

Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF081916\  
 Data File : BF089799.D  
 Acq On : 19 Aug 2016 16:55  
 Operator : UM/SJ  
 Sample : PB92924BL  
 Misc :  
 ALS Vial : 15 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 PB92924BL

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

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

Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF081916.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         | 1.656       | 4             | 6           | 15           | rBV      | 3620268        | 6673737       | 32.07%          | 4.414%        |
| 2         | 1.781       | 15            | 17          | 27           | rVV      | 8981324        | 20807701      | 100.00%         | 13.763%       |
| 3         | 1.918       | 27            | 29          | 76           | rVB      | 828586         | 4638651       | 22.29%          | 3.068%        |
| 4         | 4.844       | 281           | 285         | 297          | rBV      | 2165689        | 3724180       | 17.90%          | 2.463%        |
| 5         | 5.279       | 319           | 323         | 325          | rBV      | 8546173        | 13088995      | 62.90%          | 8.658%        |
| 6         | 6.319       | 411           | 414         | 417          | rBV      | 8577923        | 11737952      | 56.41%          | 7.764%        |
| 7         | 6.445       | 422           | 425         | 428          | rBV      | 9178856        | 12900951      | 62.00%          | 8.533%        |
| 8         | 6.685       | 444           | 446         | 448          | rBV      | 3793769        | 3238814       | 15.57%          | 2.142%        |
| 9         | 6.845       | 457           | 460         | 462          | rBV      | 9717536        | 10862010      | 52.20%          | 7.185%        |
| 10        | 7.245       | 492           | 495         | 498          | rBV      | 5941271        | 7681571       | 36.92%          | 5.081%        |
| 11        | 7.965       | 556           | 558         | 561          | rBV      | 4513246        | 4080632       | 19.61%          | 2.699%        |
| 12        | 9.051       | 650           | 653         | 655          | rBV      | 14535361       | 15129690      | 72.71%          | 10.007%       |
| 13        | 9.713       | 708           | 711         | 713          | rBV      | 5444153        | 4751777       | 22.84%          | 3.143%        |
| 14        | 10.502      | 777           | 780         | 782          | rBV      | 7857907        | 8641627       | 41.53%          | 5.716%        |
| 15        | 11.188      | 838           | 840         | 842          | rBV      | 5454286        | 4547834       | 21.86%          | 3.008%        |
| 16        | 12.777      | 976           | 979         | 982          | rBV      | 9220130        | 13135031      | 63.13%          | 8.688%        |
| 17        | 13.840      | 1069          | 1072        | 1075         | rBV      | 3285528        | 3014058       | 14.49%          | 1.994%        |
| 18        | 15.303      | 1197          | 1200        | 1203         | rBV      | 2208212        | 2529067       | 12.15%          | 1.673%        |

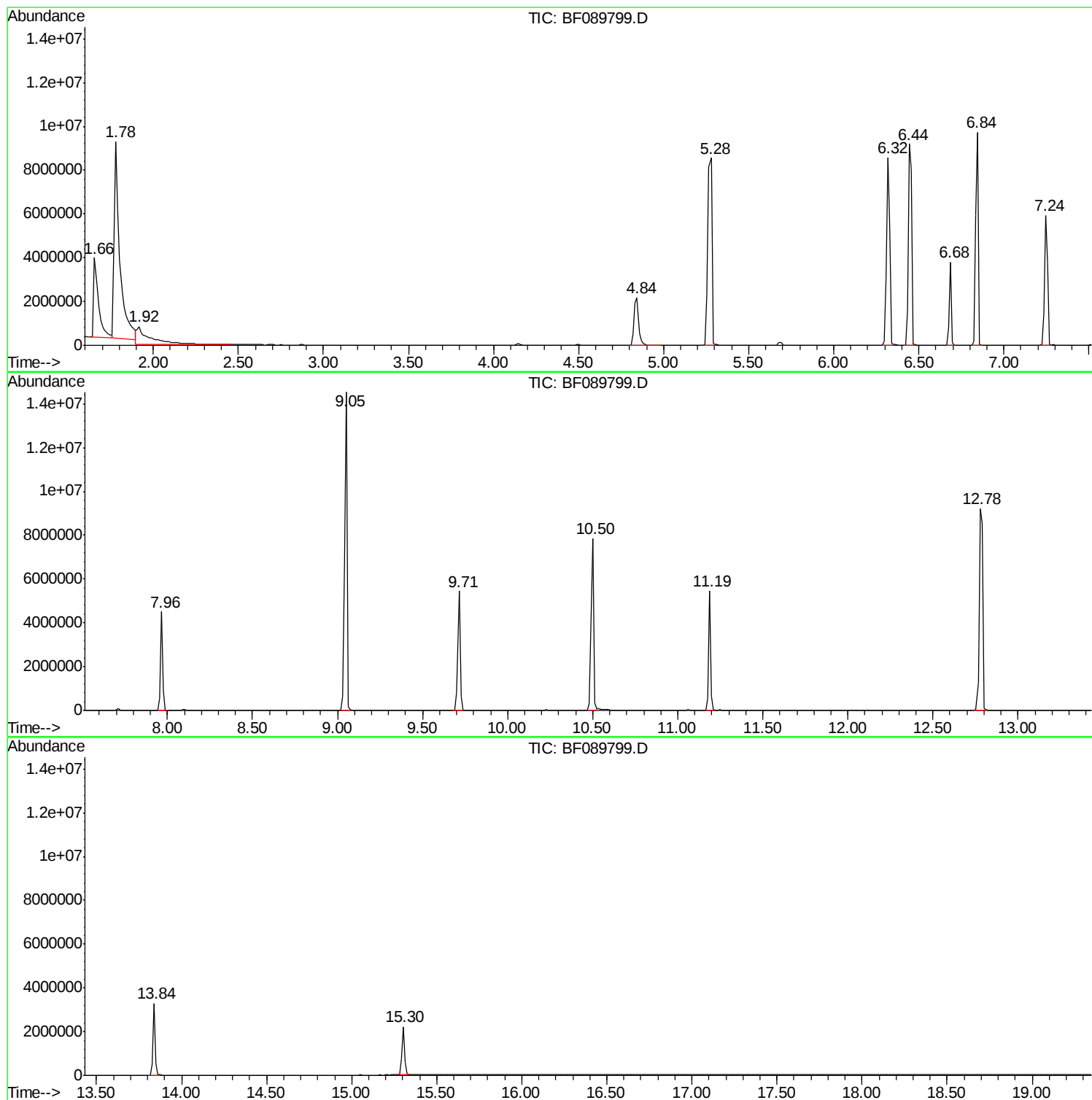
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TIC Library : C:\Database\NIST11.L  
TIC Integration Parameters: LSCINT.P



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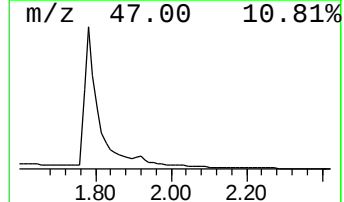
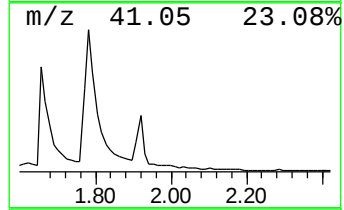
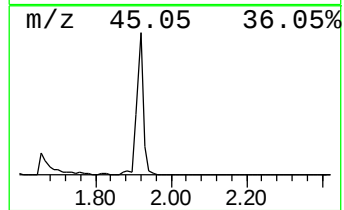
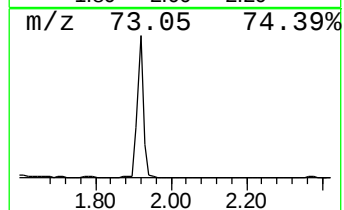
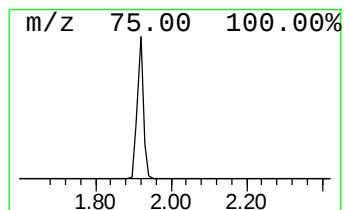
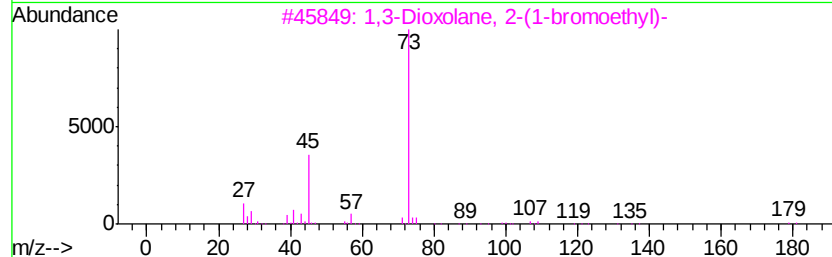
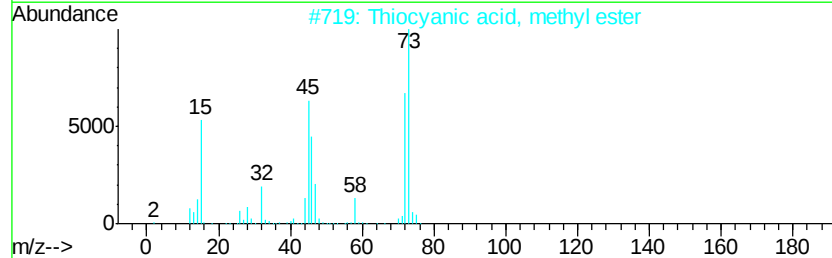
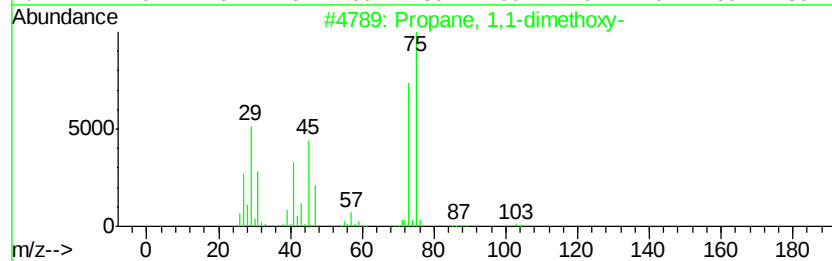
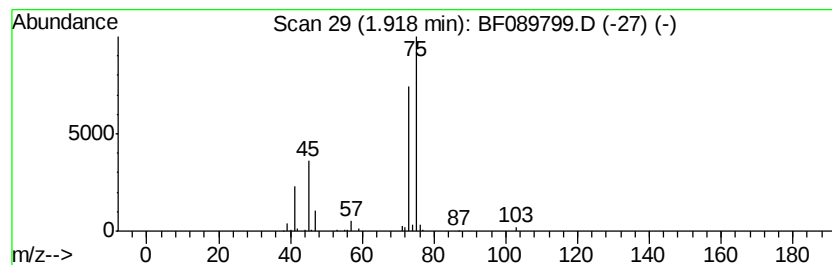
Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF081916.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 5

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 1.92 | 28.64 ng | 4638650 | 1,4-Dichlorobenzene-d4 | 6.68 |

| Hit# | of | Tentative ID                     | MW  | MolForm  | CAS#        | Qual |
|------|----|----------------------------------|-----|----------|-------------|------|
| 1    | 5  | Propane, 1,1-dimethoxy-          | 104 | C5H12O2  | 004744-10-9 | 56   |
| 2    |    | Thiocyanic acid, methyl ester    | 73  | C2H3NS   | 000556-64-9 | 22   |
| 3    |    | 1,3-Dioxolane, 2-(1-bromoethyl)- | 180 | C5H9BrO2 | 005267-73-2 | 10   |
| 4    |    | Pentane, 3-methoxy-              | 102 | C6H14O   | 036839-67-5 | 10   |
| 5    |    | 2,2'-Bi-1,3-dioxolane            | 146 | C6H10O4  | 006705-89-1 | 9    |



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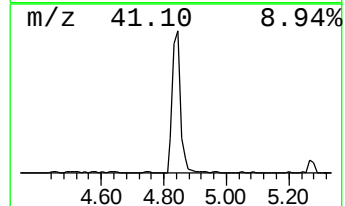
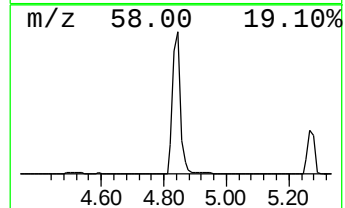
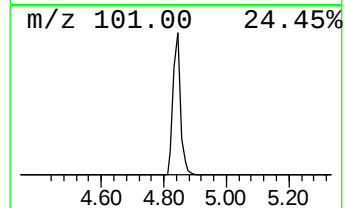
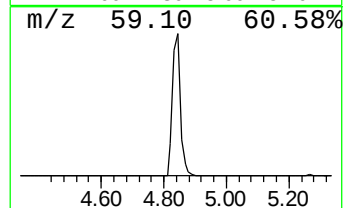
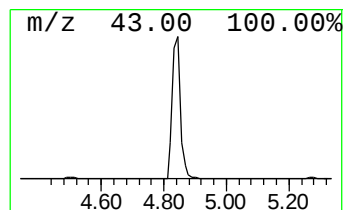
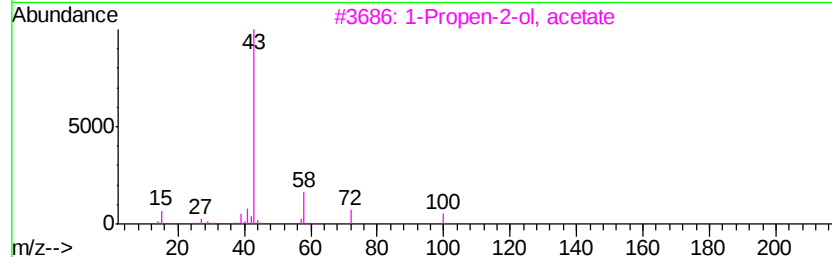
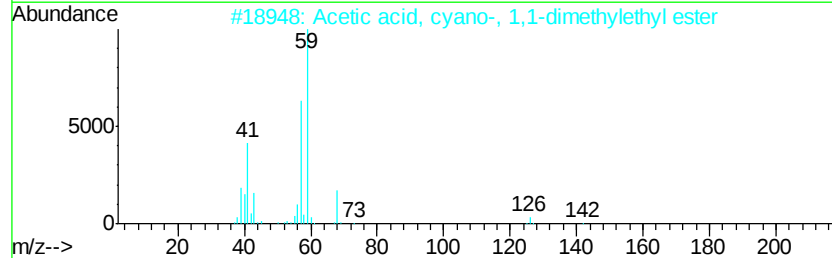
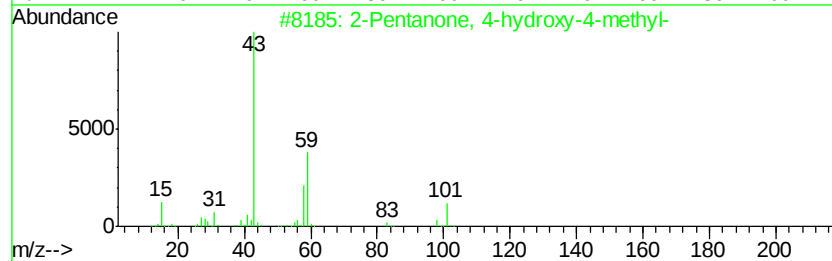
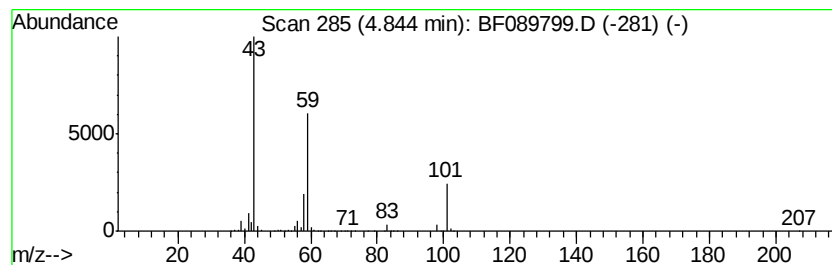
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Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 4.84 | 23.00 ng | 3724180 | 1,4-Dichlorobenzene-d4 | 6.68 |

| Hit# | of | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|-------------------------------------|-----|----------|-------------|------|
| 1    | 5  | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2  | 000123-42-2 | 53   |
| 2    |    | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 17   |
| 3    |    | 1-Propen-2-ol, acetate              | 100 | C5H8O2   | 000108-22-5 | 10   |
| 4    |    | 5-Hexen-2-one                       | 98  | C6H10O   | 000109-49-9 | 9    |
| 5    |    | Morpholine, 4-methyl-               | 101 | C5H11NO  | 000109-02-4 | 9    |



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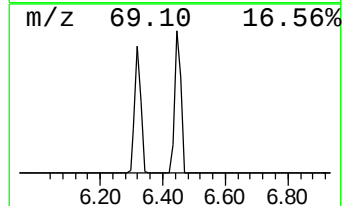
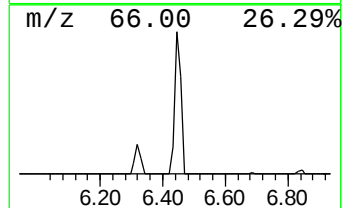
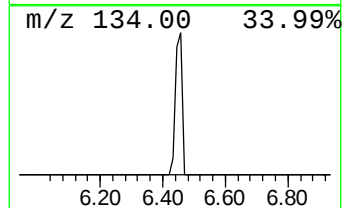
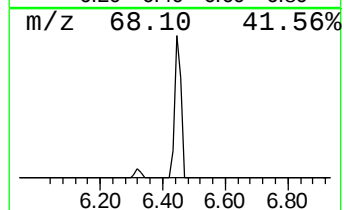
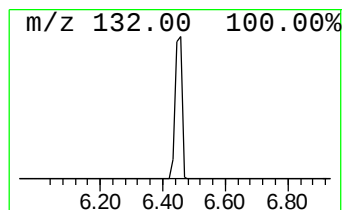
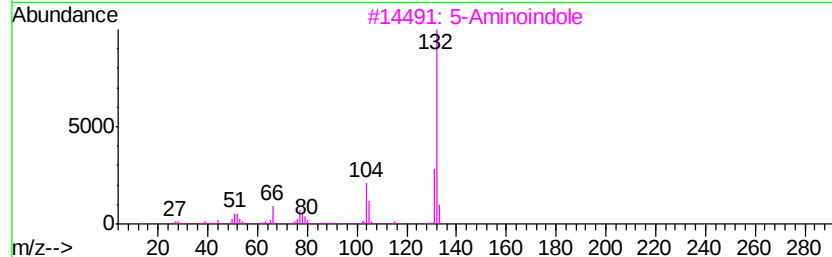
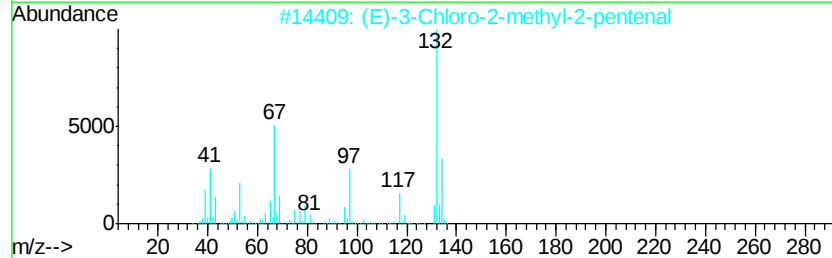
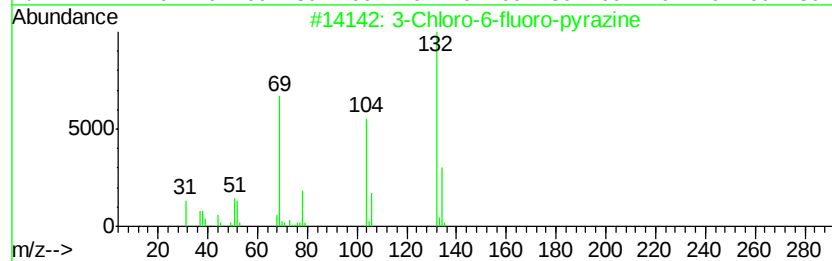
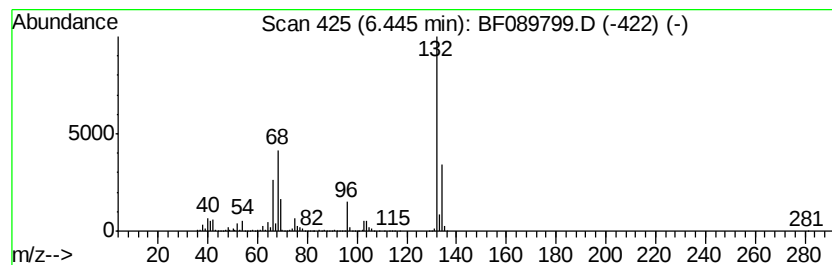
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TIC Integration Parameters: LSCINT.P

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Peak Number 5 unknown6.44 Concentration Rank 2

| R.T. | EstConc  | Area     | Relative to ISTD       | R.T. |
|------|----------|----------|------------------------|------|
| 6.44 | 79.66 ng | 12901000 | 1,4-Dichlorobenzene-d4 | 6.68 |

| 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    |    | 5-Aminoindole                    | 132 | C8H8N2    | 005192-03-0  | 12   |
| 4    |    | 4-Chloro-2-fluoro-pyrimidine     | 132 | C4H2ClFN2 | 051422-00-5  | 9    |
| 5    |    | 4-Chloro-6-fluoro-pyrimidine     | 132 | C4H2ClFN2 | 051422-01-6  | 9    |



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| TIC Top Hit name     | RT   | EstConc | Units | Response | --Internal Standard-- |      |         |      |
|----------------------|------|---------|-------|----------|-----------------------|------|---------|------|
|                      |      |         |       |          | #                     | RT   | Resp    | Conc |
| Propane, 1,1-dime... | 1.92 | 28.6    | ng    | 4638650  | 1                     | 6.68 | 3238810 | 20.0 |
| 2-Pentanone, 4-hy... | 4.84 | 23.0    | ng    | 3724180  | 1                     | 6.68 | 3238810 | 20.0 |
| unknown6.44          | 6.44 | 79.7    | ng    | 12901000 | 1                     | 6.68 | 3238810 | 20.0 |