

Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF081716\  
 Data File : BF089764.D  
 Acq On : 17 Aug 2016 15:49  
 Operator : UM/SJ  
 Sample : H4476-09  
 Misc :  
 ALS Vial : 34 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 LOCATION-16A

Integration Parameters: rteint.p  
 Integrator: RTE  
 Smoothing : ON Filtering: 5  
 Sampling : 1 Min Area: 3 % of largest Peak  
 Start Thrs: 0.2 Max Peaks: 100  
 Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >  
 Peak separation: 5

Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF081616.M  
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

| peak<br># | R.T.<br>min | first<br>scan | max<br>scan | last<br>scan | PK<br>TY | peak<br>height | corr.<br>area | corr.<br>% max. | % of<br>total |
|-----------|-------------|---------------|-------------|--------------|----------|----------------|---------------|-----------------|---------------|
| 1         | 1.667       | 6             | 7           | 16           | rVV      | 1656133        | 2921125       | 9.19%           | 1.640%        |
| 2         | 1.793       | 16            | 18          | 64           | rVB      | 12766119       | 31800102      | 100.00%         | 17.853%       |
| 3         | 4.844       | 282           | 285         | 292          | rBV      | 1157266        | 1675371       | 5.27%           | 0.941%        |
| 4         | 5.279       | 320           | 323         | 325          | rBV      | 8157595        | 8028582       | 25.25%          | 4.507%        |
| 5         | 6.330       | 412           | 415         | 417          | rBV      | 5175512        | 5239749       | 16.48%          | 2.942%        |
| 6         | 6.467       | 424           | 427         | 429          | rBV      | 12662020       | 15316008      | 48.16%          | 8.598%        |
| 7         | 6.696       | 445           | 447         | 449          | rBV      | 4444675        | 3728273       | 11.72%          | 2.093%        |
| 8         | 6.776       | 452           | 454         | 458          | rBV      | 188113         | 327370        | 1.03%           | 0.184%        |
| 9         | 6.856       | 458           | 461         | 463          | rVB      | 14107476       | 13234659      | 41.62%          | 7.430%        |
| 10        | 7.267       | 493           | 497         | 499          | rBV      | 10115304       | 11650372      | 36.64%          | 6.541%        |
| 11        | 7.908       | 551           | 553         | 557          | rBV      | 241588         | 430916        | 1.36%           | 0.242%        |
| 12        | 7.988       | 557           | 560         | 562          | rVB      | 4983112        | 5235671       | 16.46%          | 2.939%        |
| 13        | 8.262       | 581           | 584         | 586          | rVB      | 614747         | 674589        | 2.12%           | 0.379%        |
| 14        | 9.073       | 652           | 655         | 657          | rVB      | 18187426       | 21734743      | 68.35%          | 12.202%       |
| 15        | 9.462       | 686           | 689         | 691          | rBV      | 1073311        | 880397        | 2.77%           | 0.494%        |
| 16        | 9.736       | 710           | 713         | 715          | rBV      | 6786001        | 6052249       | 19.03%          | 3.398%        |
| 17        | 10.525      | 777           | 782         | 784          | rBV      | 10708773       | 12891269      | 40.54%          | 7.237%        |
| 18        | 11.211      | 839           | 842         | 844          | rBV      | 6731432        | 5881683       | 18.50%          | 3.302%        |
| 19        | 11.531      | 868           | 870         | 876          | rBV      | 139537         | 320173        | 1.01%           | 0.180%        |
| 20        | 11.759      | 888           | 890         | 892          | rBV      | 508413         | 523469        | 1.65%           | 0.294%        |
| 21        | 12.548      | 957           | 959         | 965          | rBV      | 390261         | 472404        | 1.49%           | 0.265%        |
| 22        | 12.811      | 978           | 982         | 984          | rBV      | 15454650       | 19424013      | 61.08%          | 10.905%       |
| 23        | 13.862      | 1071          | 1074        | 1076         | rVV      | 4162128        | 5440881       | 17.11%          | 3.055%        |
| 24        | 15.314      | 1198          | 1201        | 1203         | rBV      | 3085829        | 4241993       | 13.34%          | 2.381%        |

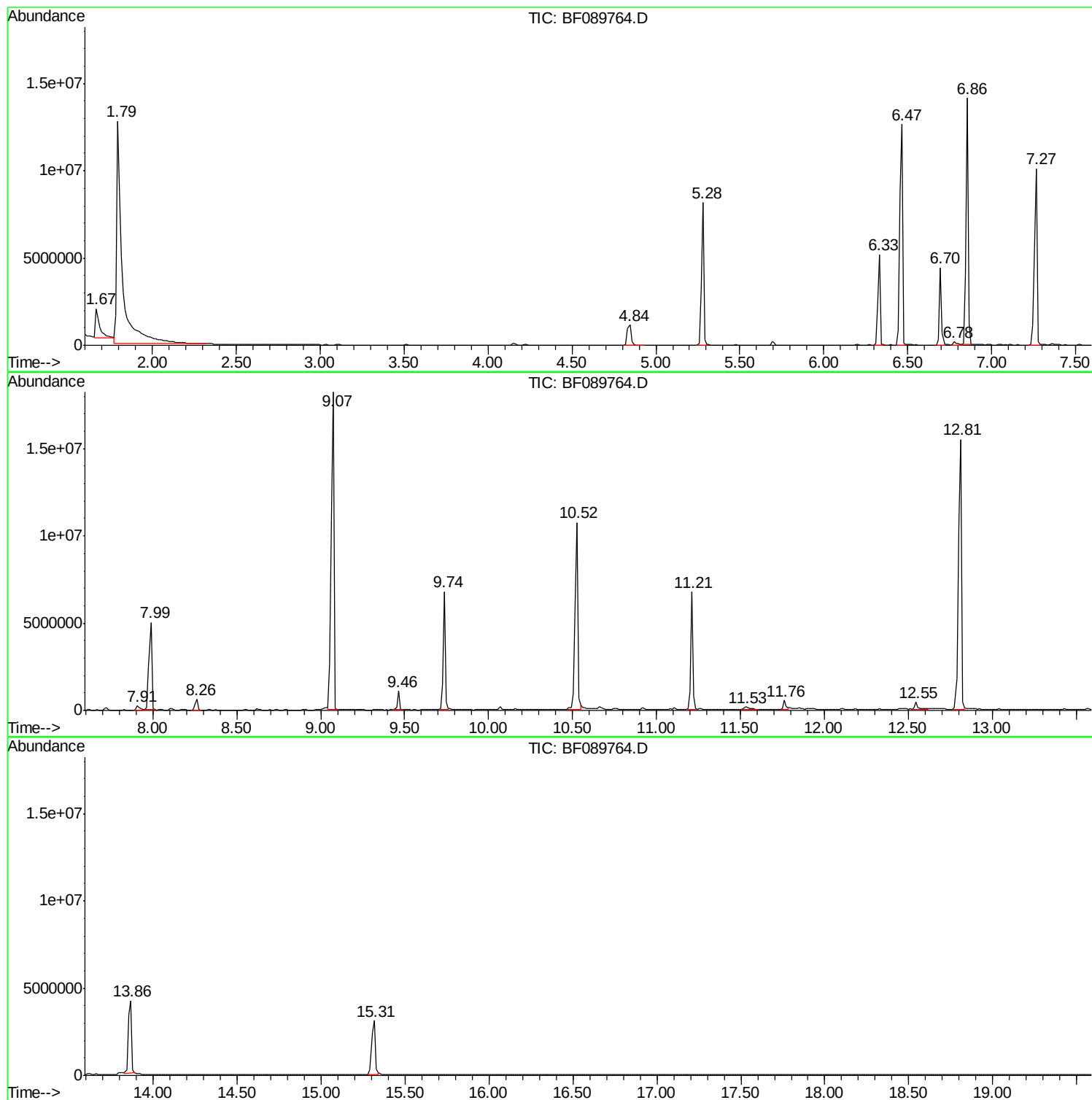
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ClientSampleId :  
LOCATION-16A

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF081616.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L  
TIC Integration Parameters: LSCINT.P



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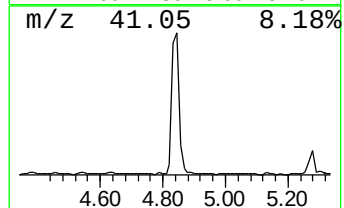
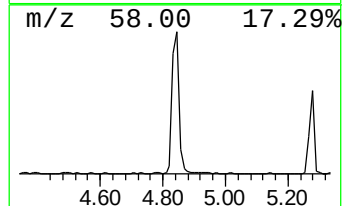
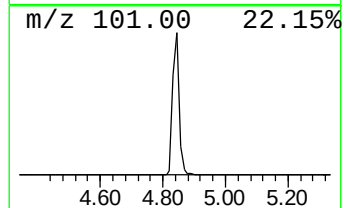
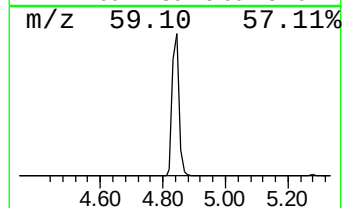
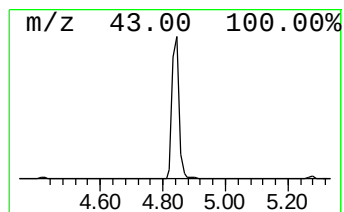
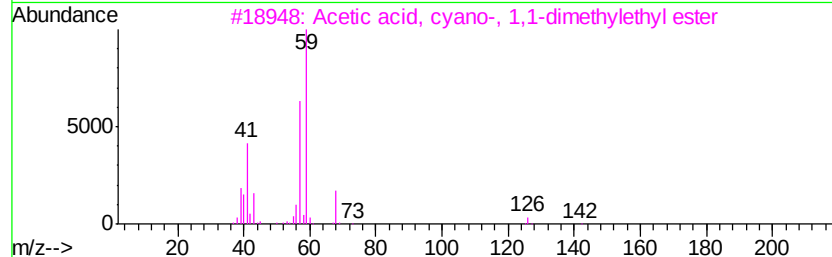
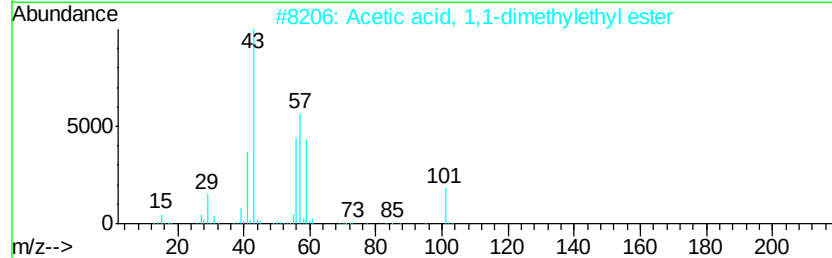
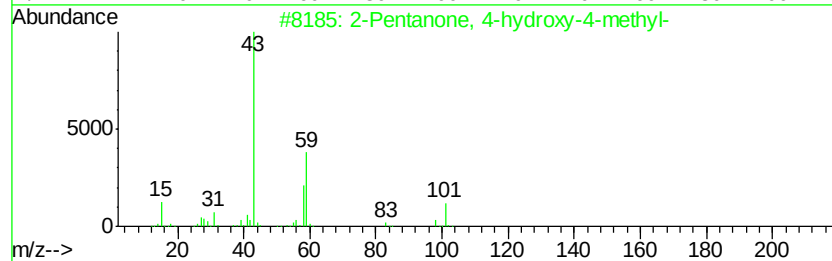
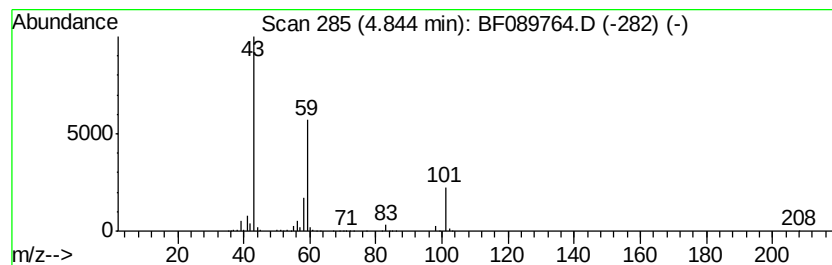
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TIC Integration Parameters: LSCINT.P

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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

| R.T. | EstConc | Area    | Relative to ISTD       | R.T. |
|------|---------|---------|------------------------|------|
| 4.84 | 8.99 ng | 1675370 | 1,4-Dichlorobenzene-d4 | 6.70 |

| Hit# | of | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|-------------------------------------|-----|----------|-------------|------|
| 1    | 5  | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2  | 000123-42-2 | 50   |
| 2    |    | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2  | 000540-88-5 | 39   |
| 3    |    | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 32   |
| 4    |    | Morpholine, 4-methyl-               | 101 | C5H11NO  | 000109-02-4 | 9    |
| 5    |    | 5-Hexen-2-one                       | 98  | C6H10O   | 000109-49-9 | 9    |



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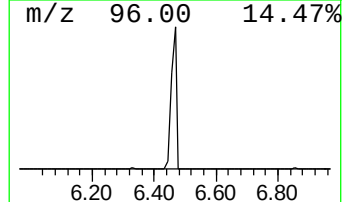
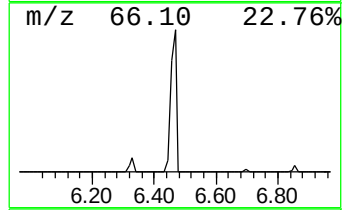
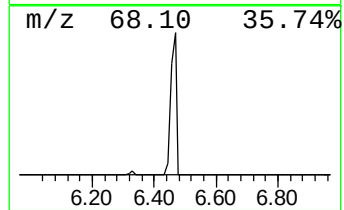
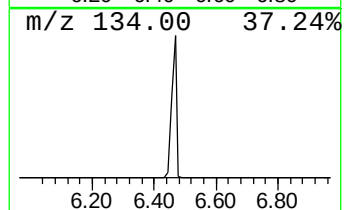
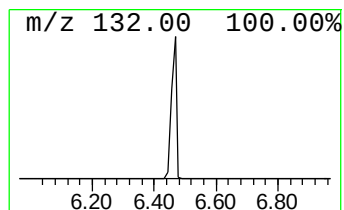
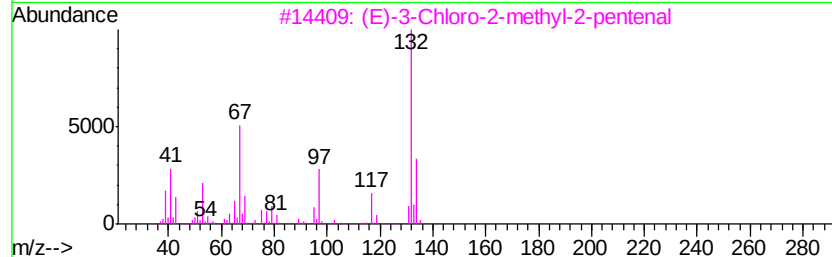
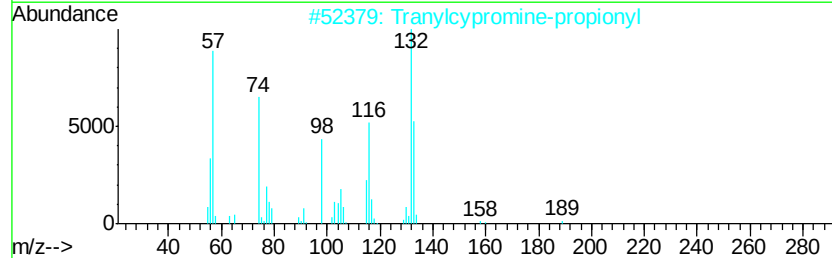
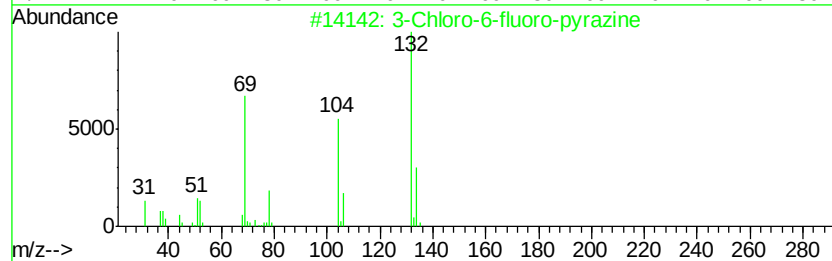
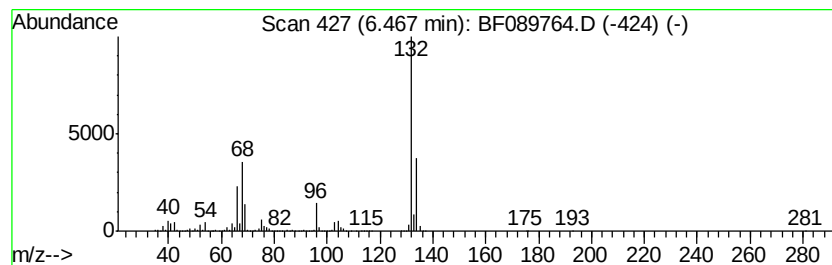
Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF081616.M  
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Peak Number 4 unknown6.47 Concentration Rank 2

| R.T. | EstConc  | Area     | Relative to ISTD       | R.T. |
|------|----------|----------|------------------------|------|
| 6.47 | 82.16 ng | 15316000 | 1,4-Dichlorobenzene-d4 | 6.70 |

| Hit# | of | Tentative ID                     | MW  | MolForm   | CAS#         | Qual |
|------|----|----------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 3-Chloro-6-fluoro-pyrazine       | 132 | C4H2ClFN2 | 1000146-10-7 | 38   |
| 2    |    | Tranylcypromine-propionyl        | 189 | C12H15NO  | 1000123-86-3 | 16   |
| 3    |    | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO   | 031357-76-3  | 12   |
| 4    |    | Amphetaminil                     | 250 | C17H18N2  | 017590-01-1  | 12   |
| 5    |    | 4-Methylpyrrolo[1,2-a]pyrazine   | 132 | C8H8N2    | 064608-60-2  | 9    |



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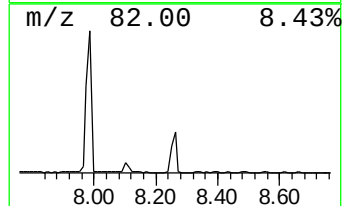
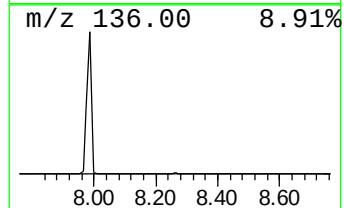
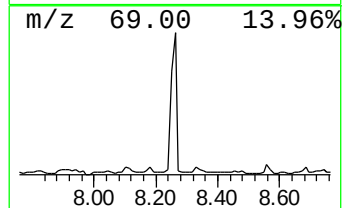
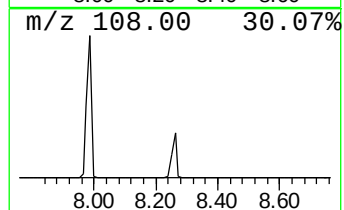
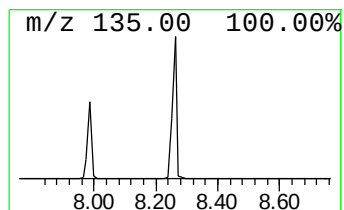
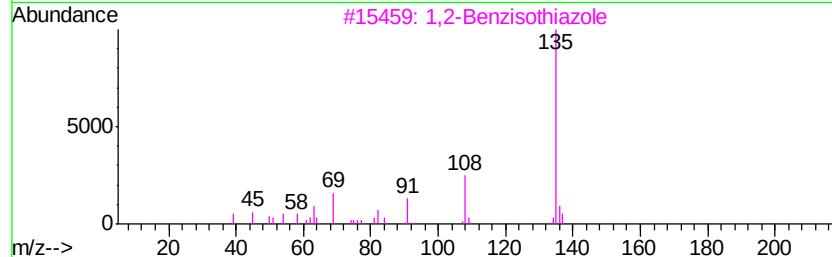
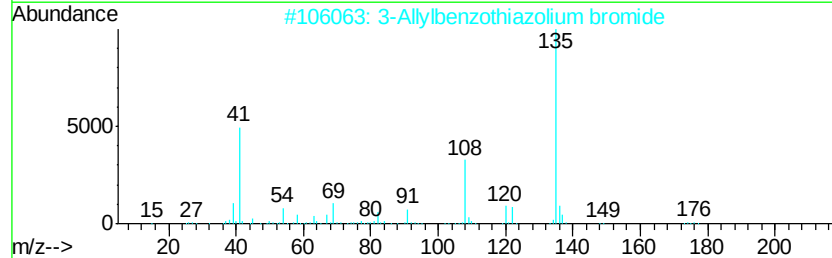
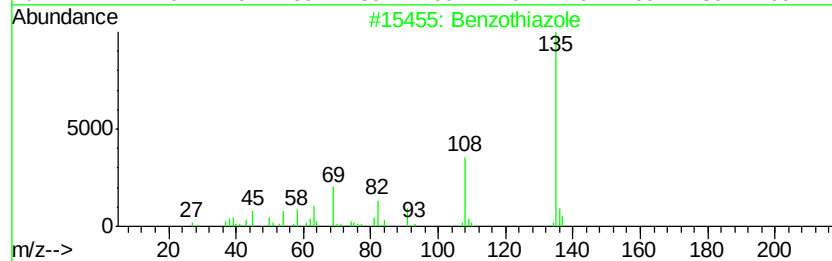
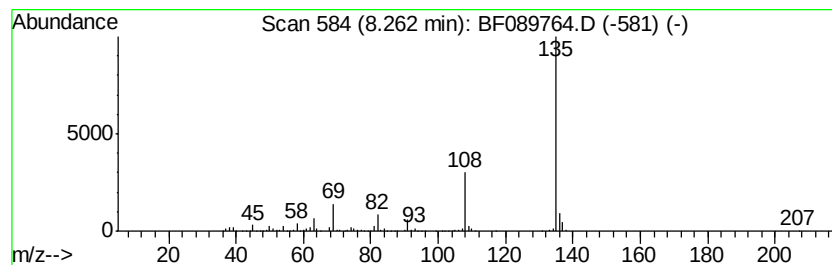
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TIC Integration Parameters: LSCINT.P

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Peak Number 6 Benzothiazole Concentration Rank 6

| R.T. | EstConc | Area   | Relative to ISTD | R.T. |
|------|---------|--------|------------------|------|
| 8.26 | 2.58 ng | 674589 | Napthalene-d8    | 7.99 |

| Hit# of 5 | Tentative ID                        | MW  | MolForm    | CAS#        | Qual |
|-----------|-------------------------------------|-----|------------|-------------|------|
| 1         | Benzothiazole                       | 135 | C7H5NS     | 000095-16-9 | 95   |
| 2         | 3-Allylbenzothiazolium bromide      | 255 | C10H10BrNS | 016407-55-9 | 90   |
| 3         | 1,2-Benzisothiazole                 | 135 | C7H5NS     | 000272-16-2 | 78   |
| 4         | 1H-Pyrazolo[3,4-d]pyrimidin-4-amine | 135 | C5H5N5     | 002380-63-4 | 72   |
| 5         | Adenine                             | 135 | C5H5N5     | 000073-24-5 | 64   |



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TIC Library : C:\Database\NIST11.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name     | RT   | EstConc | Units | Response | --Internal Standard-- |      |         |      |
|----------------------|------|---------|-------|----------|-----------------------|------|---------|------|
|                      |      |         |       |          | #                     | RT   | Resp    | Conc |
| 2-Pentanone, 4-hy... | 4.84 | 9.0     | ng    | 1675370  | 1                     | 6.70 | 3728270 | 20.0 |
| unknown6.47          | 6.47 | 82.2    | ng    | 15316000 | 1                     | 6.70 | 3728270 | 20.0 |
| Benzothiazole        | 8.26 | 2.6     | ng    | 674589   | 2                     | 7.99 | 5235670 | 20.0 |