

Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF060416\  
 Data File : BF087658.D  
 Acq On : 4 Jun 2016 11:13  
 Operator : UM/SJ  
 Sample : PB90993BL  
 Misc :  
 ALS Vial : 3 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 PB90993BL

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-BF060416.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         | 1.770       | 14            | 16          | 17           | rBV      | 583804         | 973329        | 28.90%          | 2.725%        |
| 2         | 1.804       | 17            | 19          | 21           | rVB      | 2843659        | 3229410       | 95.88%          | 9.041%        |
| 3         | 1.895       | 26            | 27          | 52           | rVB      | 1705565        | 3295837       | 97.85%          | 9.227%        |
| 4         | 2.204       | 52            | 54          | 75           | rVB      | 103454         | 223150        | 6.62%           | 0.625%        |
| 5         | 5.061       | 301           | 304         | 313          | rVB      | 268059         | 382140        | 11.35%          | 1.070%        |
| 6         | 5.461       | 336           | 339         | 342          | rBV      | 2418983        | 2621479       | 77.83%          | 7.339%        |
| 7         | 6.490       | 425           | 429         | 431          | rBV      | 2466963        | 3178620       | 94.37%          | 8.899%        |
| 8         | 6.627       | 438           | 441         | 443          | rBV      | 2873155        | 2980826       | 88.50%          | 8.345%        |
| 9         | 6.856       | 459           | 461         | 464          | rBV      | 848638         | 737164        | 21.89%          | 2.064%        |
| 10        | 7.016       | 472           | 475         | 477          | rBV      | 2546266        | 2324385       | 69.01%          | 6.508%        |
| 11        | 7.416       | 507           | 510         | 513          | rBV      | 1285498        | 1921401       | 57.04%          | 5.379%        |
| 12        | 8.147       | 571           | 574         | 576          | rBV      | 884055         | 1019073       | 30.25%          | 2.853%        |
| 13        | 9.222       | 664           | 668         | 671          | rBV      | 2810804        | 3368310       | 100.00%         | 9.430%        |
| 14        | 9.896       | 724           | 727         | 730          | rVB      | 1158489        | 1113879       | 33.07%          | 3.119%        |
| 15        | 10.685      | 793           | 796         | 798          | rBV      | 2008982        | 2058374       | 61.11%          | 5.763%        |
| 16        | 11.382      | 854           | 857         | 859          | rBV      | 1235596        | 1189299       | 35.31%          | 3.330%        |
| 17        | 12.971      | 993           | 996         | 998          | rBV      | 3200951        | 3215353       | 95.46%          | 9.002%        |
| 18        | 14.011      | 1084          | 1087        | 1089         | rBV      | 1201746        | 1071276       | 31.80%          | 2.999%        |
| 19        | 15.440      | 1209          | 1212        | 1215         | rBV      | 701774         | 815114        | 24.20%          | 2.282%        |

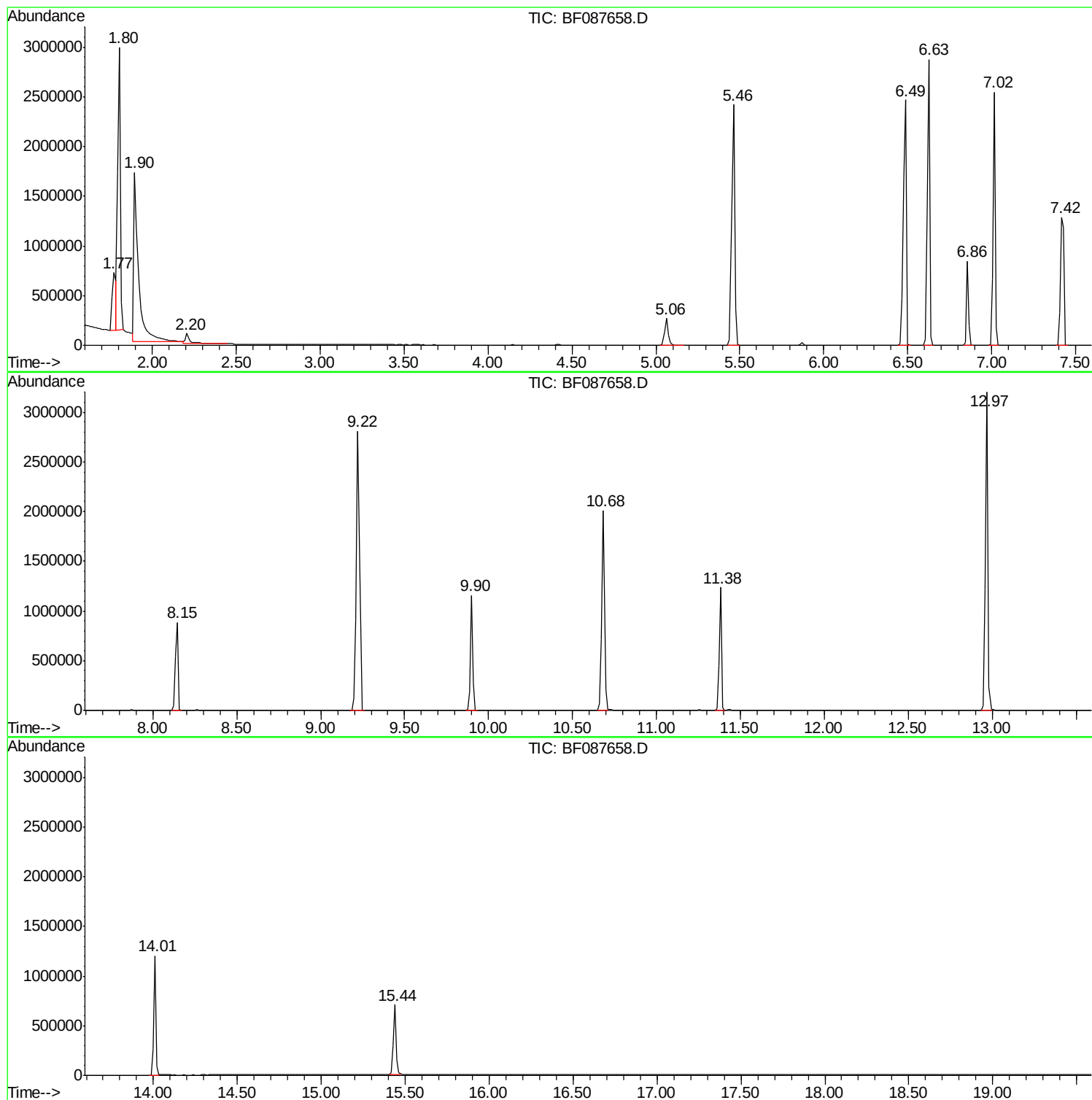
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ClientSampleId :  
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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF060416.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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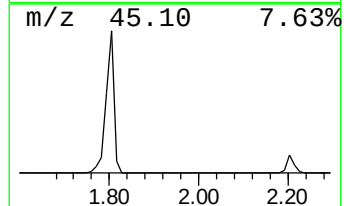
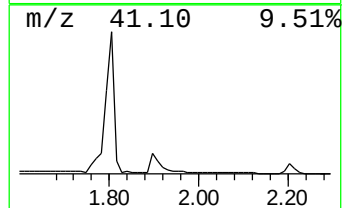
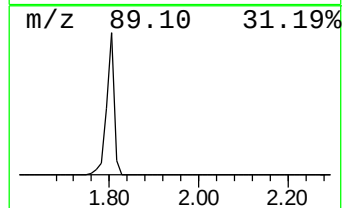
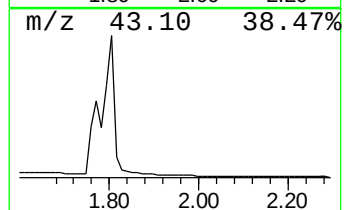
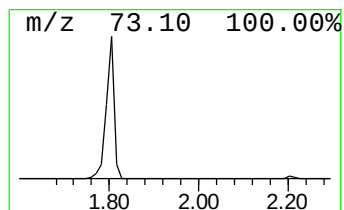
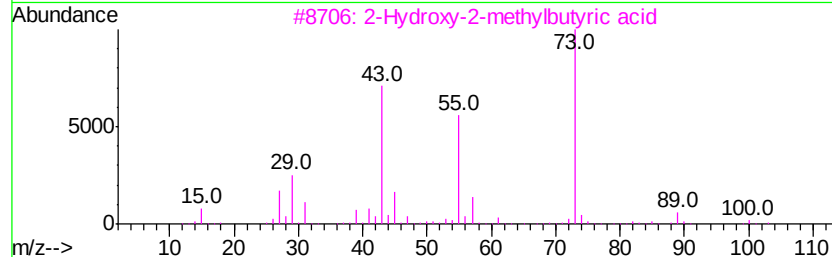
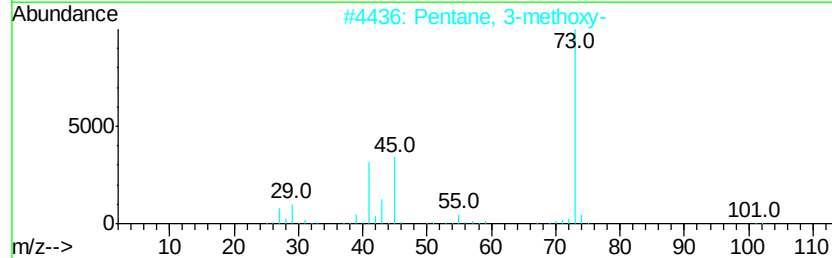
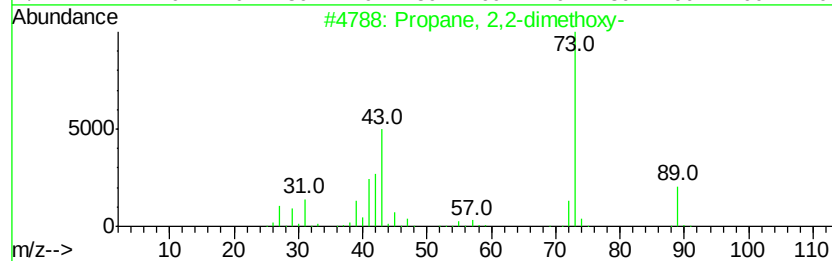
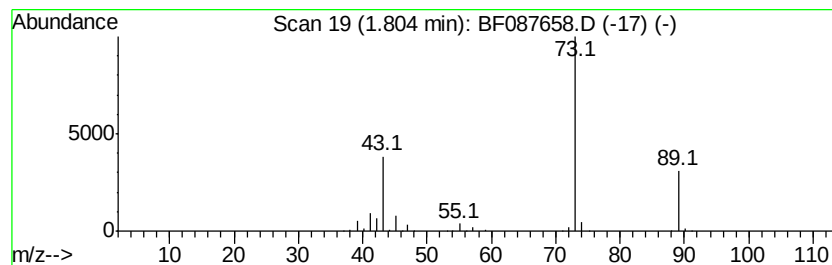
TIC Library : C:\Database\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 Propane, 2,2-dimethoxy- Concentration Rank 2

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 1.80 | 87.62 ng | 3229410 | 1,4-Dichlorobenzene-d4 | 6.86 |

| Hit# | of | Tentative ID                   | MW  | MolForm | CAS#        | Qual |
|------|----|--------------------------------|-----|---------|-------------|------|
| 1    | 5  | Propane, 2,2-dimethoxy-        | 104 | C5H12O2 | 000077-76-9 | 56   |
| 2    |    | Pentane, 3-methoxy-            | 102 | C6H14O  | 036839-67-5 | 17   |
| 3    |    | 2-Hydroxy-2-methylbutyric acid | 118 | C5H10O3 | 003739-30-8 | 9    |
| 4    |    | Propane, 2-methoxy-2-methyl-   | 88  | C5H12O  | 001634-04-4 | 9    |
| 5    |    | Methane, isothiocyanato-       | 73  | C2H3NS  | 000556-61-6 | 7    |



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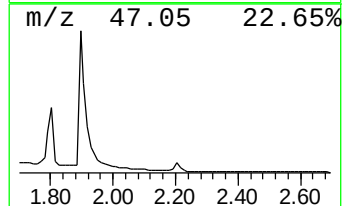
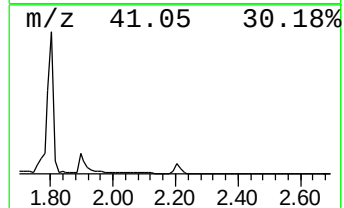
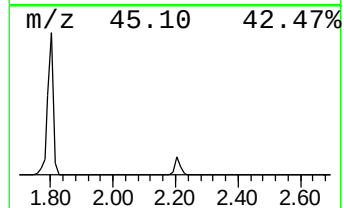
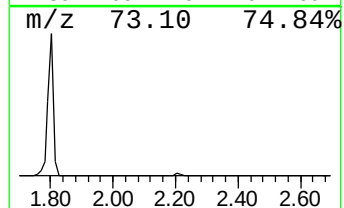
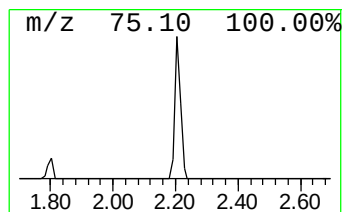
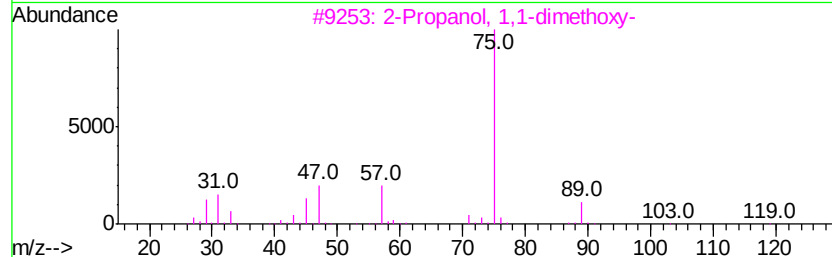
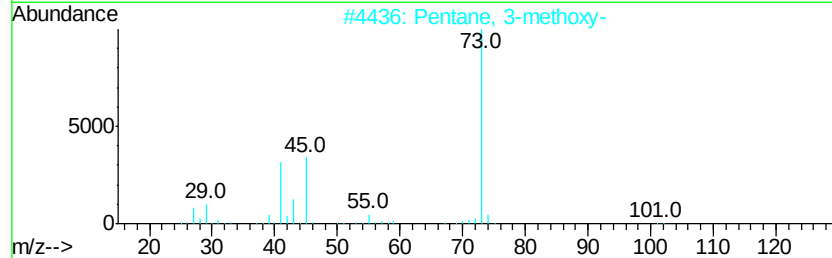
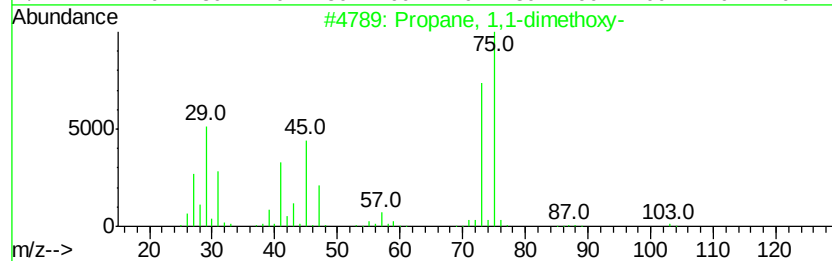
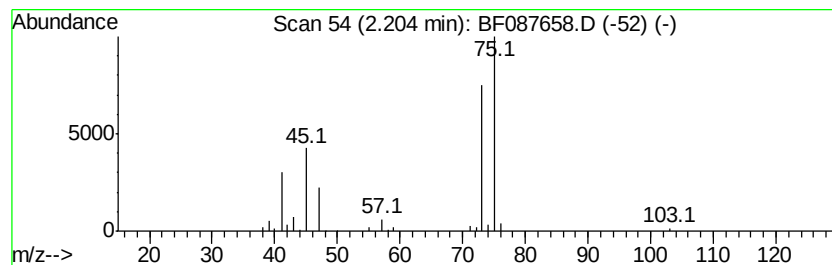
Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF060416.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 4 Propane, 1,1-dimethoxy- Concentration Rank 7

| R.T. | EstConc | Area   | Relative to ISTD       | R.T. |
|------|---------|--------|------------------------|------|
| 2.20 | 6.05 ng | 223150 | 1,4-Dichlorobenzene-d4 | 6.86 |

| Hit# | of | Tentative ID                      | MW  | MolForm  | CAS#        | Qual |
|------|----|-----------------------------------|-----|----------|-------------|------|
| 1    | 5  | Propane, 1,1-dimethoxy-           | 104 | C5H12O2  | 004744-10-9 | 64   |
| 2    |    | Pentane, 3-methoxy-               | 102 | C6H14O   | 036839-67-5 | 16   |
| 3    |    | 2-Propanol, 1,1-dimethoxy-        | 120 | C5H12O3  | 042919-42-6 | 9    |
| 4    |    | Ethane, 2-chloro-1,1-dimethoxy-   | 124 | C4H9ClO2 | 000097-97-2 | 9    |
| 5    |    | Aminoacetaldehyde dimethyl acetal | 105 | C4H11NO2 | 022483-09-6 | 9    |



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ClientSampleId :  
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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF060416.M  
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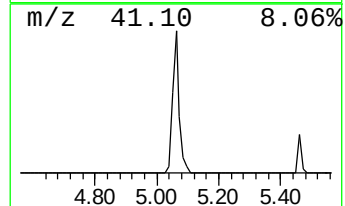
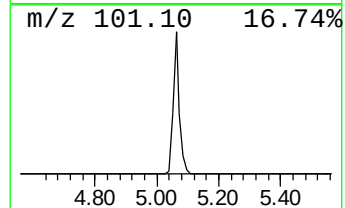
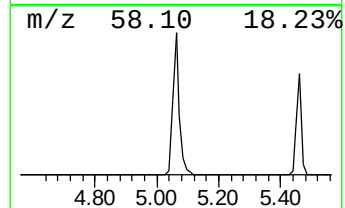
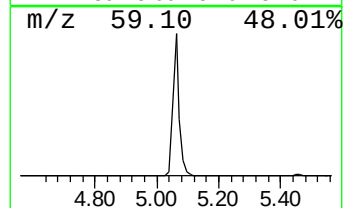
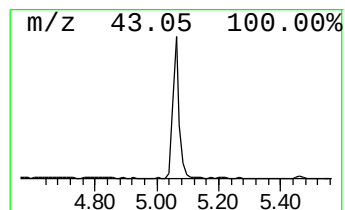
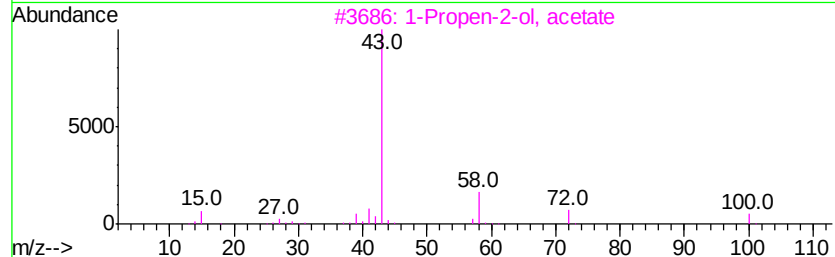
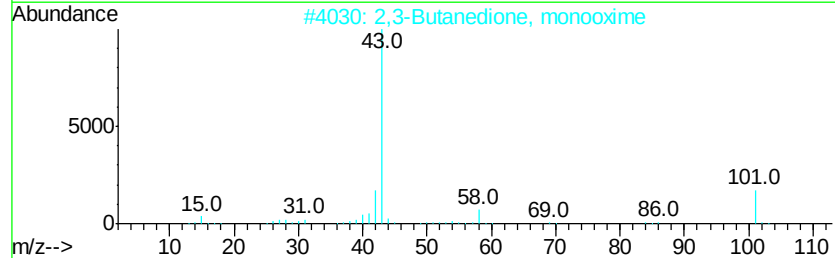
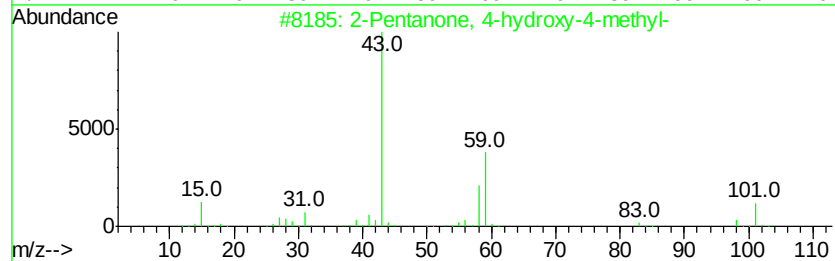
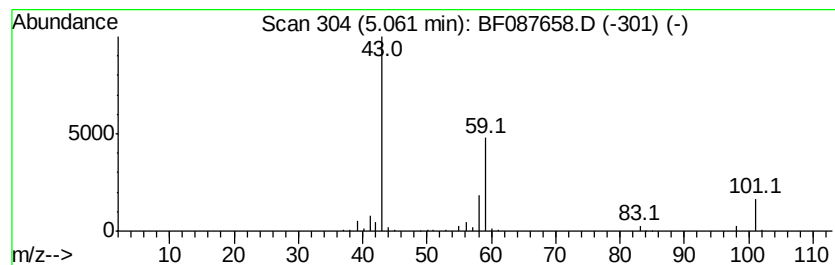
TIC Library : C:\Database\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

| R.T. | EstConc  | Area   | Relative to ISTD       | R.T. |
|------|----------|--------|------------------------|------|
| 5.06 | 10.37 ng | 382140 | 1,4-Dichlorobenzene-d4 | 6.86 |

| Hit# | of | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|-------------------------------------|-----|---------|-------------|------|
| 1    | 5  | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2 | 000123-42-2 | 59   |
| 2    |    | 2,3-Butanedione, monooxime          | 101 | C4H7NO2 | 000057-71-6 | 16   |
| 3    |    | 1-Propen-2-ol, acetate              | 100 | C5H8O2  | 000108-22-5 | 10   |
| 4    |    | Allyl acetate                       | 100 | C5H8O2  | 000591-87-7 | 9    |
| 5    |    | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 9    |



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PB90993BL

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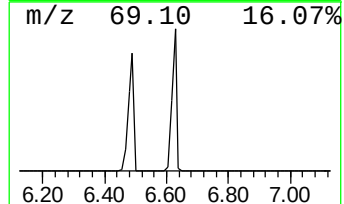
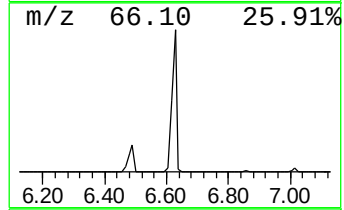
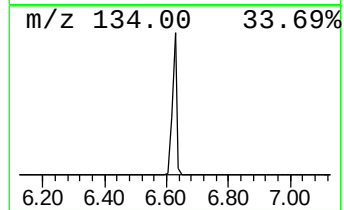
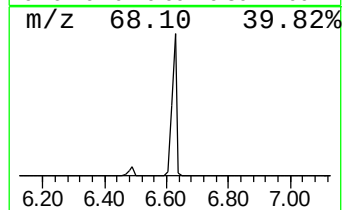
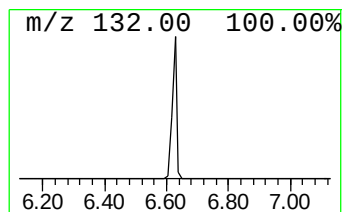
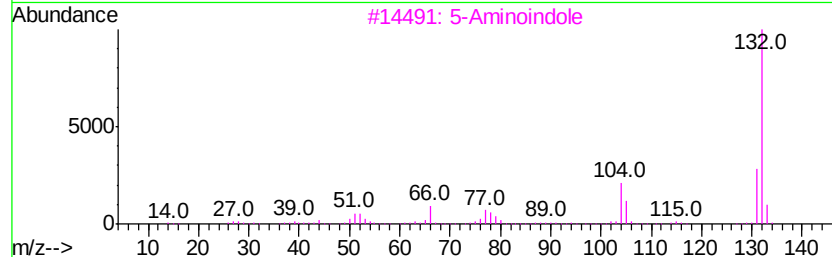
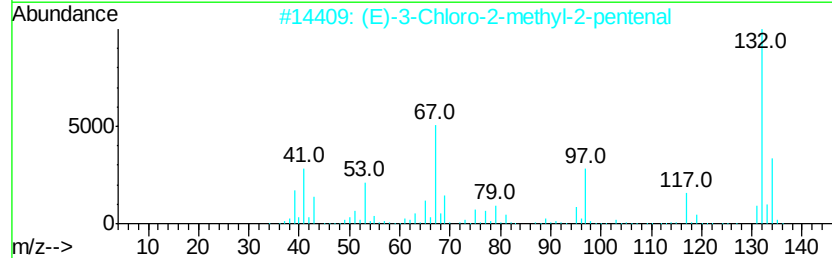
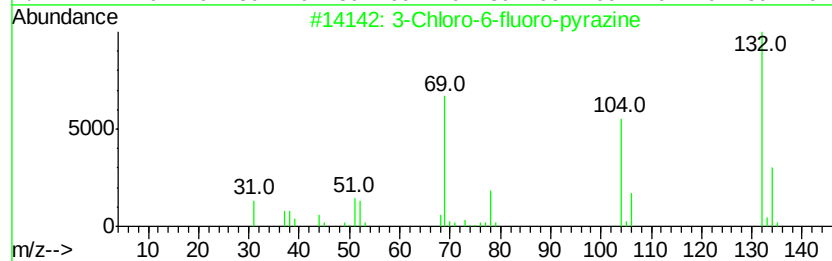
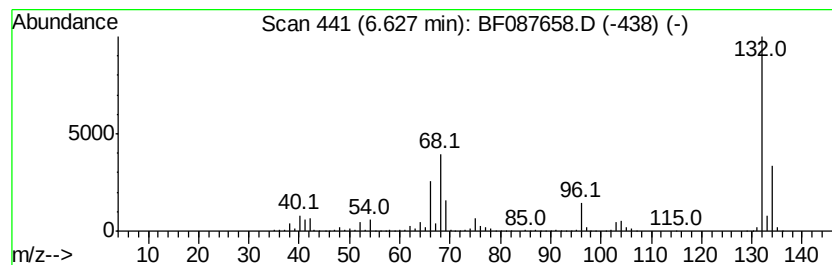
TIC Library : C:\Database\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 6 unknown6.63 Concentration Rank 3

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.63 | 80.87 ng | 2980830 | 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  | 16   |
| 3    |    | 5-Aminoindole                       | 132 | C8H8N2    | 005192-03-0  | 12   |
| 4    |    | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12    | 028749-81-7  | 9    |
| 5    |    | 5-Fluoro-2-chloropyrimidine         | 132 | C4H2ClFN2 | 062802-42-0  | 9    |



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| TIC Top Hit name     | RT   | EstConc | Units | Response | --Internal Standard-- |      |        |      |
|----------------------|------|---------|-------|----------|-----------------------|------|--------|------|
|                      |      |         |       |          | #                     | RT   | Resp   | Conc |
| Propane, 2,2-dime... | 1.80 | 87.6    | ng    | 3229410  | 1                     | 6.86 | 737164 | 20.0 |
| Propane, 1,1-dime... | 2.20 | 6.0     | ng    | 223150   | 1                     | 6.86 | 737164 | 20.0 |
| 2-Pentanone, 4-hy... | 5.06 | 10.4    | ng    | 382140   | 1                     | 6.86 | 737164 | 20.0 |
| unknown6.63          | 6.63 | 80.9    | ng    | 2980830  | 1                     | 6.86 | 737164 | 20.0 |