

Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF112217\  
 Data File : BF100864.D  
 Acq On : 23 Nov 2017 10:13  
 Operator : SJ/JU  
 Sample : I6541-06  
 Misc :  
 ALS Vial : 35 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 111717-SIDI-F-D-M

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-BF110817.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         | 2.146       | 7             | 10          | 39           | rVB4     | 62119          | 192430        | 7.57%           | 1.383%        |
| 2         | 5.075       | 504           | 508         | 517          | rBV      | 147744         | 156412        | 6.15%           | 1.124%        |
| 3         | 5.475       | 572           | 576         | 579          | rBV      | 859783         | 729306        | 28.67%          | 5.240%        |
| 4         | 6.481       | 743           | 747         | 756          | rBB      | 607423         | 514811        | 20.24%          | 3.699%        |
| 5         | 6.628       | 767           | 772         | 775          | rBV      | 1434000        | 1244345       | 48.92%          | 8.940%        |
| 6         | 6.857       | 807           | 811         | 815          | rBB      | 525633         | 412443        | 16.21%          | 2.963%        |
| 7         | 7.016       | 833           | 838         | 841          | rBV      | 1879566        | 1667393       | 65.55%          | 11.980%       |
| 8         | 7.428       | 902           | 908         | 910          | rBV      | 1219815        | 1376301       | 54.11%          | 9.888%        |
| 9         | 8.139       | 1025          | 1029        | 1032         | rBV      | 670189         | 532316        | 20.93%          | 3.825%        |
| 10        | 9.216       | 1207          | 1212        | 1215         | rBV      | 2562193        | 2543640       | 100.00%         | 18.275%       |
| 11        | 9.892       | 1322          | 1327        | 1331         | rBV      | 613298         | 583642        | 22.95%          | 4.193%        |
| 12        | 10.686      | 1458          | 1462        | 1465         | rBV      | 960952         | 901837        | 35.45%          | 6.479%        |
| 13        | 10.792      | 1476          | 1480        | 1485         | rBV      | 29228          | 28606         | 1.12%           | 0.206%        |
| 14        | 11.380      | 1576          | 1580        | 1583         | rBV      | 627271         | 510169        | 20.06%          | 3.665%        |
| 15        | 12.968      | 1845          | 1850        | 1853         | rBV      | 1903045        | 1788132       | 70.30%          | 12.847%       |
| 16        | 14.021      | 2025          | 2029        | 2032         | rBV      | 387506         | 348686        | 13.71%          | 2.505%        |
| 17        | 15.492      | 2273          | 2279        | 2288         | rVB      | 315251         | 387961        | 15.25%          | 2.787%        |

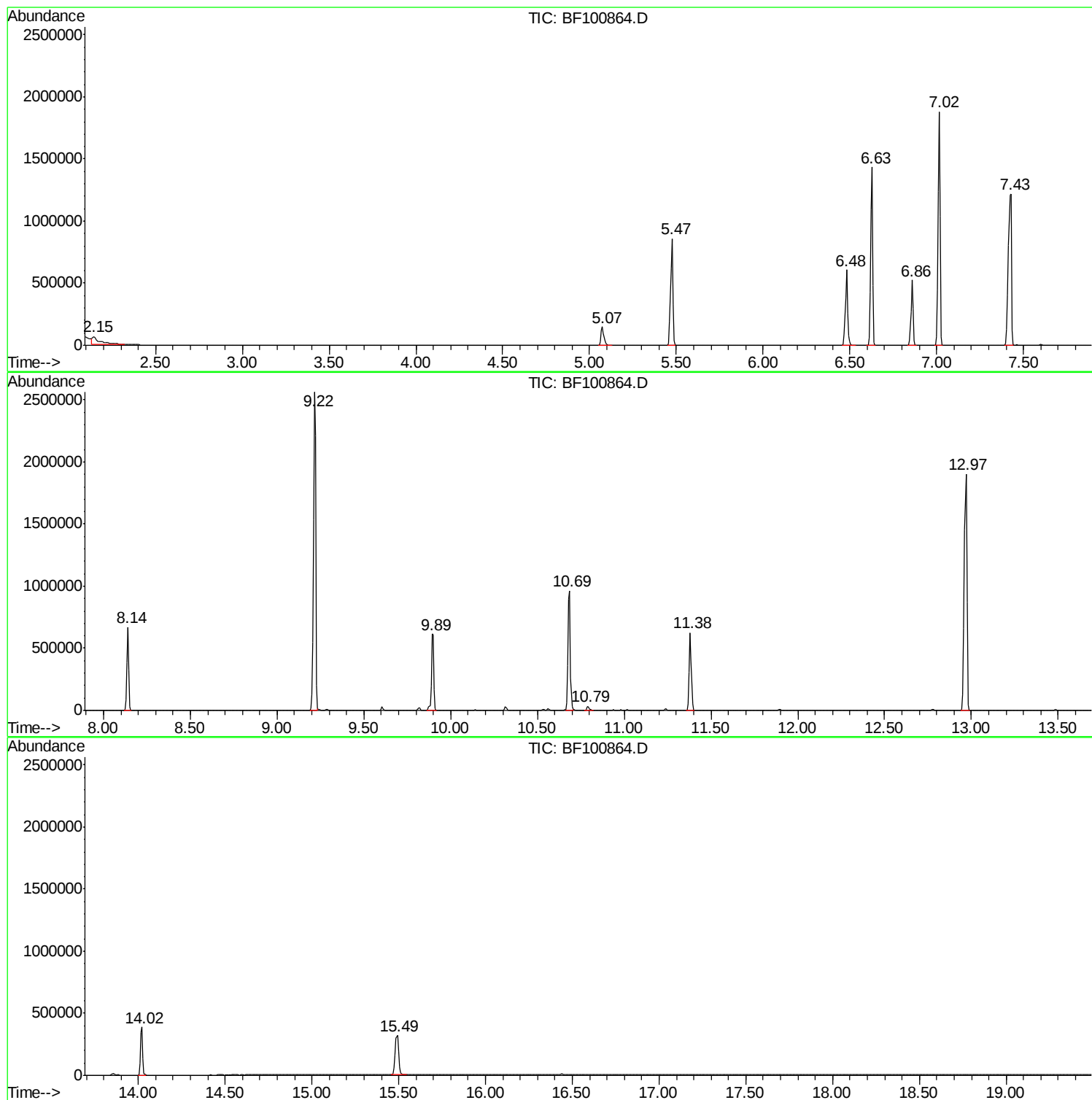
Sum of corrected areas: 13918430

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ClientSampleId :  
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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF110817.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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BNA\_F  
ClientSampleId :  
111717-SIDI-F-D-M

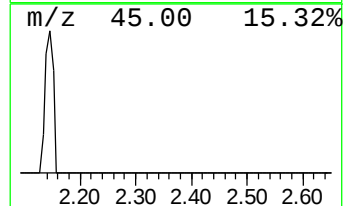
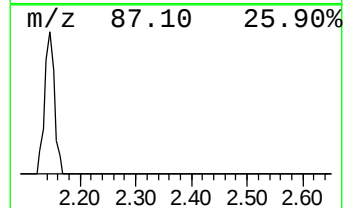
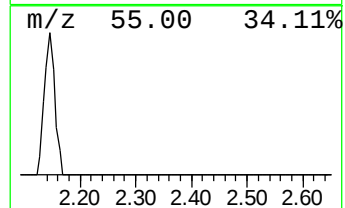
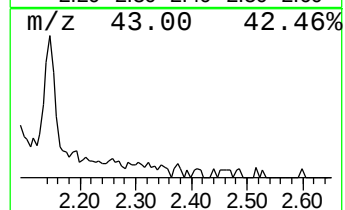
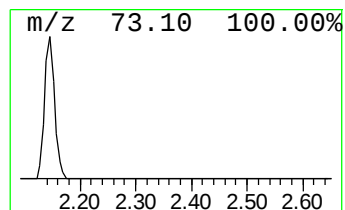
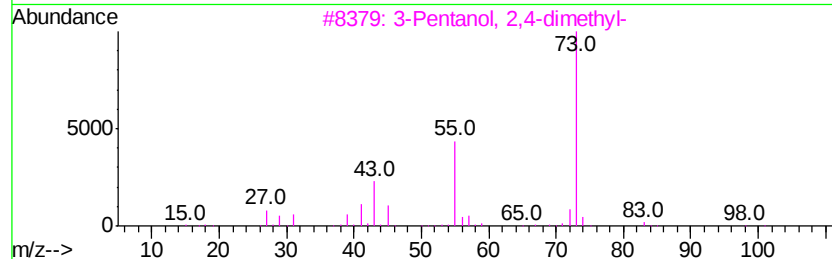
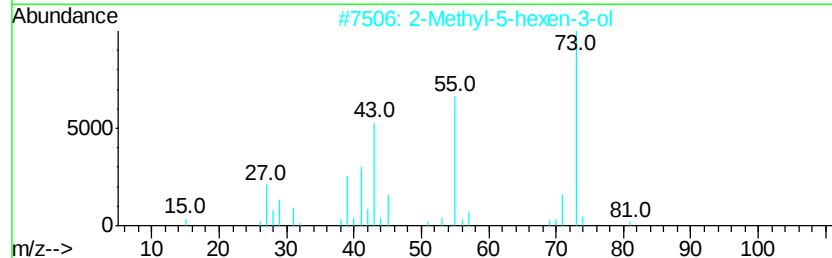
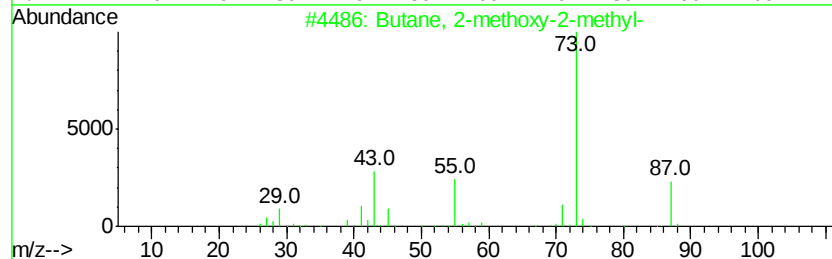
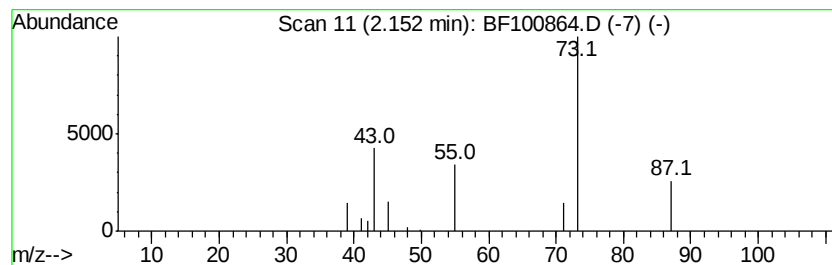
Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF110817.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

| R.T. | EstConc | Area   | Relative to ISTD       | R.T. |
|------|---------|--------|------------------------|------|
| 2.15 | 9.33 ng | 192430 | 1,4-Dichlorobenzene-d4 | 6.86 |

| Hit# | of | Tentative ID                | MW  | MolForm | CAS#        | Qual |
|------|----|-----------------------------|-----|---------|-------------|------|
| 1    | 5  | Butane, 2-methoxy-2-methyl- | 102 | C6H14O  | 000994-05-8 | 72   |
| 2    |    | 2-Methyl-5-hexen-3-ol       | 114 | C7H14O  | 032815-70-6 | 42   |
| 3    |    | 3-Pentanol, 2,4-dimethyl-   | 116 | C7H16O  | 000600-36-2 | 9    |
| 4    |    | Isobutylamine               | 73  | C4H11N  | 000078-81-9 | 5    |
| 5    |    | N-Ethylformamide            | 73  | C3H7NO  | 000627-45-2 | 5    |



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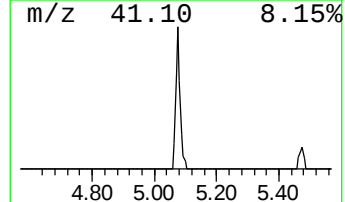
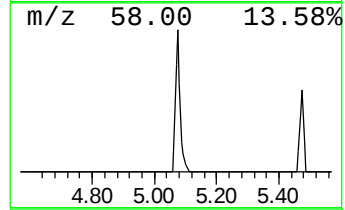
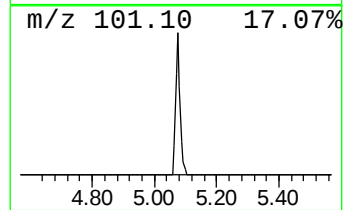
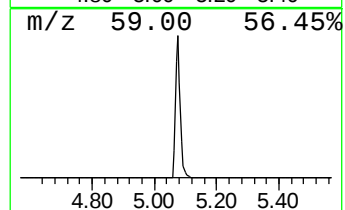
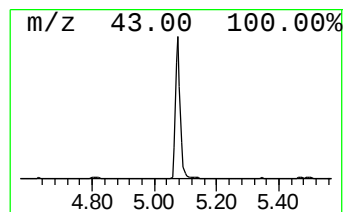
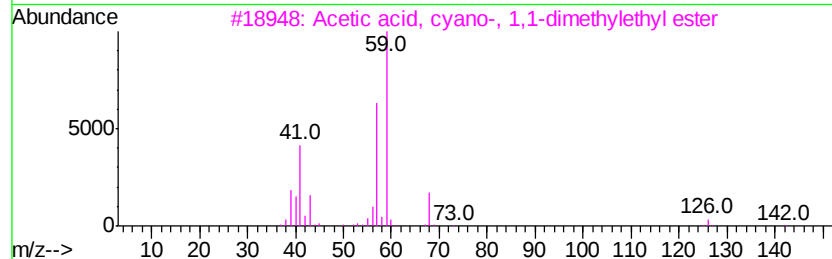
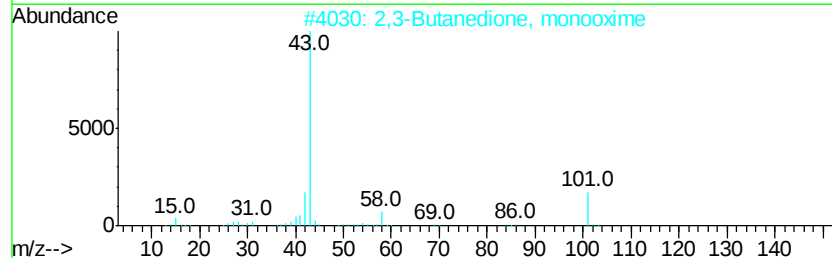
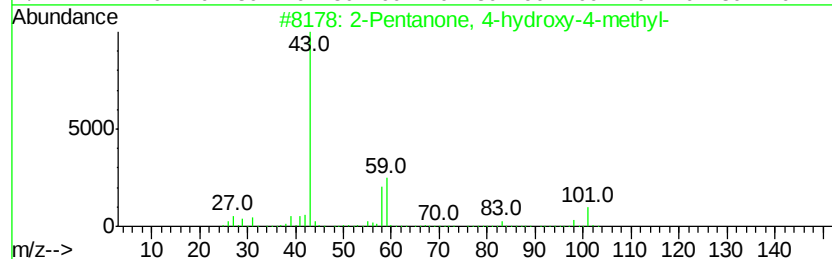
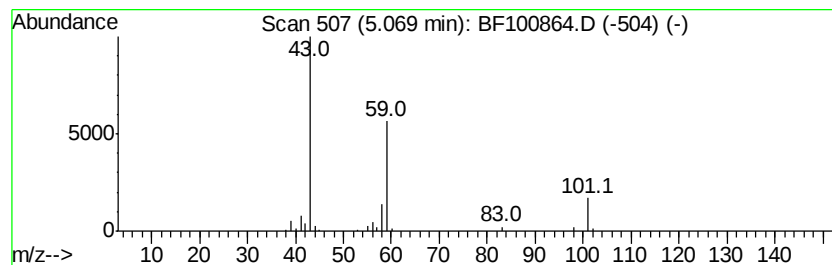
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

| R.T. | EstConc | Area   | Relative to ISTD       | R.T. |
|------|---------|--------|------------------------|------|
| 5.07 | 7.58 ng | 156412 | 1,4-Dichlorobenzene-d4 | 6.86 |

| Hit# | of | 5 | Tentative ID                         | MW  | MolForm  | CAS#        | Qual |
|------|----|---|--------------------------------------|-----|----------|-------------|------|
| 1    |    |   | 2-Pentanone, 4-hydroxy-4-methyl-     | 116 | C6H12O2  | 000123-42-2 | 64   |
| 2    |    |   | 2,3-Butanedione, monooxime           | 101 | C4H7NO2  | 000057-71-6 | 35   |
| 3    |    |   | Acetic acid, cyano-, 1,1-dimethyl... | 141 | C7H11NO2 | 001116-98-9 | 17   |
| 4    |    |   | Morpholine, 4-methyl-                | 101 | C5H11NO  | 000109-02-4 | 9    |
| 5    |    |   | Butane, 1-ethoxy-                    | 102 | C6H14O   | 000628-81-9 | 9    |



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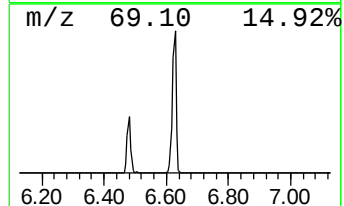
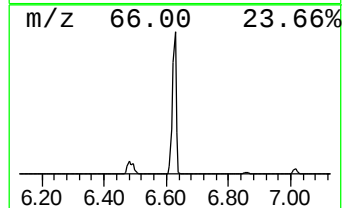
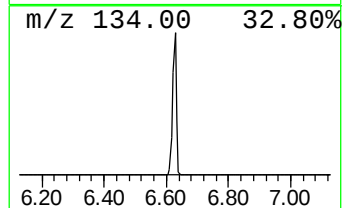
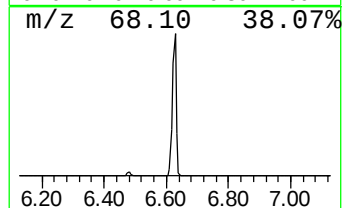
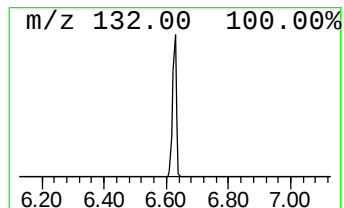
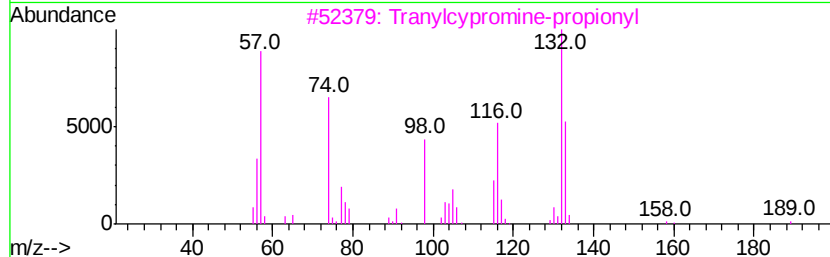
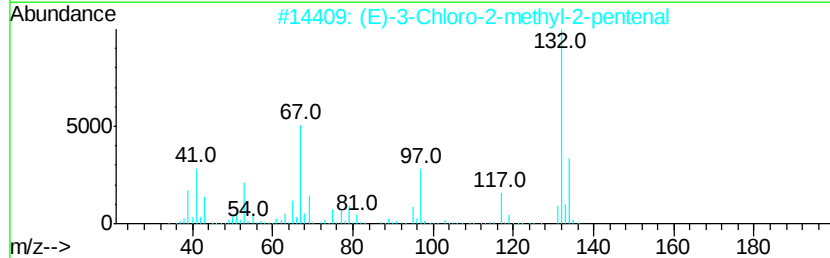
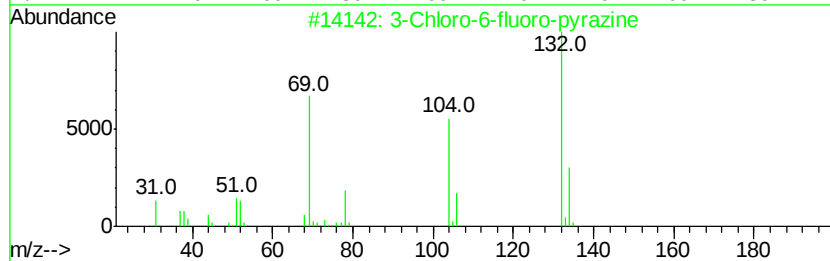
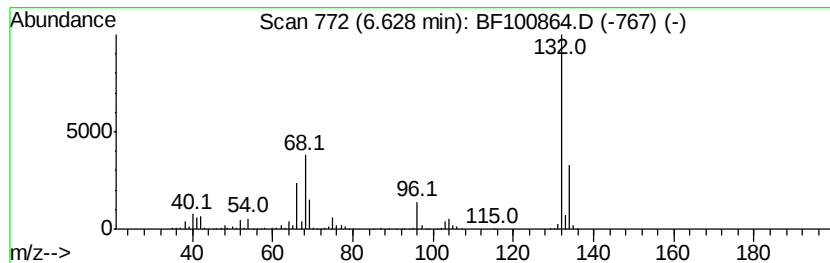
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TIC Integration Parameters: LSCINT.P

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Peak Number 3 unknown6.63 Concentration Rank 2

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.63 | 60.34 ng | 1244350 | 1,4-Dichlorobenzene-d4 | 6.86 |

| Hit# | of | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|-------------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 3-Chloro-6-fluoro-pyrazine          | 132 | C4H2ClFN2 | 1000146-10-7 | 27   |
| 2    |    | (E)-3-Chloro-2-methyl-2-pentenal    | 132 | C6H9ClO   | 031357-76-3  | 17   |
| 3    |    | Tranvlcypropine-propionyl           | 189 | C12H15NO  | 1000123-86-3 | 10   |
| 4    |    | 5-Fluoro-2-chloropyrimidine         | 132 | C4H2ClFN2 | 062802-42-0  | 9    |
| 5    |    | 2H-Cyclopenta[d]pyridazine, 2-me... | 132 | C8H8N2    | 022291-85-6  | 9    |



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| TIC Top Hit name     | RT   | EstConc | Units | Response | --Internal Standard-- |      |        |      |
|----------------------|------|---------|-------|----------|-----------------------|------|--------|------|
|                      |      |         |       |          | #                     | RT   | Resp   | Conc |
| Butane, 2-methoxy... | 2.15 | 9.3     | ng    | 192430   | 1                     | 6.86 | 412443 | 20.0 |
| 2-Pentanone, 4-hy... | 5.07 | 7.6     | ng    | 156412   | 1                     | 6.86 | 412443 | 20.0 |
| unknown6.63          | 6.63 | 60.3    | ng    | 1244350  | 1                     | 6.86 | 412443 | 20.0 |