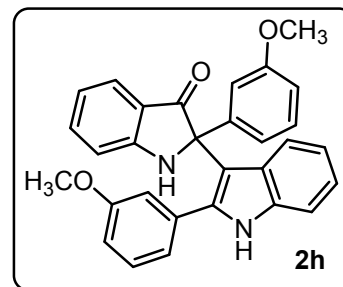
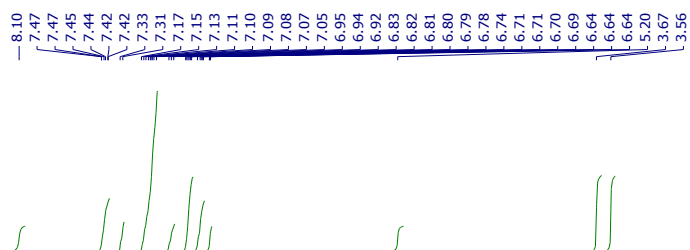
## MS Zoomed Spectrum



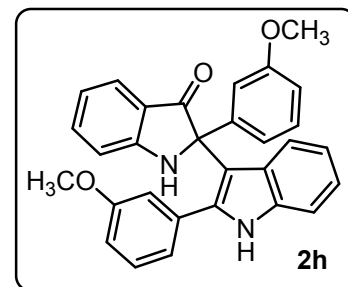
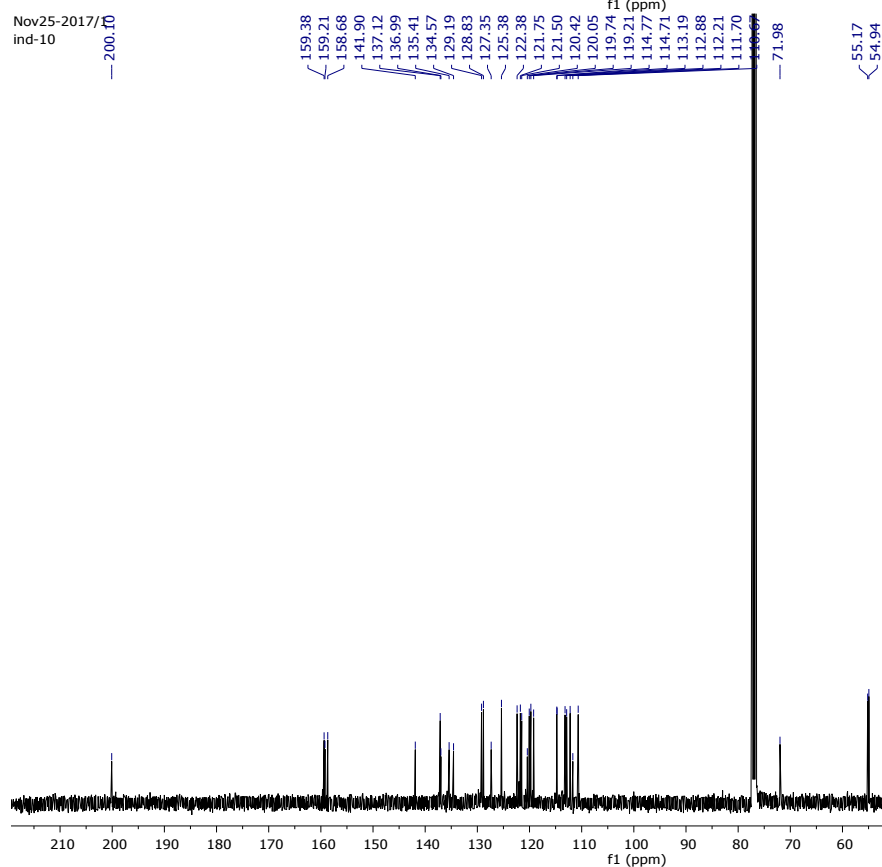
## MS Spectrum Peak List

| m/z     | Calc m/z | Diff(ppm) | z | Abund | Formula   | Ion     |
|---------|----------|-----------|---|-------|-----------|---------|
| 451.176 | 451.1781 | 4.66      | 1 | 59.44 | C30H24N2O | (M+Na)+ |

Nov24-2017/2  
IND-10



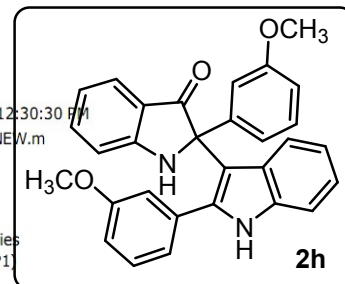
Nov25-2017/10  
ind-10



## Qualitative Compound Report

|                               |                            |                      |                      |
|-------------------------------|----------------------------|----------------------|----------------------|
| <b>Data File</b>              | IND 10.d                   | <b>Sample Name</b>   | IND 10               |
| <b>Sample Type</b>            | Sample                     | <b>Position</b>      | P2-D9                |
| <b>Instrument Name</b>        | Instrument 1               | <b>User Name</b>     |                      |
| <b>Acq Method</b>             | water_meoh_grad_6min_reg.m | <b>Acquired Time</b> | 1/5/2018 12:30:30 PM |
| <b>IRM Calibration Status</b> | Success                    | <b>DA Method</b>     | PROCESSNEW.m         |
| <b>Comment</b>                |                            |                      |                      |

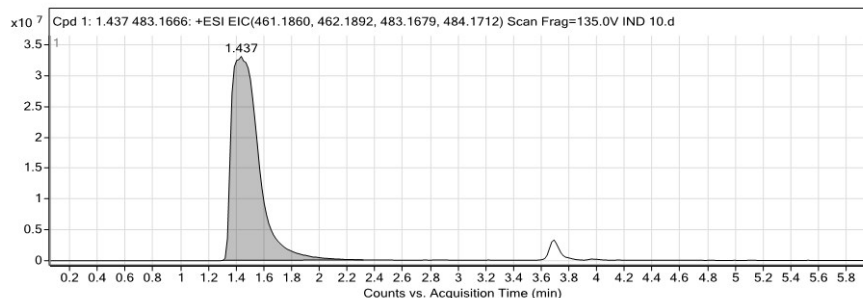
|                     |      |                             |
|---------------------|------|-----------------------------|
| <b>Sample Group</b> | LC 1 | <b>Info.</b>                |
| <b>Stream Name</b>  |      | <b>Acquisition SW</b>       |
|                     |      | 6200 series TOF/6500 series |
|                     |      | Q-TOF B.06.01 (B6172 SP1)   |



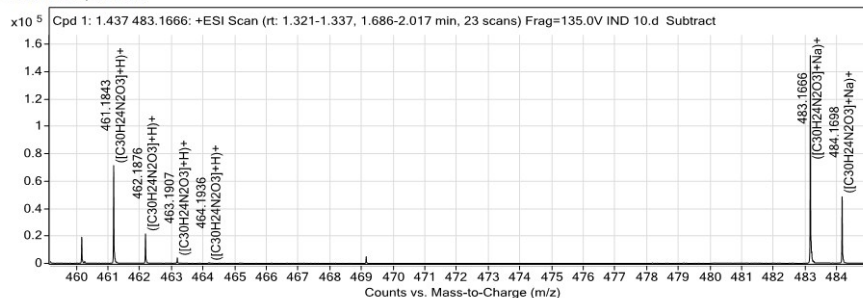
### Compound Table

| Compound Label        | RT    | Mass     | Abund  | Formula       | Tgt Mass | Diff (ppm) |
|-----------------------|-------|----------|--------|---------------|----------|------------|
| Cpd 1: 1.437 483.1666 | 1.437 | 460.1773 | 155498 | C30 H24 N2 O3 | 460.1787 | -3.11      |

| Compound Label        | m/z      | RT    | Algorithm       | Mass     |
|-----------------------|----------|-------|-----------------|----------|
| Cpd 1: 1.437 483.1666 | 483.1666 | 1.437 | Find By Formula | 460.1773 |

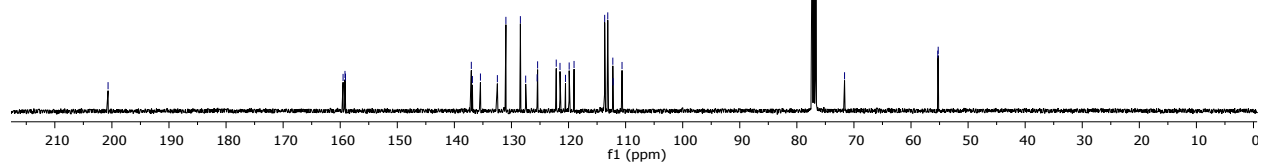
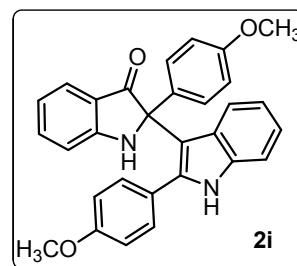
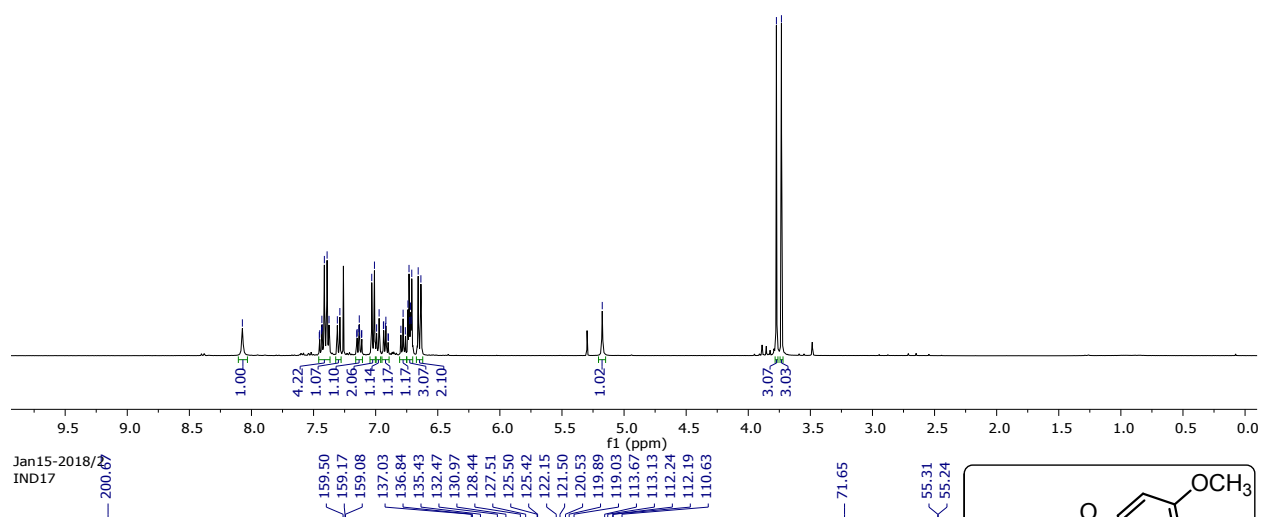
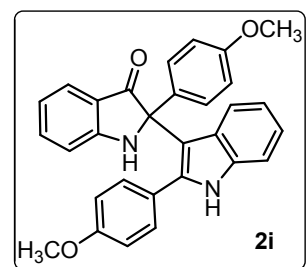
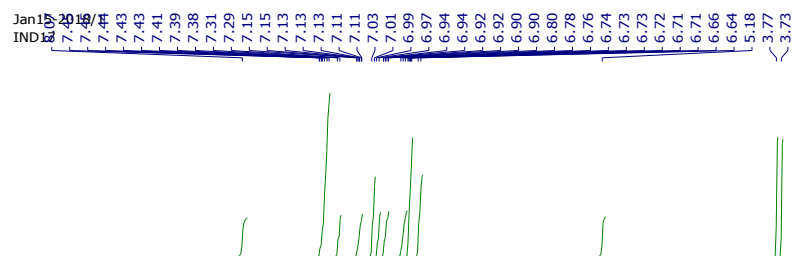


### MS Zoomed Spectrum



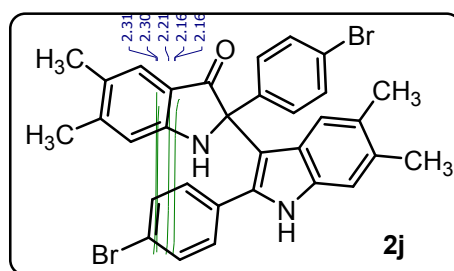
### MS Spectrum Peak List

| m/z      | Calc m/z | Diff(ppm) | z | Abund    | Formula    | Ion    |
|----------|----------|-----------|---|----------|------------|--------|
| 461.1843 | 461.186  | 3.58      | 1 | 71739.17 | C30H24N2O3 | (M+H)+ |
| 462.1876 | 462.1892 | 3.42      | 1 | 22086.86 | C30H24N2O3 | (M+H)+ |



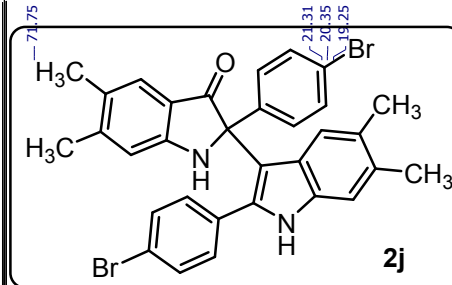
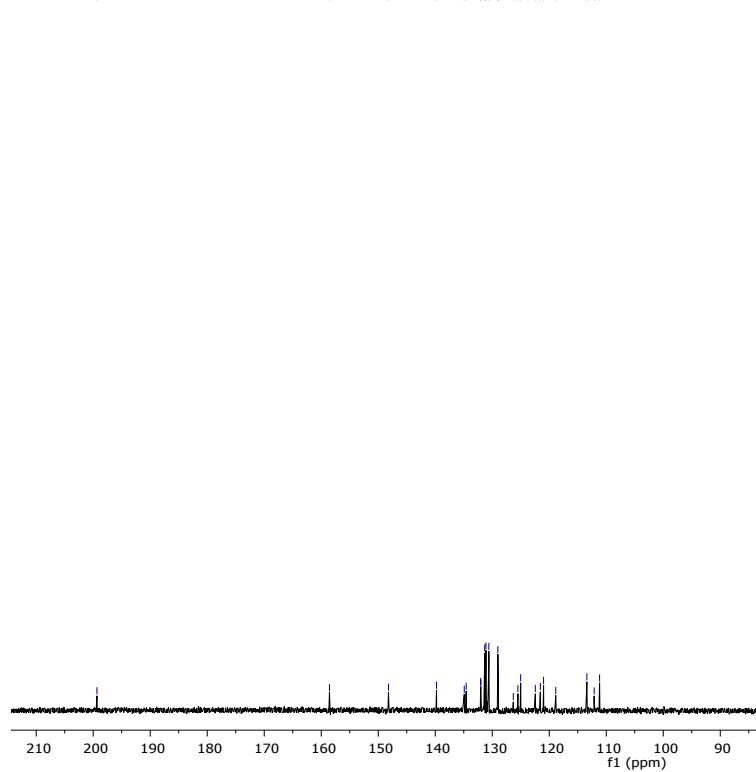
Dec16-2017/2  
IND13

7.85  
7.37  
7.35  
7.28  
7.25  
7.24  
7.16  
7.11  
6.95  
6.65  
4.94



Dec27-2017/2  
IND 13

199.72  
158.56  
148.21  
139.78  
134.91  
134.57  
132.03  
131.99  
131.32  
131.11  
130.60  
129.01  
128.93  
126.31  
125.49  
125.02  
122.44  
121.56  
121.00  
118.86  
113.40  
112.12  
111.17

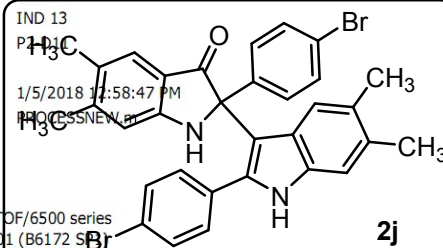


# Qualitative Compound Report

**Data File**  
**Sample Type**  
**Instrument Name**  
**Acq Method**  
**IRM Calibration Status**  
**Comment**

IND 13.d  
Sample  
Instrument 1  
water\_meoh\_grad\_6min\_reg.m  
Success

**Sample Name**  
**Position**  
**User Name**  
**Acquired Time**  
**DA Method**



**Sample Group**  
**Stream Name**

LC 1

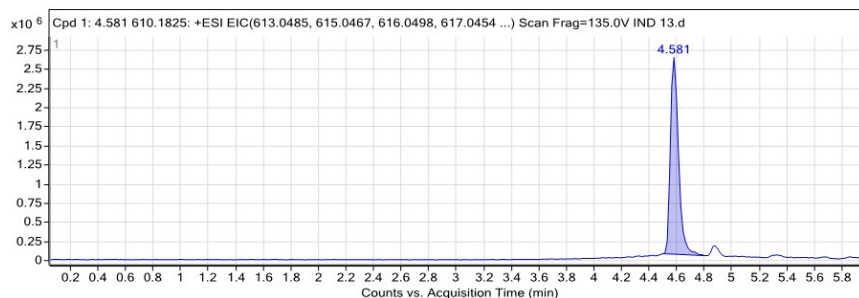
**Info.**  
**Acquisition SW**  
**Version**

6200 series TOF/6500 series  
Q-TOF B.06.01 (B6172 S

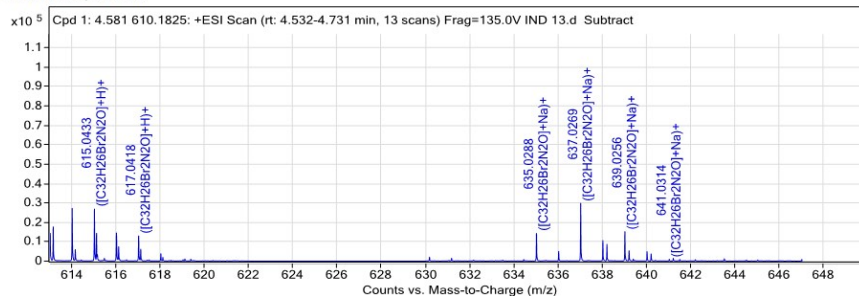
## Compound Table

| Compound Label        | RT    | Mass    | Abund | Formula          | Tgt Mass | Diff (ppm) |
|-----------------------|-------|---------|-------|------------------|----------|------------|
| Cpd 1: 4.581 610.1825 | 4.581 | 612.038 | 29875 | C32 H26 Br2 N2 O | 612.0412 | -5.27      |

| Compound Label        | m/z      | RT    | Algorithm       | Mass    |
|-----------------------|----------|-------|-----------------|---------|
| Cpd 1: 4.581 610.1825 | 637.0269 | 4.581 | Find By Formula | 612.038 |

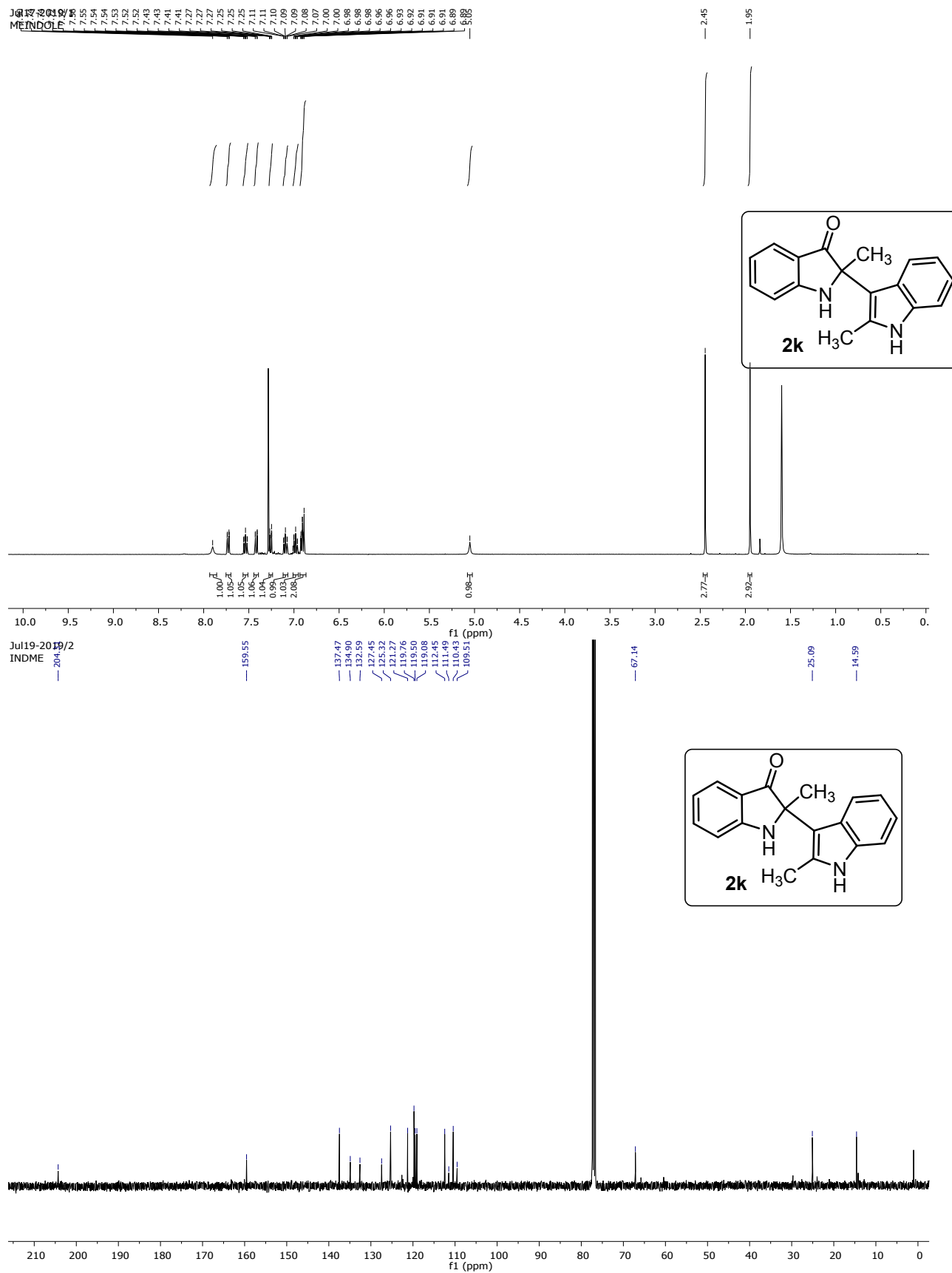


## MS Zoomed Spectrum



## MS Spectrum Peak List

| m/z      | Calc m/z | Diff(ppm) | z | Abund    | Formula      | Ion    |
|----------|----------|-----------|---|----------|--------------|--------|
| 615.0433 | 615.0467 | 5.5       | 1 | 27156.81 | C32H26Br2N2O | (M+H)+ |
| 616.0391 | 616.0498 | 17.24     | 1 | 14915.89 | C32H26Br2N2O | (M+H)+ |

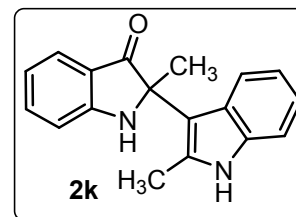


# HRMS Facility, BITS Pilani, Pilani Campus

## Compound Report

|                        |                                                |               |                      |
|------------------------|------------------------------------------------|---------------|----------------------|
| Data File              | VS-INDD.d                                      | Sample Name   | VS-INDD              |
| Sample Type            | Sample                                         | Position      | P2-D1                |
| Instrument Name        | Instrument 1                                   | User Name     |                      |
| Acq Method             | Ch860ChD40_Isocratic_esi_positive_3min.bintu.m | Acquired Time | 7/19/2019 5:34:30 PM |
| IRM Calibration Status | Success                                        | DA Method     | PROCESSNEW.m         |
| Comment                |                                                |               |                      |

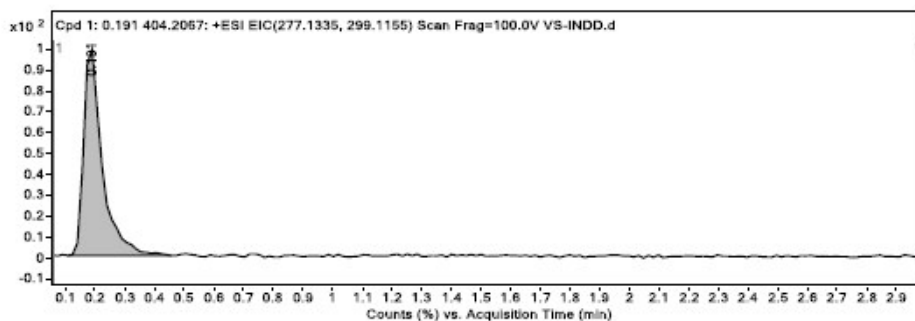
|              |      |                        |                                                       |
|--------------|------|------------------------|-------------------------------------------------------|
| Sample Group |      | Info.                  |                                                       |
| Stream Name  | LC 1 | Acquisition SW Version | 6200 series TOF/6500 series Q-TOF 8.06.01 (B6172 SP1) |



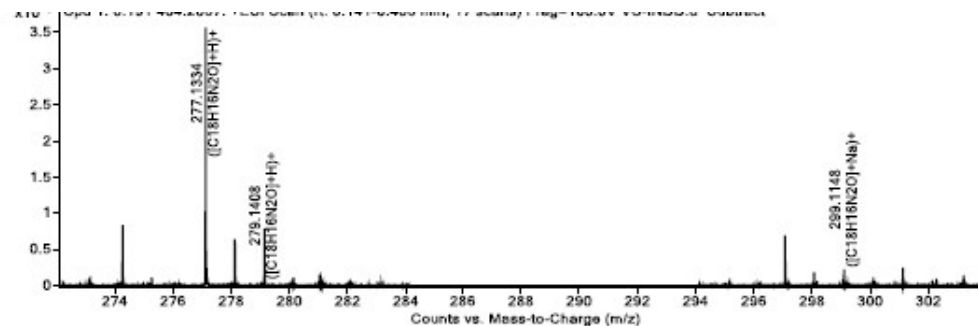
### Compound Table

| Compound Label        | RT    | Mass     | Abund | Formula      | Tgt Mass | Diff (ppm) |
|-----------------------|-------|----------|-------|--------------|----------|------------|
| Cpd 1: 0.191 404.2067 | 0.191 | 276.1262 | 36358 | C18 H16 N2 O | 276.1263 | -0.27      |

| Compound Label        | m/z      | RT    | Algorithm       | Mass     |
|-----------------------|----------|-------|-----------------|----------|
| Cpd 1: 0.191 404.2067 | 277.1334 | 0.191 | Find By Formula | 276.1262 |



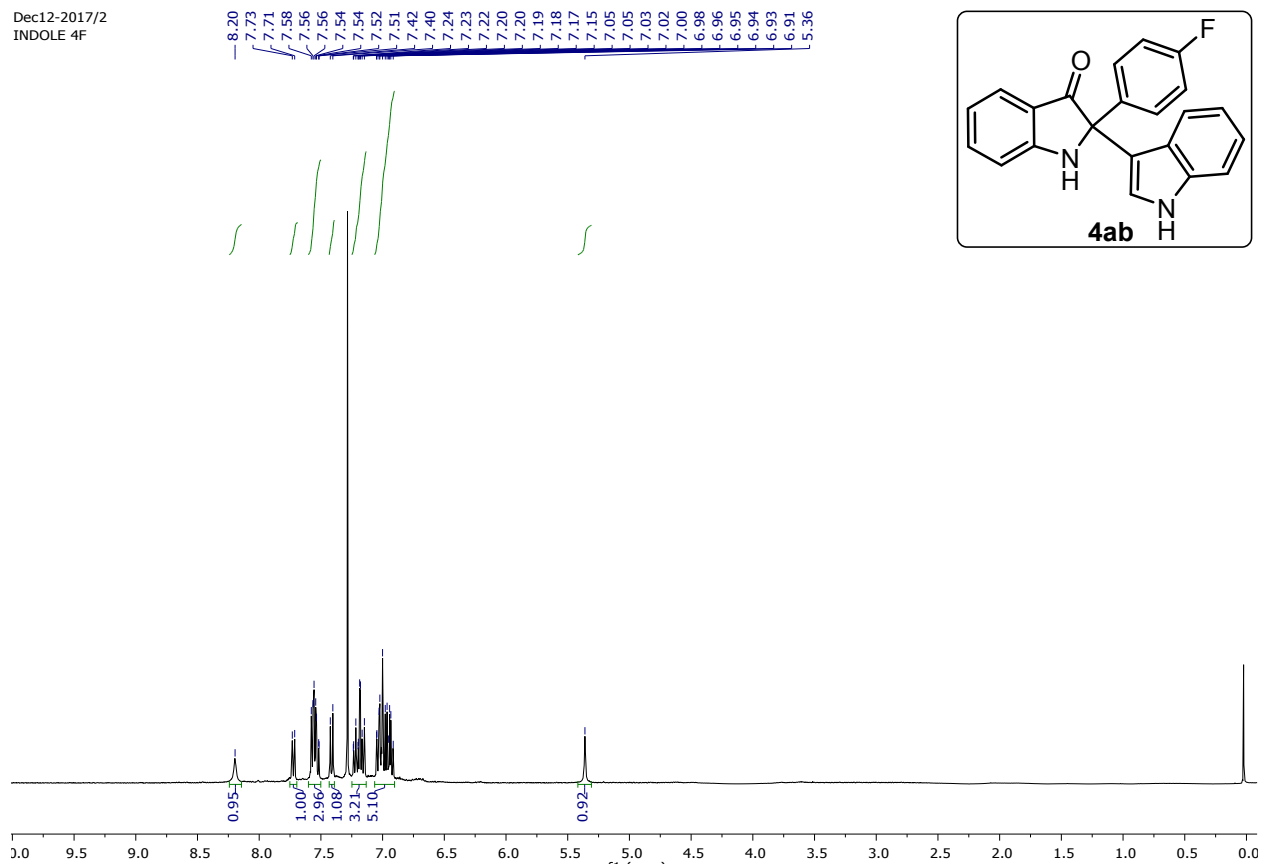
### MS Zoomed Spectrum



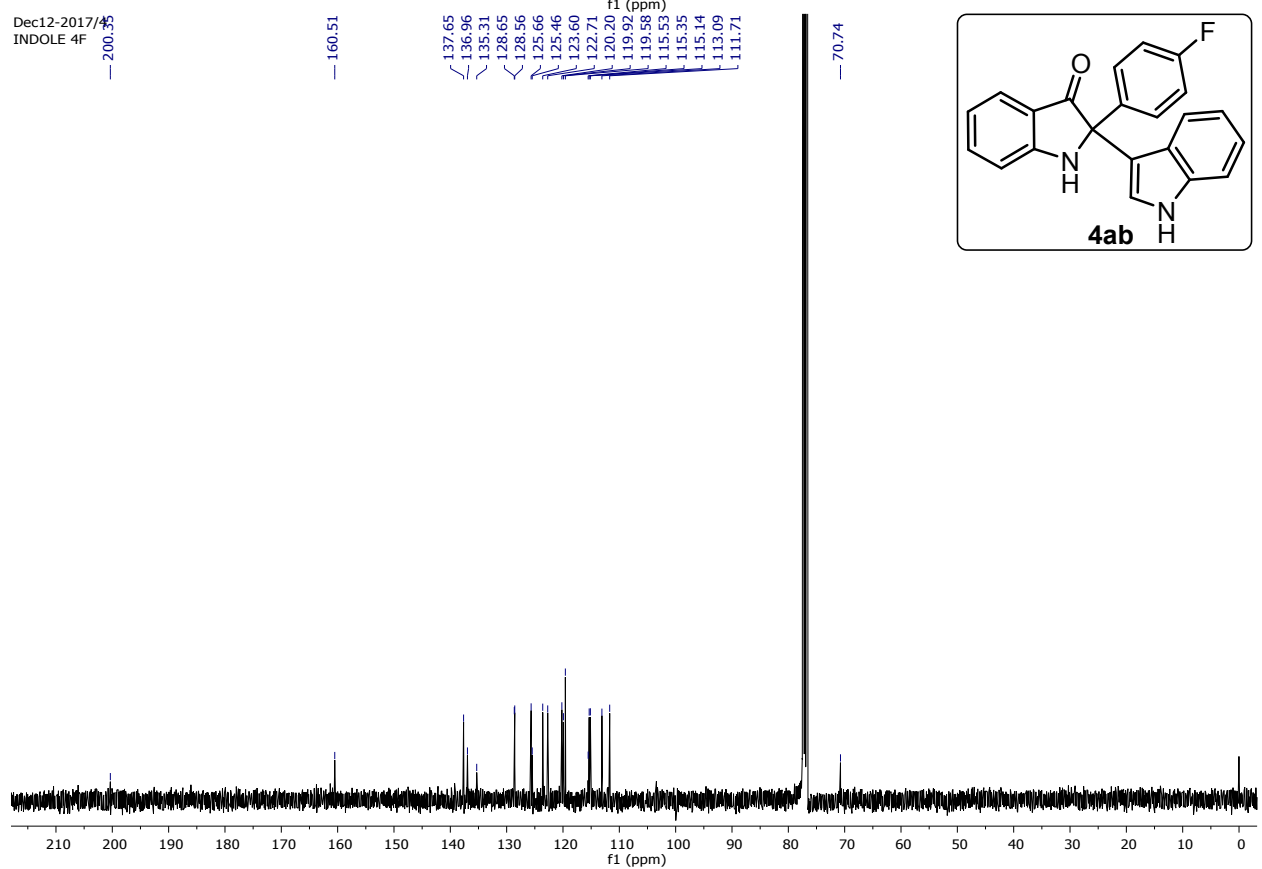
### MS Spectrum Peak List

| m/z      | Calc m/z | Diff(ppm) | z | Abund    | Formula   | Ion     |
|----------|----------|-----------|---|----------|-----------|---------|
| 277.1334 | 277.1335 | 0.37      | 1 | 36358.38 | C18H16N2O | (M+H)+  |
| 278.137  | 278.1367 | -0.91     | 1 | 6537.04  | C18H16N2O | (M+H)+  |
| 279.1408 | 279.1397 | -4.27     | 1 | 996.3    | C18H16N2O | (M+H)+  |
| 299.1148 | 299.1155 | 2.44      | 1 | 2278.87  | C18H16N2O | (M+Na)+ |
| 300.1177 | 300.1186 | 3         | 1 | 478.05   | C18H16N2O | (M+Na)+ |

Dec12-2017/2  
INDOLE 4F

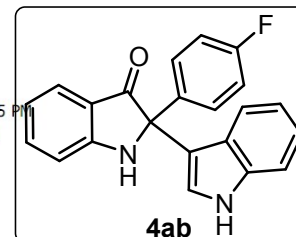


Dec12-2017/43  
INDOLE 4F



## Qualitative Compound Report

|                               |                            |                      |                     |
|-------------------------------|----------------------------|----------------------|---------------------|
| <b>Data File</b>              | INDOLE 4F.d                | <b>Sample Name</b>   | INDOLE 4F           |
| <b>Sample Type</b>            | Sample                     | <b>Position</b>      | P2-E2               |
| <b>Instrument Name</b>        | Instrument 1               | <b>User Name</b>     |                     |
| <b>Acq Method</b>             | water_meoh_grad_6min_reg.m | <b>Acquired Time</b> | 1/5/2018 1:27:05 PM |
| <b>IRM Calibration Status</b> | Success                    | <b>DA Method</b>     | PROCESSNEW.m        |
| <b>Comment</b>                |                            |                      |                     |

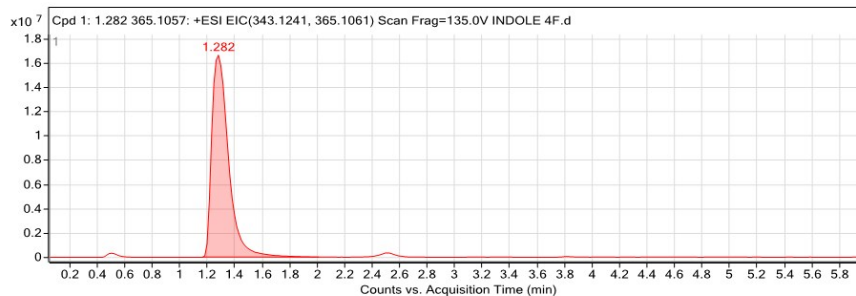


|                     |      |                               |                                                       |
|---------------------|------|-------------------------------|-------------------------------------------------------|
| <b>Sample Group</b> | LC 1 | <b>Info.</b>                  |                                                       |
| <b>Stream Name</b>  | LC 1 | <b>Acquisition SW Version</b> | 6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1) |

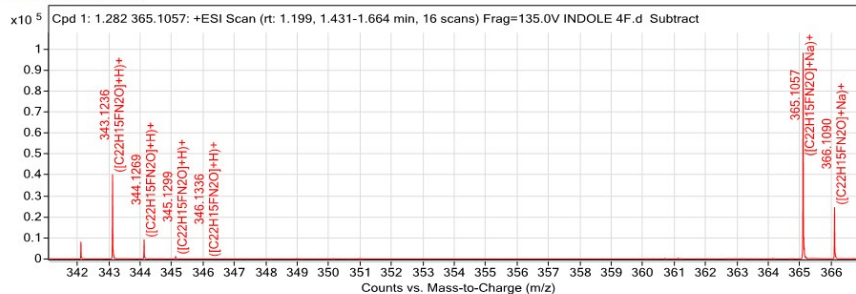
### Compound Table

| Compound Label        | RT    | Mass     | Abund  | Formula        | Tgt Mass | Diff (ppm) |
|-----------------------|-------|----------|--------|----------------|----------|------------|
| Cpd 1: 1.282 365.1057 | 1.282 | 342.1165 | 101297 | C22 H15 F N2 O | 342.1168 | -1.06      |

| Compound Label        | m/z      | RT    | Algorithm       | Mass     |
|-----------------------|----------|-------|-----------------|----------|
| Cpd 1: 1.282 365.1057 | 365.1057 | 1.282 | Find By Formula | 342.1165 |



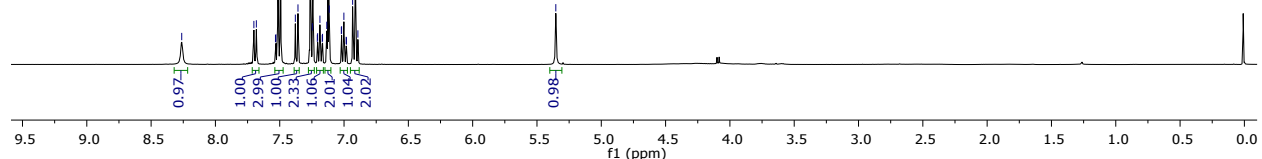
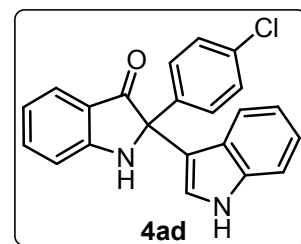
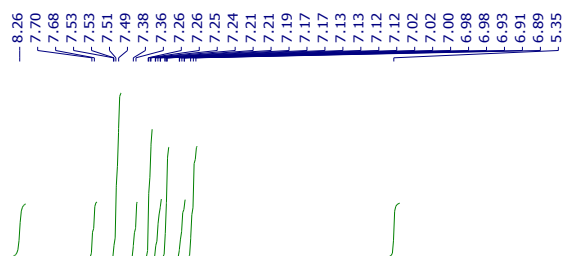
### MS Zoomed Spectrum



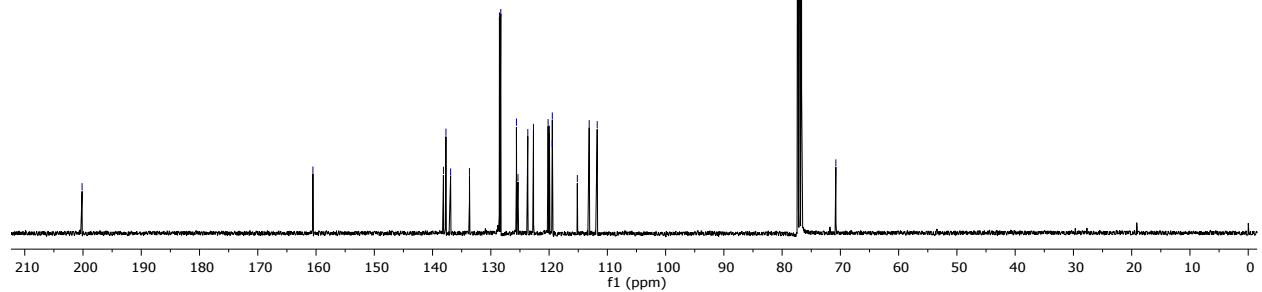
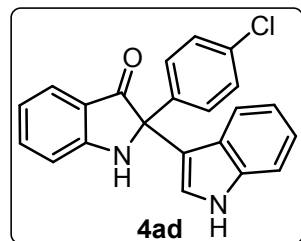
### MS Spectrum Peak List

| m/z      | Calc m/z | Diff(ppm) | z | Abund    | Formula    | Ion    |
|----------|----------|-----------|---|----------|------------|--------|
| 343.1236 | 343.1241 | 1.41      | 1 | 40267.52 | C22H15FN2O | (M+H)+ |
| 344.1269 | 344.1273 | 1.08      | 1 | 9355.85  | C22H15FN2O | (M+H)+ |

Dec16-2017/1  
INDOLE4CL

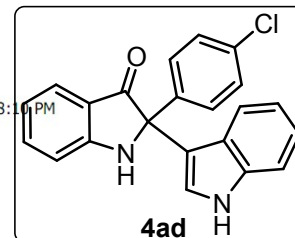


Dec16-2017/3  
INDOLE4CL



## Qualitative Compound Report

|                               |                           |                      |                        |
|-------------------------------|---------------------------|----------------------|------------------------|
| <b>Data File</b>              | Indole 4 Cl.d             | <b>Sample Name</b>   | Indole 4 Cl            |
| <b>Sample Type</b>            | Sample                    | <b>Position</b>      | P1-F9                  |
| <b>Instrument Name</b>        | Instrument 1              | <b>User Name</b>     |                        |
| <b>Acq Method</b>             | water_acn_grad_6min_reg.m | <b>Acquired Time</b> | 10/18/2017 10:28:16 PM |
| <b>IRM Calibration Status</b> | Success                   | <b>DA Method</b>     | PROCESSNEW.m           |
| <b>Comment</b>                |                           |                      |                        |

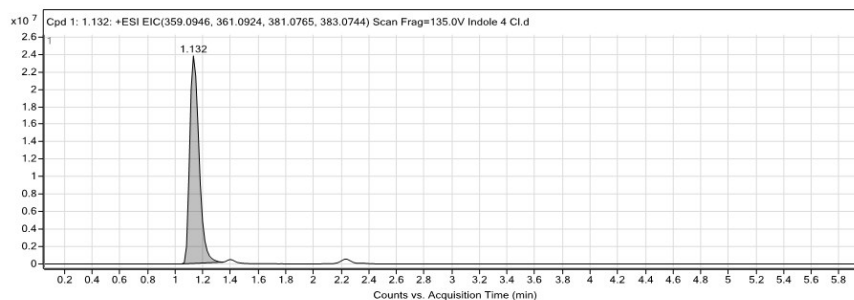


|                     |      |                               |                                                       |
|---------------------|------|-------------------------------|-------------------------------------------------------|
| <b>Sample Group</b> | LC 1 | <b>Info.</b>                  |                                                       |
| <b>Stream Name</b>  | LC 1 | <b>Acquisition SW Version</b> | 6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1) |

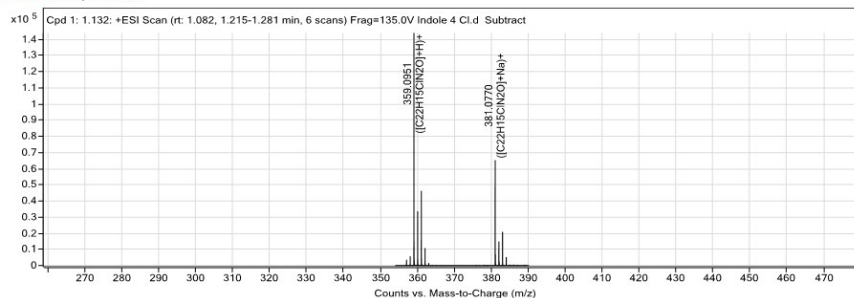
### Compound Table

| Compound Label | RT    | Mass     | Abund | Formula         | Tgt Mass | Diff (ppm) |
|----------------|-------|----------|-------|-----------------|----------|------------|
| Cpd 1: 1.132   | 1.132 | 358.0877 | 65442 | C22 H15 Cl N2 O | 358.0873 | 1.2        |

| Compound Label | m/z     | RT    | Algorithm       | Mass     |
|----------------|---------|-------|-----------------|----------|
| Cpd 1: 1.132   | 381.077 | 1.132 | Find By Formula | 358.0877 |



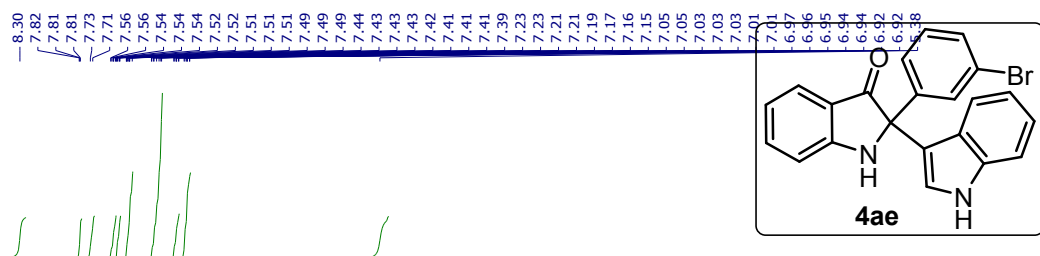
### MS Zoomed Spectrum



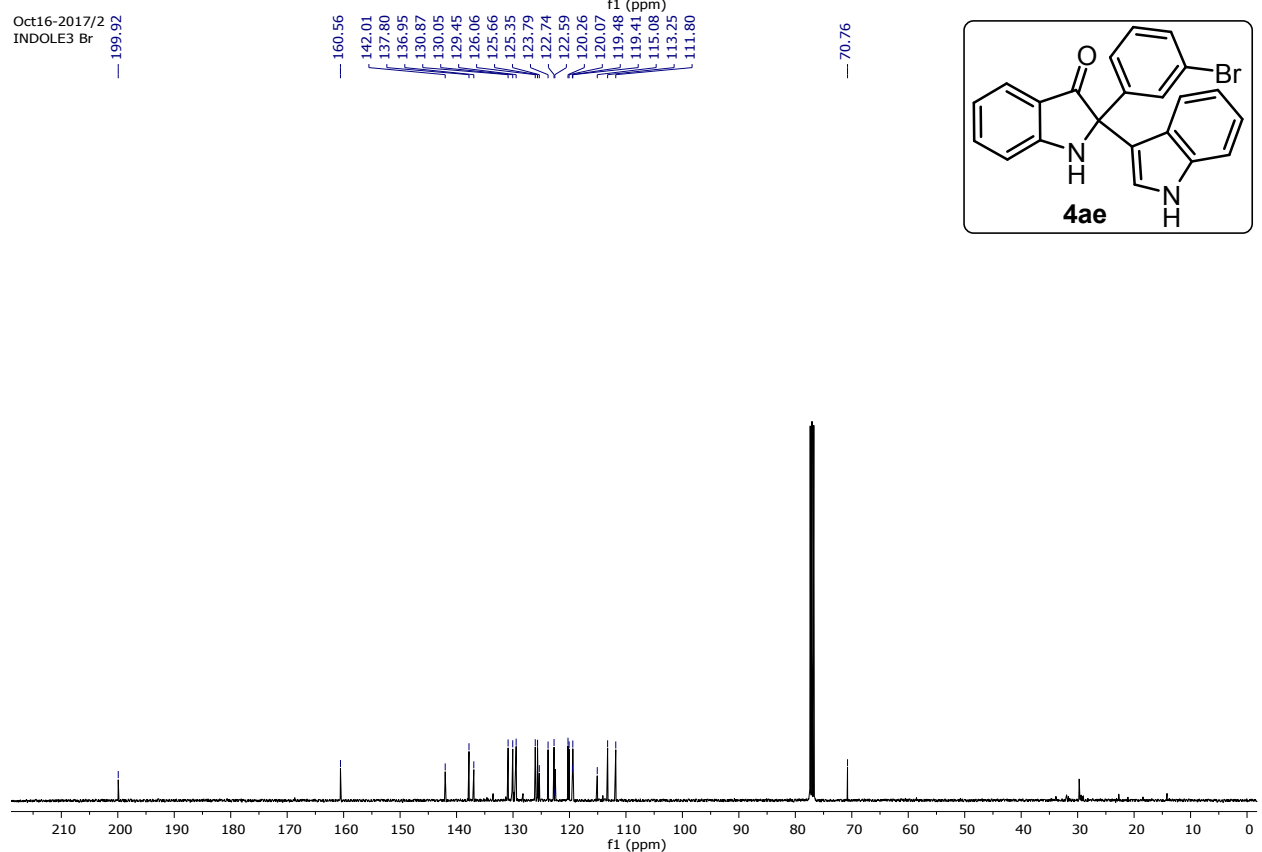
### MS Spectrum Peak List

| m/z      | Calc m/z | Diff(ppm) | z | Abund     | Formula     | Ion    |
|----------|----------|-----------|---|-----------|-------------|--------|
| 359.0951 | 359.0946 | -1.47     | 1 | 144883.69 | C22H15ClN2O | (M+H)+ |
| 360.0982 | 360.0978 | -1.13     | 1 | 34112.25  | C22H15ClN2O | (M+H)+ |

Oct16-2017/1  
INDOLE3 Br

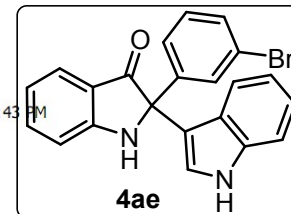


Oct16-2017/2  
INDOLE3 Br



## Qualitative Compound Report

|                               |                           |                      |                       |
|-------------------------------|---------------------------|----------------------|-----------------------|
| <b>Data File</b>              | Inodle 3 Br.d             | <b>Sample Name</b>   | Indole 3 Br           |
| <b>Sample Type</b>            | Sample                    | <b>Position</b>      | P1-F7                 |
| <b>Instrument Name</b>        | Instrument 1              | <b>User Name</b>     |                       |
| <b>Acq Method</b>             | water_acn_grad_6min_reg.m | <b>Acquired Time</b> | 10/18/2017 9:59:43 AM |
| <b>IRM Calibration Status</b> | Success                   | <b>DA Method</b>     | PROCESSNEW.m          |
| <b>Comment</b>                |                           |                      |                       |

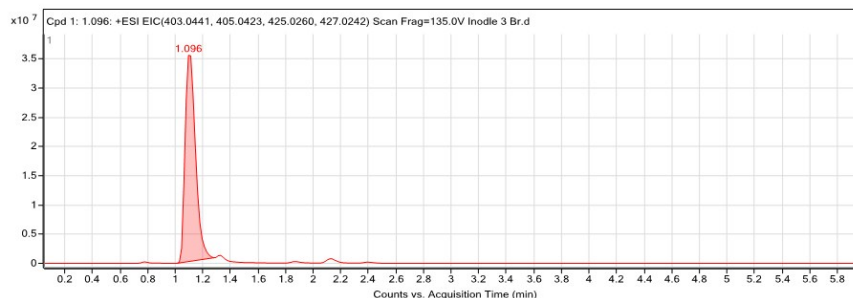


|                     |      |                               |                                                       |
|---------------------|------|-------------------------------|-------------------------------------------------------|
| <b>Sample Group</b> | LC 1 | <b>Info.</b>                  |                                                       |
| <b>Stream Name</b>  | LC 1 | <b>Acquisition SW Version</b> | 6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1) |

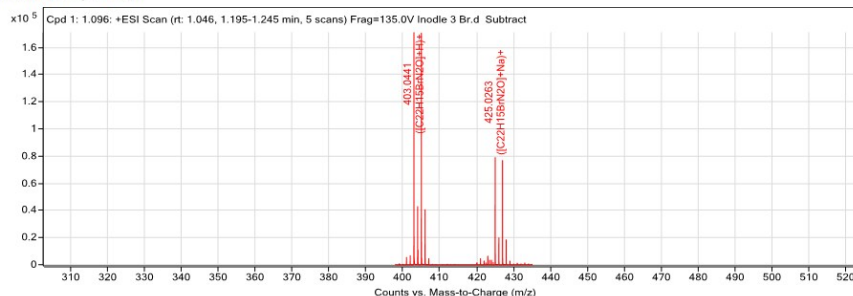
### Compound Table

| Compound Label | RT    | Mass     | Abund  | Formula         | Tgt Mass | Diff (ppm) |
|----------------|-------|----------|--------|-----------------|----------|------------|
| Cpd 1: 1.096   | 1.096 | 402.0368 | 172822 | C22 H15 Br N2 O | 402.0368 | 0.14       |

| Compound Label | m/z      | RT    | Algorithm       | Mass     |
|----------------|----------|-------|-----------------|----------|
| Cpd 1: 1.096   | 403.0441 | 1.096 | Find By Formula | 402.0368 |



### MS Zoomed Spectrum



### MS Spectrum Peak List

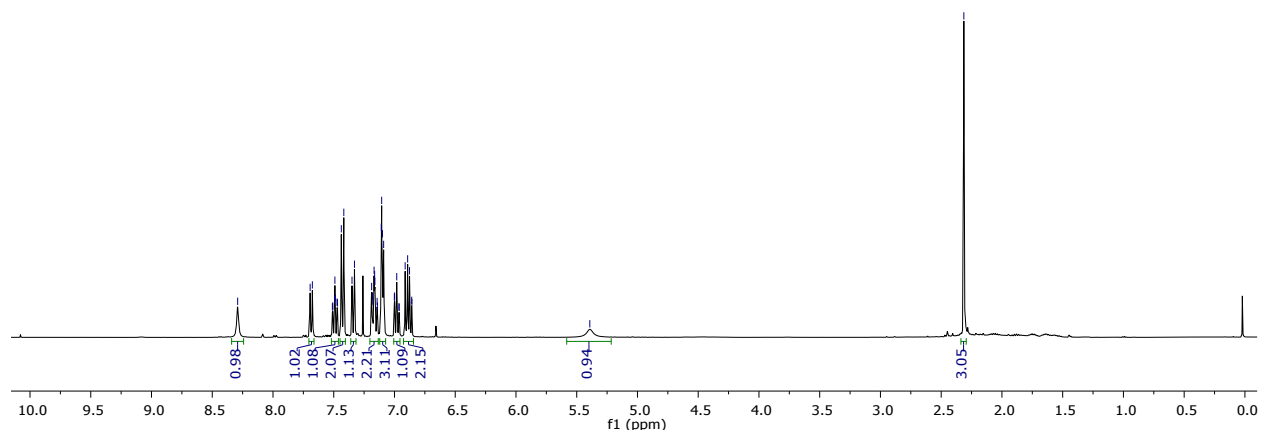
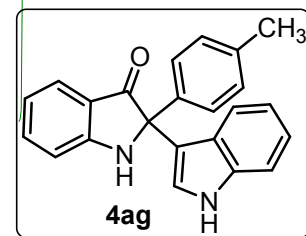
| m/z      | Calc m/z | Diff(ppm) | z | Abund     | Formula     | Ion    |
|----------|----------|-----------|---|-----------|-------------|--------|
| 403.0441 | 403.0441 | -0.18     | 1 | 172821.62 | C22H15BrN2O | (M+H)+ |
| 404.0469 | 404.0472 | 0.97      | 1 | 43398.09  | C22H15BrN2O | (M+H)+ |

Dec07-2017/1  
INDOLE4CH3

8.29  
7.69  
7.68  
7.51  
7.49  
7.49  
7.49  
7.47  
7.44  
7.42  
7.35  
7.33  
7.19  
7.18  
7.18  
7.17  
7.16  
7.16  
7.14  
7.14  
7.11  
7.11  
7.10  
7.09  
7.00  
7.00  
6.98  
6.96  
6.96  
6.91  
6.89  
6.88  
6.86  
6.86  
5.39

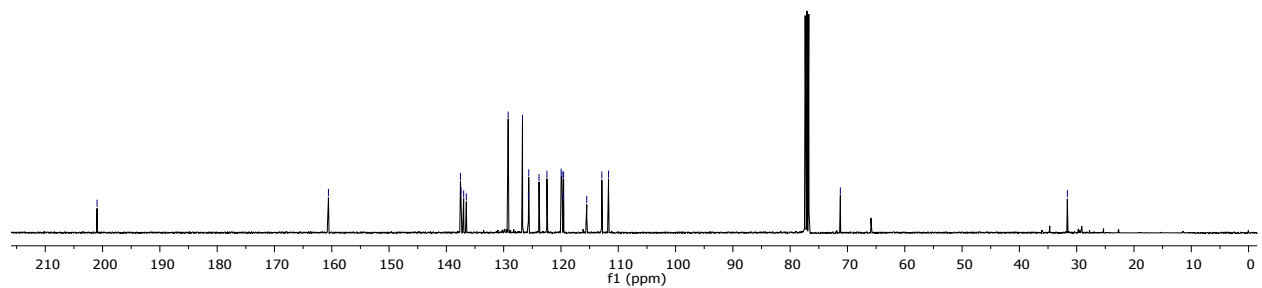
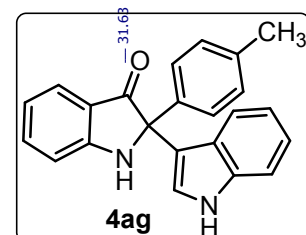


2.31



Dec08-2017/1  
INDOLE4CH3

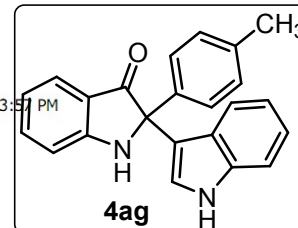
200.58  
160.58  
137.54  
137.46  
136.98  
136.52  
129.22  
126.72  
125.68  
125.62  
123.83  
122.45  
119.97  
119.82  
119.59  
119.54  
115.50  
112.87  
111.70  
71.24



## Qualitative Compound Report

**Data File** Indole 4 Me.d  
**Sample Type** Sample  
**Instrument Name** Instrument 1  
**Acq Method** water\_acn\_grad\_6min\_reg.m  
**IRM Calibration Status** Success  
**Comment**

**Sample Name** Indole 4 Me  
**Position** P1-F8  
**User Name**  
**Acquired Time** 10/18/2017 10:13:57 PM  
**DA Method** PROCESSNEW.m



**Sample Group**

**Stream Name** LC 1

**Info.**

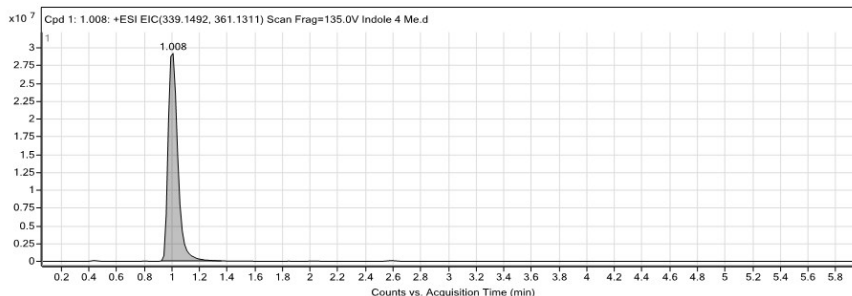
**Acquisition SW Version**

6200 series TOF/6500 series  
Q-TOF B.06.01 (B6172 SP1)

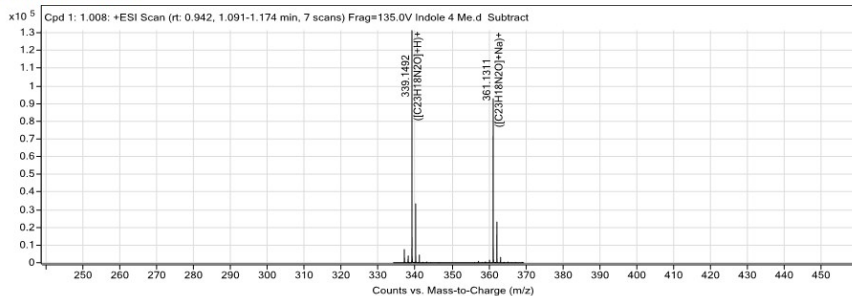
### Compound Table

| Compound Label | RT    | Mass     | Abund  | Formula      | Tgt Mass | Diff (ppm) |
|----------------|-------|----------|--------|--------------|----------|------------|
| Cpd 1: 1.008   | 1.008 | 338.1419 | 133416 | C23 H18 N2 O | 338.1419 | -0.11      |

| Compound Label | m/z      | RT    | Algorithm       | Mass     |
|----------------|----------|-------|-----------------|----------|
| Cpd 1: 1.008   | 339.1492 | 1.008 | Find By Formula | 338.1419 |



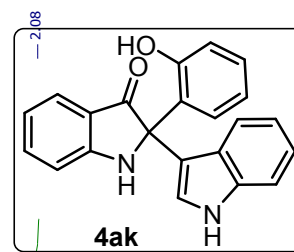
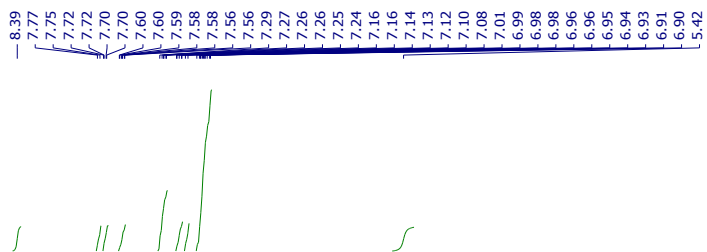
### MS Zoomed Spectrum



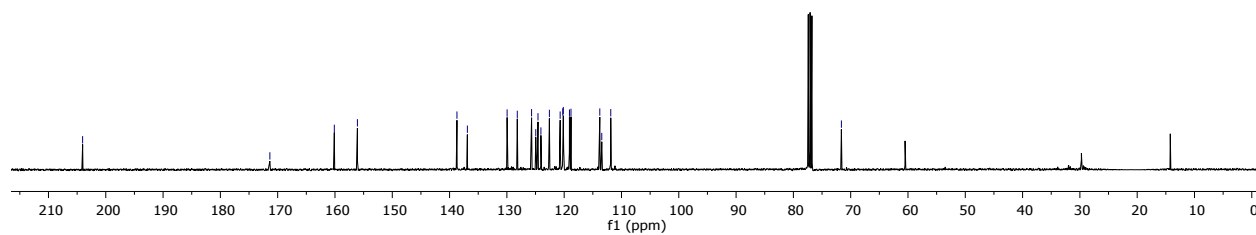
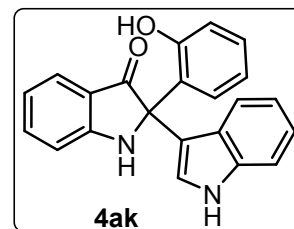
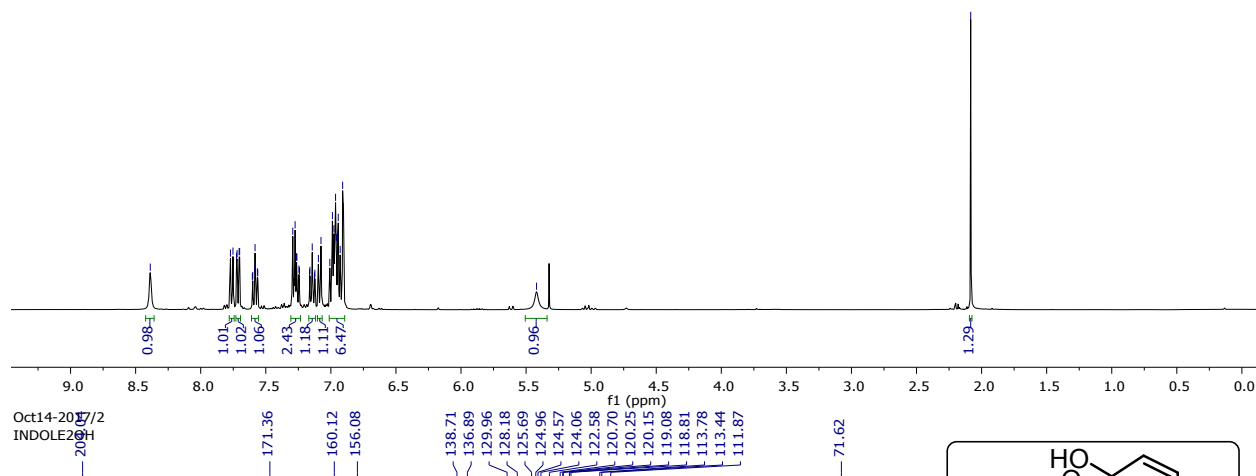
### MS Spectrum Peak List

| m/z      | Calc m/z | Diff(ppm) | z | Abund     | Formula   | Ion    |
|----------|----------|-----------|---|-----------|-----------|--------|
| 339.1492 | 339.1492 | 0.11      | 1 | 133415.77 | C23H18N2O | (M+H)+ |
| 340.1524 | 340.1524 | 0.12      | 1 | 34113.54  | C23H18N2O | (M+H)+ |

Oct14-2017/1  
INDOLE2OH

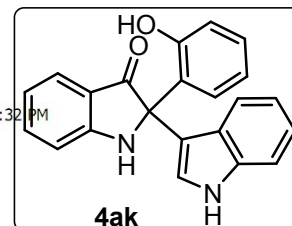


Oct14-2017/2  
INDOLE2OH



## Qualitative Compound Report

|                               |                           |                      |                       |
|-------------------------------|---------------------------|----------------------|-----------------------|
| <b>Data File</b>              | indole 2 OH.d             | <b>Sample Name</b>   | Indole 2 OH           |
| <b>Sample Type</b>            | Sample                    | <b>Position</b>      | P1-F6                 |
| <b>Instrument Name</b>        | Instrument 1              | <b>User Name</b>     |                       |
| <b>Acq Method</b>             | water_acn_grad_6min_reg.m | <b>Acquired Time</b> | 10/18/2017 9:45:32 PM |
| <b>IRM Calibration Status</b> | Success                   | <b>DA Method</b>     | PROCESSNEW.m          |
| <b>Comment</b>                |                           |                      |                       |

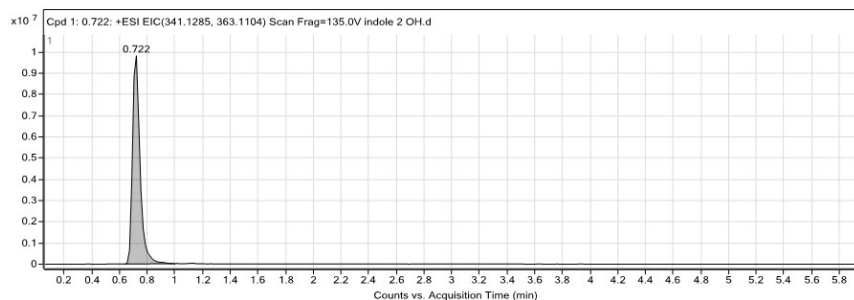


|                     |      |                               |                                                       |
|---------------------|------|-------------------------------|-------------------------------------------------------|
| <b>Sample Group</b> |      | <b>Info.</b>                  |                                                       |
| <b>Stream Name</b>  | LC 1 | <b>Acquisition SW Version</b> | 6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1) |

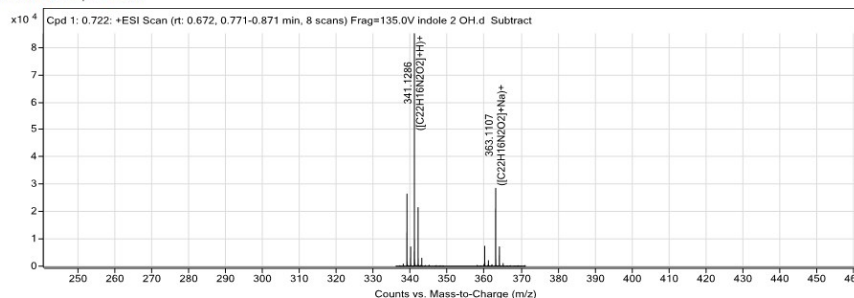
### Compound Table

| Compound Label | RT    | Mass     | Abund | Formula       | Tgt Mass | Diff (ppm) |
|----------------|-------|----------|-------|---------------|----------|------------|
| Cpd 1: 0.722   | 0.722 | 340.1214 | 88191 | C22 H16 N2 O2 | 340.1212 | 0.51       |

| Compound Label | m/z      | RT    | Algorithm       | Mass     |
|----------------|----------|-------|-----------------|----------|
| Cpd 1: 0.722   | 341.1286 | 0.722 | Find By Formula | 340.1214 |



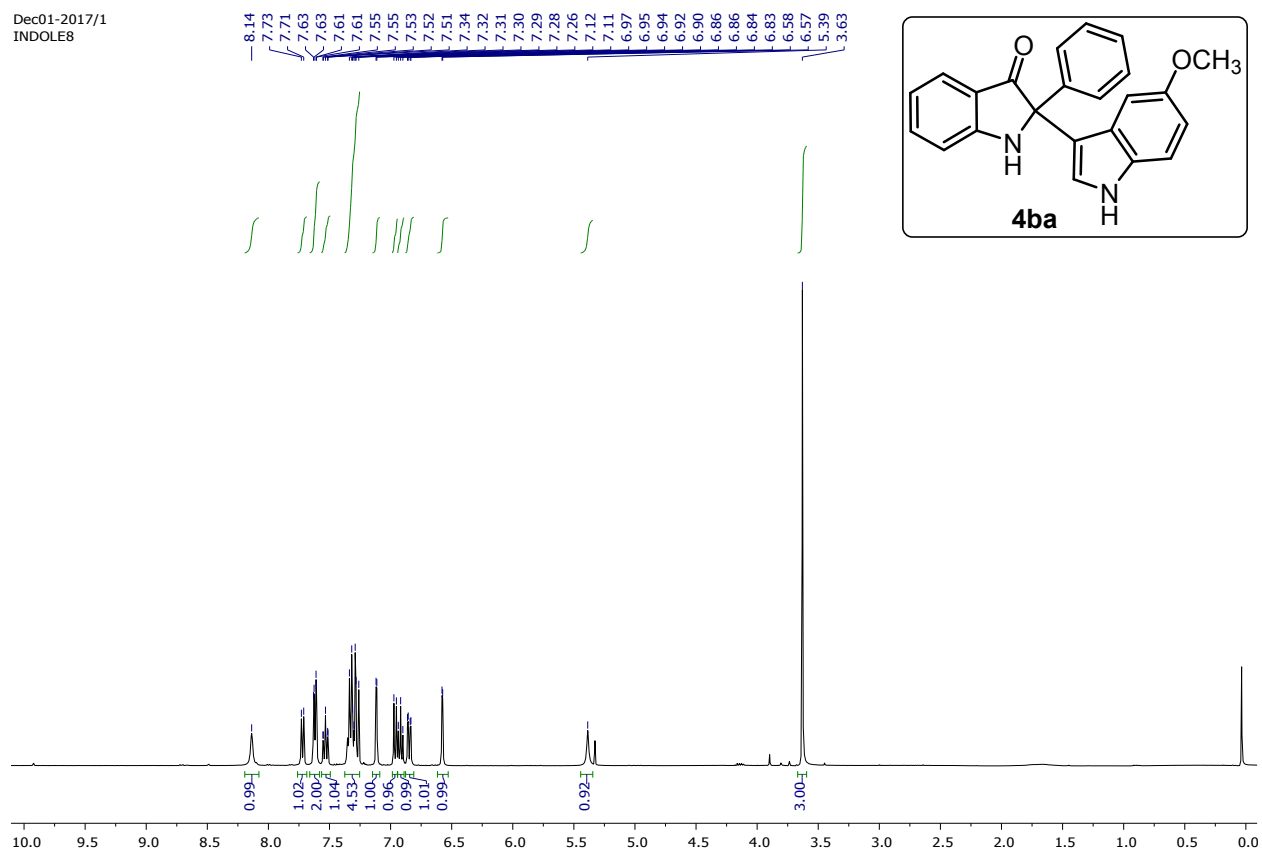
### MS Zoomed Spectrum



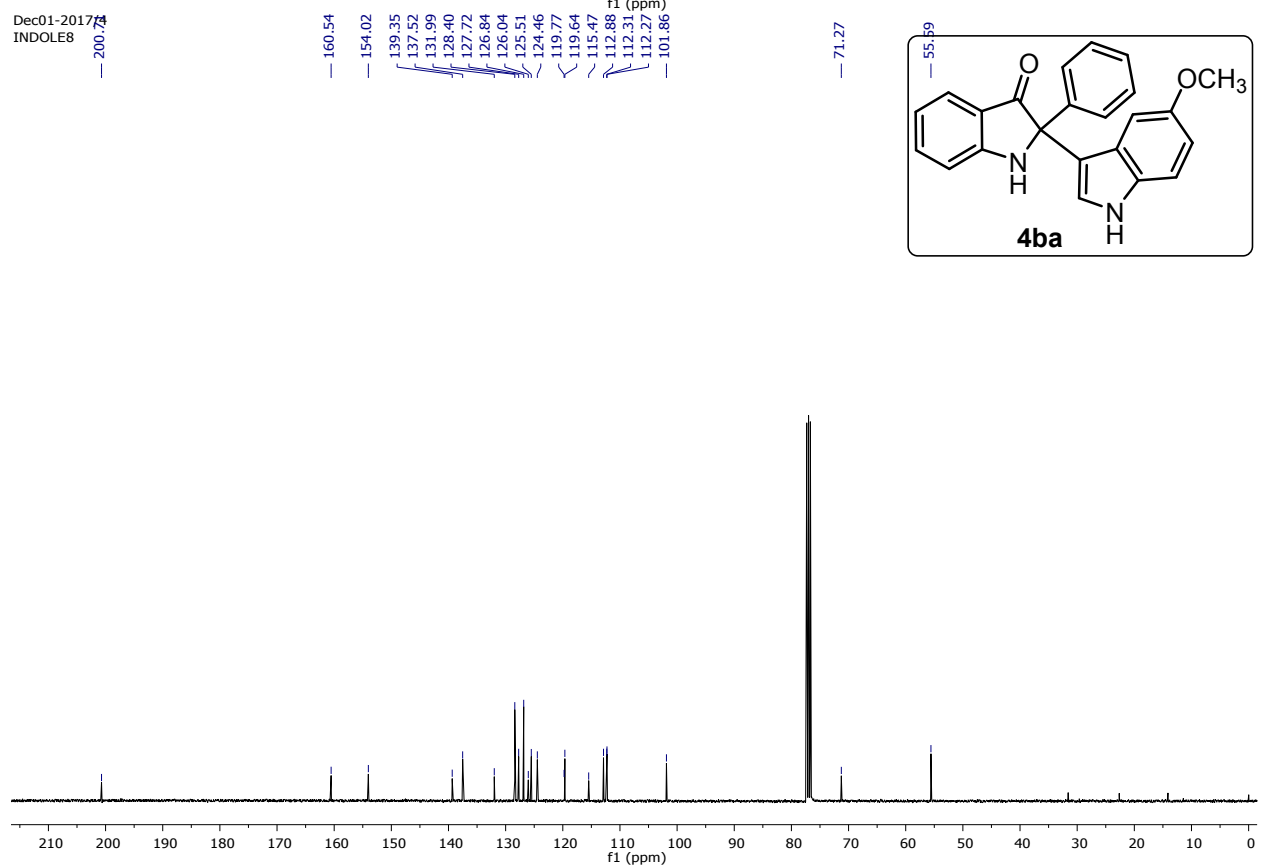
### MS Spectrum Peak List

| m/z      | Calc m/z | Diff(ppm) | z | Abund    | Formula    | Ion                |
|----------|----------|-----------|---|----------|------------|--------------------|
| 341.1286 | 341.1285 | -0.31     | 1 | 88191    | C22H16N2O2 | (M+H) <sup>+</sup> |
| 342.1318 | 342.1316 | -0.51     | 1 | 21964.47 | C22H16N2O2 | (M+H) <sup>+</sup> |

Dec01-2017/1  
INDOLE8



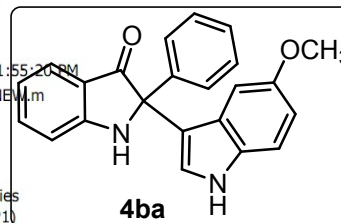
Dec01-2017/1  
INDOLE8



## Qualitative Compound Report

**Data File** INDOLE 8.d  
**Sample Type** Sample  
**Instrument Name** Instrument 1  
**Acq Method** water\_meoh\_grad\_6min\_reg.m  
**IRM Calibration Status** Success  
**Comment**

**Sample Name** INDOLE 8  
**Position** P2-E4  
**User Name**  
**Acquired Time** 1/5/2018 1:55:20 PM  
**DA Method** PROCESSNEW.m

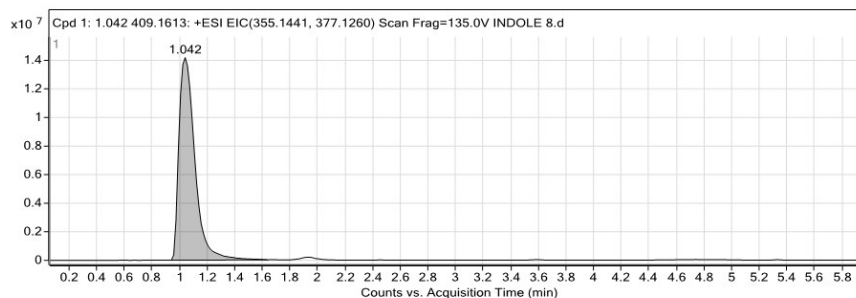


**Sample Group**  
**Stream Name** LC 1  
**Info.**  
**Acquisition SW Version** 6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

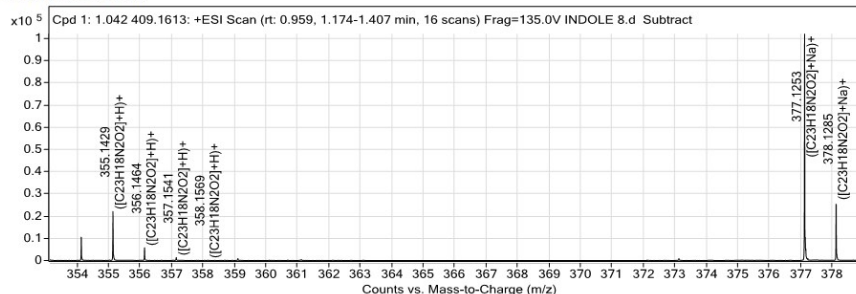
### Compound Table

| Compound Label        | RT    | Mass    | Abund  | Formula       | Tgt Mass | Diff (ppm) |
|-----------------------|-------|---------|--------|---------------|----------|------------|
| Cpd 1: 1.042 409.1613 | 1.042 | 354.136 | 103571 | C23 H18 N2 O2 | 354.1368 | -2.22      |

| Compound Label        | m/z      | RT    | Algorithm       | Mass    |
|-----------------------|----------|-------|-----------------|---------|
| Cpd 1: 1.042 409.1613 | 377.1253 | 1.042 | Find By Formula | 354.136 |

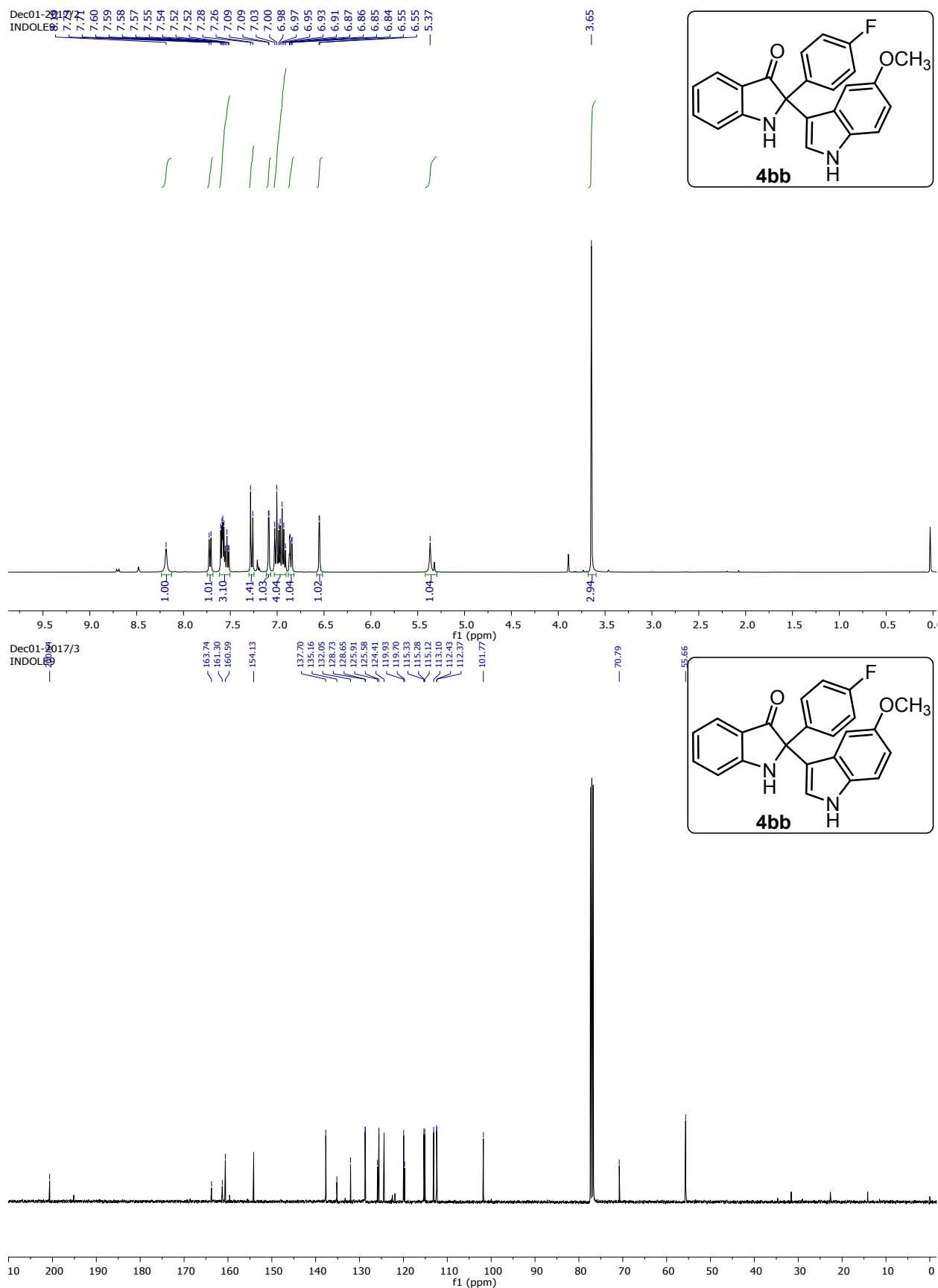


### MS Zoomed Spectrum



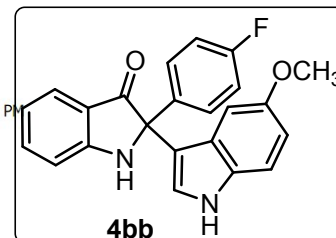
### MS Spectrum Peak List

| m/z      | Calc m/z | Diff(ppm) | z | Abund    | Formula    | Ion    |
|----------|----------|-----------|---|----------|------------|--------|
| 355.1429 | 355.1441 | 3.3       | 1 | 22090.02 | C23H18N2O2 | (M+H)+ |
| 356.1464 | 356.1473 | 2.54      | 1 | 5752     | C23H18N2O2 | (M+H)+ |



## Qualitative Compound Report

|                               |                            |                      |                     |
|-------------------------------|----------------------------|----------------------|---------------------|
| <b>Data File</b>              | INDOLE 9.d                 | <b>Sample Name</b>   | INDOLE 9            |
| <b>Sample Type</b>            | Sample                     | <b>Position</b>      | P2-E5               |
| <b>Instrument Name</b>        | Instrument 1               | <b>User Name</b>     |                     |
| <b>Acq Method</b>             | water_meoh_grad_6min_reg.m | <b>Acquired Time</b> | 1/5/2018 2:09:27 PM |
| <b>IRM Calibration Status</b> | Success                    | <b>DA Method</b>     | PROCESSNEW.m        |
| <b>Comment</b>                |                            |                      |                     |

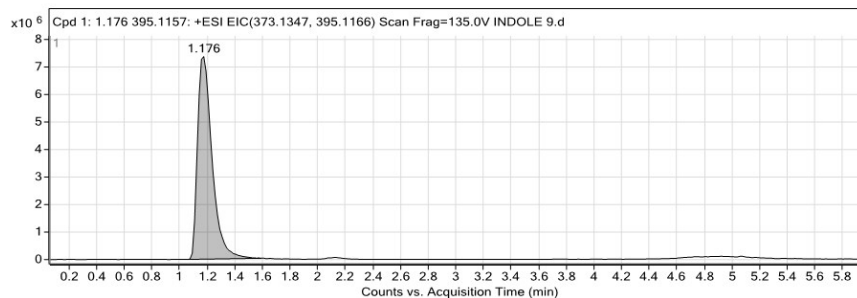


|                     |                |                             |
|---------------------|----------------|-----------------------------|
| <b>Sample Group</b> | <b>Info.</b>   |                             |
| <b>Stream Name</b>  | LC 1           | <b>Acquisition SW</b>       |
|                     |                | 6200 series TOF/6500 series |
|                     | <b>Version</b> | Q-TOF B.06.01 (B6172 SP1)   |

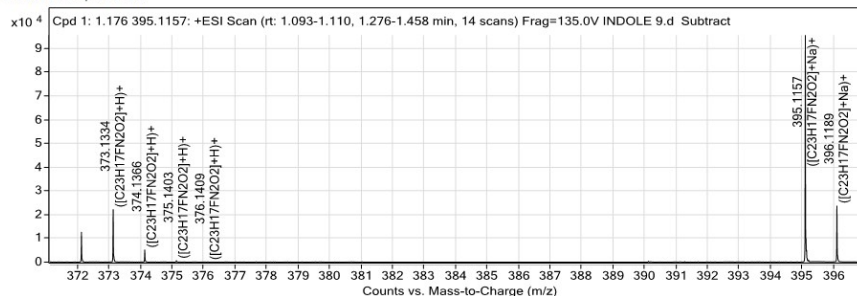
### Compound Table

| Compound Label        | RT    | Mass     | Abund | Formula         | Tgt Mass | Diff (ppm) |
|-----------------------|-------|----------|-------|-----------------|----------|------------|
| Cpd 1: 1.176 395.1157 | 1.176 | 372.1264 | 96028 | C23 H17 F N2 O2 | 372.1274 | -2.63      |

| Compound Label        | m/z      | RT    | Algorithm       | Mass     |
|-----------------------|----------|-------|-----------------|----------|
| Cpd 1: 1.176 395.1157 | 395.1157 | 1.176 | Find By Formula | 372.1264 |



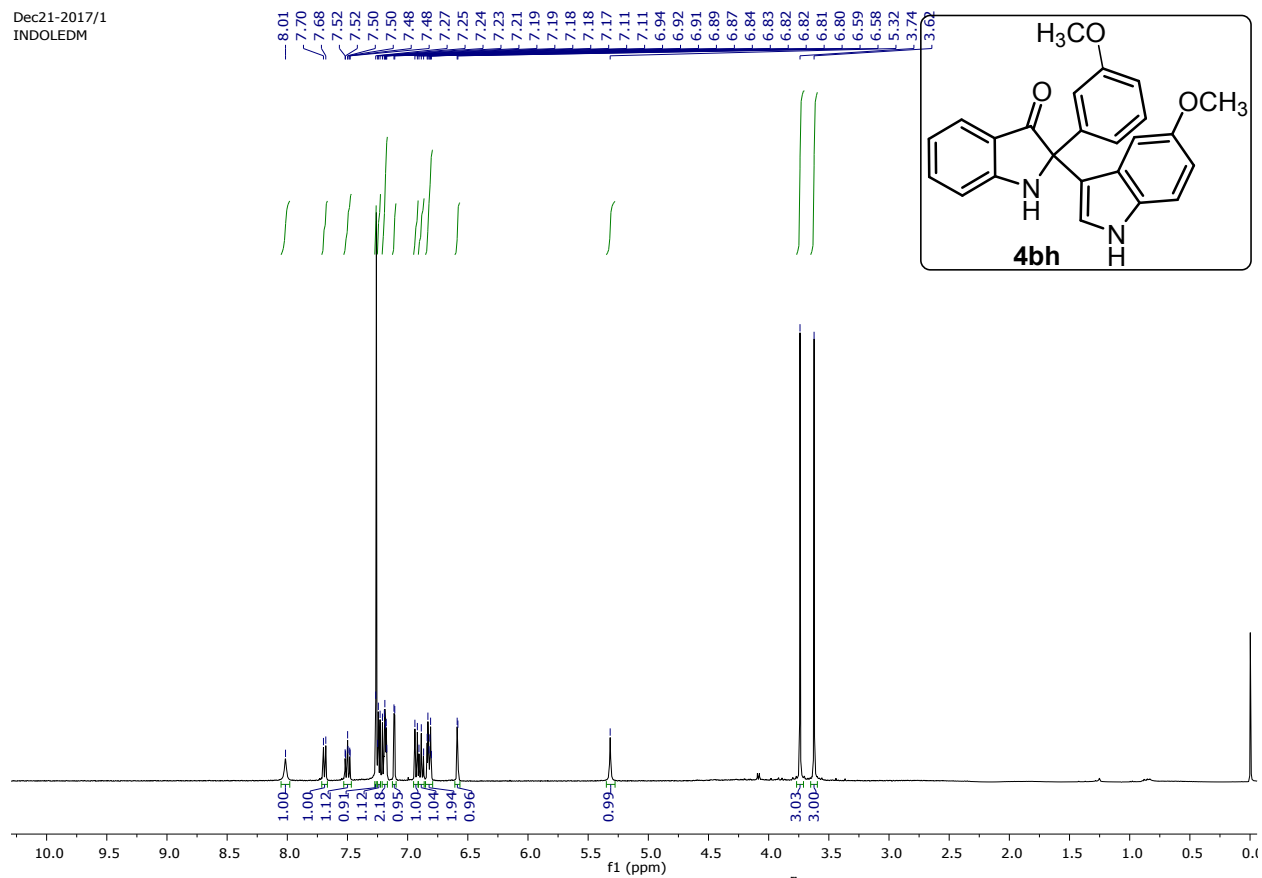
### MS Zoomed Spectrum



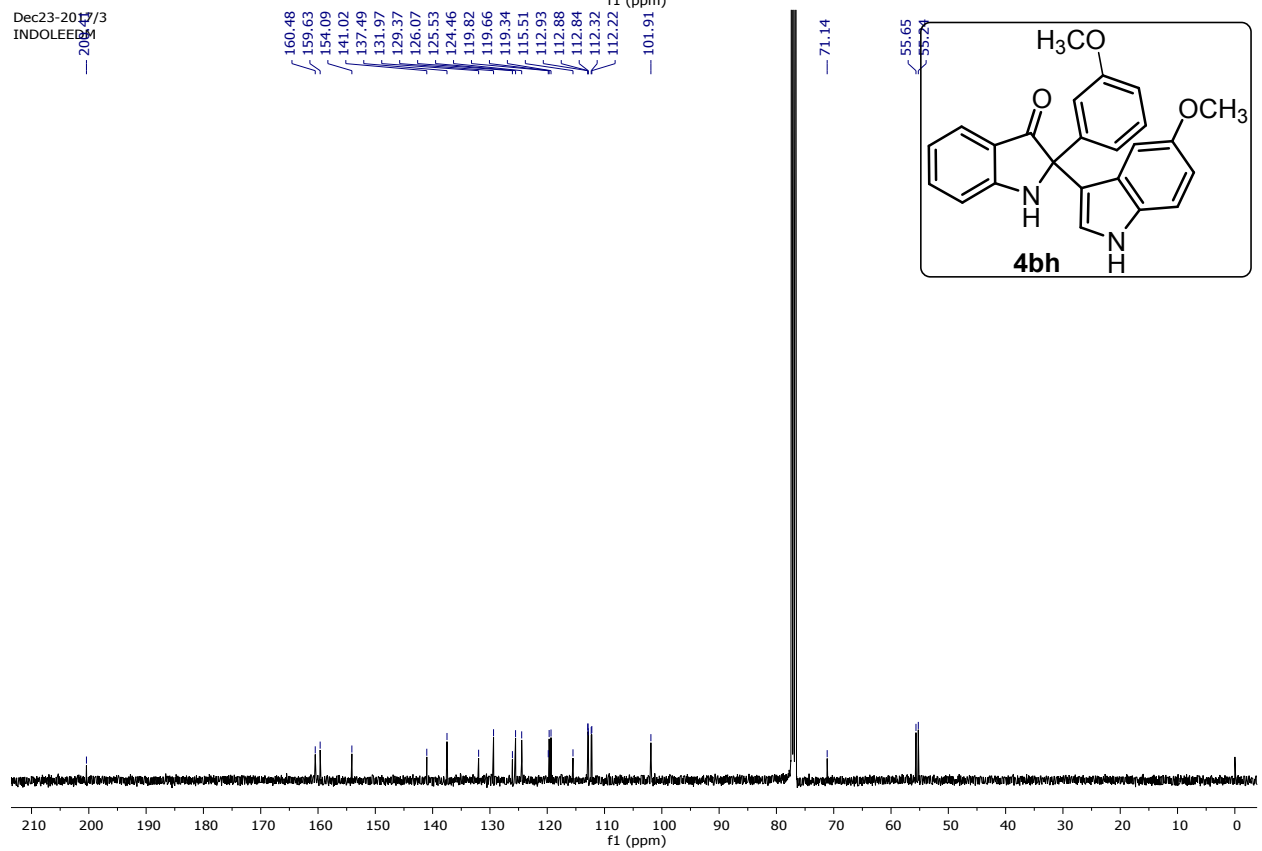
### MS Spectrum Peak List

| m/z      | Calc m/z | Diff(ppm) | z | Abund    | Formula     | Ion    |
|----------|----------|-----------|---|----------|-------------|--------|
| 373.1334 | 373.1347 | 3.51      | 1 | 22215.47 | C23H17FN2O2 | (M+H)+ |
| 374.1366 | 374.1379 | 3.53      | 1 | 5205.3   | C23H17FN2O2 | (M+H)+ |

Dec21-2017/1  
INDOLEDM



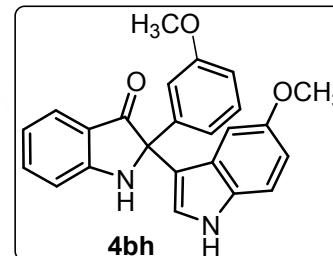
Dec23-2017/3  
INDOLEDM



# Qualitative Compound Report

**Data File** Blank 15.d  
**Sample Type** Sample  
**Instrument Name** Instrument 1  
**Acq Method** water\_meoh\_grad\_6min\_reg.m  
**IRM Calibration Status** Success  
**Comment**

**Sample Name** INDOLE DM  
**Position** P2-E6  
**User Name**  
**Acquired Time** 1/5/2018 2:23:34 PM  
**DA Method** PROCESSNEW.m



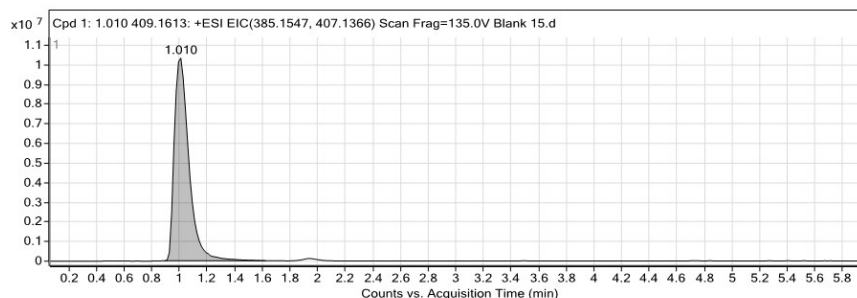
**Sample Group**  
**Stream Name** LC 1

**Info.**  
**Acquisition SW Version** 6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

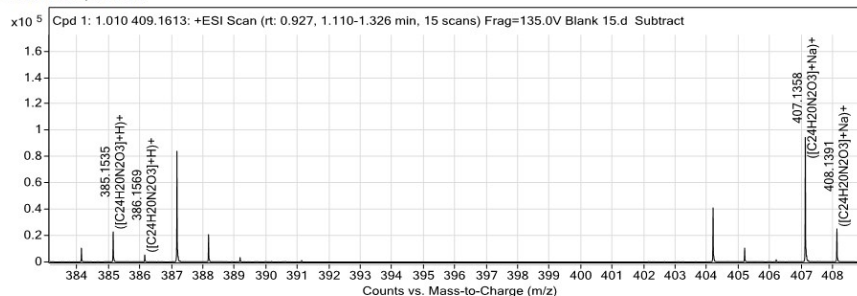
## Compound Table

| Compound Label        | RT   | Mass     | Abund | Formula                                                       | Tgt Mass | Diff (ppm) |
|-----------------------|------|----------|-------|---------------------------------------------------------------|----------|------------|
| Cpd 1: 1.010 409.1613 | 1.01 | 384.1465 | 96761 | C <sub>24</sub> H <sub>20</sub> N <sub>2</sub> O <sub>3</sub> | 384.1474 | -2.29      |

| Compound Label        | m/z      | RT   | Algorithm       | Mass     |
|-----------------------|----------|------|-----------------|----------|
| Cpd 1: 1.010 409.1613 | 407.1358 | 1.01 | Find By Formula | 384.1465 |



## MS Zoomed Spectrum

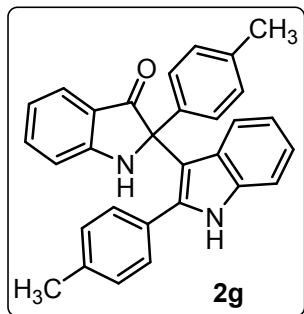


## MS Spectrum Peak List

| m/z      | Calc m/z | Diff(ppm) | z | Abund    | Formula                                                       | Ion                |
|----------|----------|-----------|---|----------|---------------------------------------------------------------|--------------------|
| 385.1535 | 385.1547 | 2.98      | 1 | 23216.58 | C <sub>24</sub> H <sub>20</sub> N <sub>2</sub> O <sub>3</sub> | (M+H) <sup>+</sup> |
| 386.1569 | 386.1579 | 2.42      | 1 | 5579     | C <sub>24</sub> H <sub>20</sub> N <sub>2</sub> O <sub>3</sub> | (M+H) <sup>+</sup> |

### Crystal structure data for (2g):

#### Crystal structure of 2-(*p*-tolyl)-2-(2-(*p*-tolyl)-1*H*-indol-3-yl)indolin-3-one(2g):



(CCDC No.1832862)

Single crystals of 2-(*p*-tolyl)-2-(2-(*p*-tolyl)-1*H*-indol-3-yl)indolin-3-one  $C_{61}H_{49}Cl_3N_4O_2$  was selected on a XtaLAB Pro: Kappa dual offset/far diffractometer. The crystal was kept at 93(2) K during data collection. Using Olex2,<sup>[1]</sup> the structure was solved with the ShelXT<sup>[2]</sup>

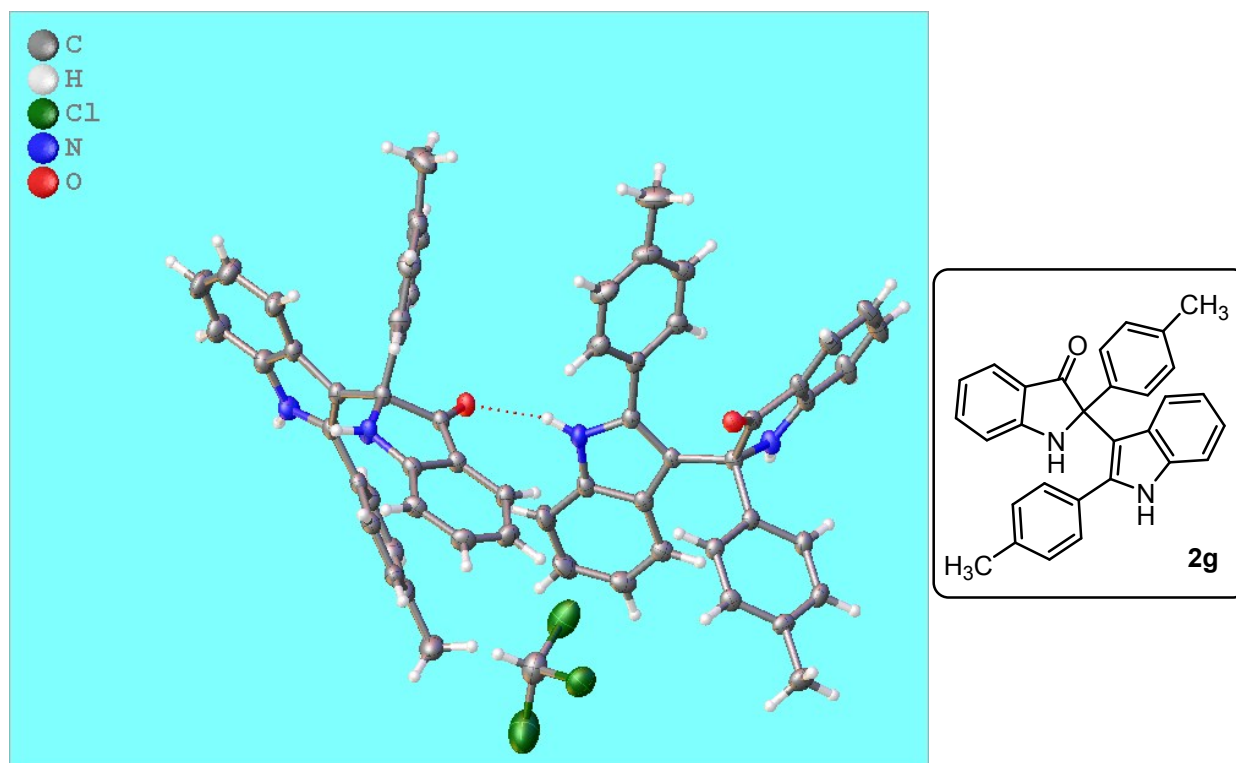
structure solution program using Intrinsic Phasing and refined with the ShelXL<sup>[3]</sup> refinement package using Least Squares minimization.

**Crystal Data** for  $C_{61}H_{49}Cl_3N_4O_2$  ( $M=976.39$  g/mol): triclinic, space group P-1 (no. 2),  $a = 13.13930(10)$  Å,  $b = 14.65600(10)$  Å,  $c = 15.47680(10)$  Å,  $\alpha = 110.2300(10)^\circ$ ,  $\beta = 91.2620(10)^\circ$ ,  $\gamma = 108.1490(10)^\circ$ ,  $V = 2629.10(4)$  Å<sup>3</sup>,  $Z = 2$ ,  $T = 93(2)$  K,  $\mu(\text{CuK}\alpha) = 1.943$  mm<sup>-1</sup>,  $D_{\text{calc}} = 1.233$  g/cm<sup>3</sup>, 28497 reflections measured ( $7.156^\circ \leq 2\theta \leq 149.04^\circ$ ), 10338 unique ( $R_{\text{int}} = 0.0246$ ,  $R_{\text{sigma}} = 0.0226$ ) which were used in all calculations. The final  $R_1$  was 0.0623 ( $I > 2\sigma(I)$ ) and  $wR_2$  was 0.1867 (all data).

| <b>TableS1:Crystal structure data of (2g): (CCDC No.1832862)</b>        |                          |
|-------------------------------------------------------------------------|--------------------------|
| <b>Table 1 Crystal data and structure refinement for exp_255-IND8a.</b> |                          |
| Identification code                                                     | <b>CCDC No.1832862</b>   |
| Empirical formula                                                       | $C_{61}H_{49}Cl_3N_4O_2$ |
| Formula weight                                                          | 976.39                   |
| Temperature/K                                                           | 93(2)                    |
| Crystal system                                                          | triclinic                |

|                                                |                                                                 |
|------------------------------------------------|-----------------------------------------------------------------|
| Space group                                    | P-1                                                             |
| a/Å                                            | 13.13930(10)                                                    |
| b/Å                                            | 14.65600(10)                                                    |
| c/Å                                            | 15.47680(10)                                                    |
| $\alpha/^\circ$                                | 110.2300(10)                                                    |
| $\beta/^\circ$                                 | 91.2620(10)                                                     |
| $\gamma/^\circ$                                | 108.1490(10)                                                    |
| Volume/Å <sup>3</sup>                          | 2629.10(4)                                                      |
| Z                                              | 2                                                               |
| $\rho_{\text{calc}}/\text{g}/\text{cm}^3$      | 1.233                                                           |
| $\mu/\text{mm}^{-1}$                           | 1.943                                                           |
| F(000)                                         | 1020.0                                                          |
| Crystal size/mm <sup>3</sup>                   | 0.2 × 0.2 × 0.1                                                 |
| Radiation                                      | CuK $\alpha$ ( $\lambda$ = 1.54184)                             |
| 2 $\Theta$ range for data collection/ $^\circ$ | 7.156 to 149.04                                                 |
| Index ranges                                   | -15 ≤ h ≤ 16, -18 ≤ k ≤ 18, -19 ≤ l ≤ 13                        |
| Reflections collected                          | 28497                                                           |
| Independent reflections                        | 10338 [ $R_{\text{int}}$ = 0.0246, $R_{\text{sigma}}$ = 0.0226] |
| Data/restraints/parameters                     | 10338/0/635                                                     |
| Goodness-of-fit on F <sup>2</sup>              | 1.069                                                           |
| Final R indexes [ $I \geq 2\sigma(I)$ ]        | $R_1$ = 0.0623, $wR_2$ = 0.1847                                 |

|                                                |                                  |
|------------------------------------------------|----------------------------------|
| Final R indexes [all data]                     | $R_1 = 0.0645$ , $wR_2 = 0.1867$ |
| Largest diff. peak/hole / $e \text{ \AA}^{-3}$ | 0.49/-0.84                       |



**FigureS2** Single crystal X-ray of **2g**(CCDC No.1832862). The thermal ellipsoids are drawn at the 50% probability level. The compound was crystalized with  $\text{CHCl}_3$ .

#### References:

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. &Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.
2. Sheldrick, G.M. (2015). ActaCryst. A71, 3-8.
3. Sheldrick, G.M. (2015). ActaCryst. C71, 3-8.