

Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF110416\  
 Data File : BF091024.D  
 Acq On : 4 Nov 2016 15:17  
 Operator : UM/SJ  
 Sample : H5526-12  
 Misc :  
 ALS Vial : 16 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 SB-103-21.5-22.0

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-BF110316.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         | 1.778       | 6             | 8           | 39           | rVB      | 2950547        | 6753019       | 100.00%         | 11.545%       |
| 2         | 4.864       | 275           | 278         | 288          | rBV      | 726660         | 1322836       | 19.59%          | 2.261%        |
| 3         | 5.299       | 313           | 316         | 319          | rBV      | 4410568        | 5097259       | 75.48%          | 8.714%        |
| 4         | 6.350       | 405           | 408         | 411          | rBV      | 4041219        | 5181463       | 76.73%          | 8.858%        |
| 5         | 6.476       | 416           | 419         | 421          | rBV      | 4421989        | 5905169       | 87.44%          | 10.095%       |
| 6         | 6.704       | 437           | 439         | 441          | rBV      | 778442         | 1014574       | 15.02%          | 1.734%        |
| 7         | 6.853       | 450           | 452         | 455          | rBV      | 3753370        | 4171994       | 61.78%          | 7.132%        |
| 8         | 7.264       | 485           | 488         | 491          | rBV      | 2434864        | 3874747       | 57.38%          | 6.624%        |
| 9         | 7.390       | 496           | 499         | 506          | rVB      | 71621          | 150753        | 2.23%           | 0.258%        |
| 10        | 7.985       | 549           | 551         | 554          | rBV      | 1400950        | 1467226       | 21.73%          | 2.508%        |
| 11        | 9.070       | 642           | 646         | 648          | rBV      | 5764649        | 6428022       | 95.19%          | 10.989%       |
| 12        | 9.470       | 677           | 681         | 683          | rBV      | 1207173        | 1420142       | 21.03%          | 2.428%        |
| 13        | 9.733       | 702           | 704         | 707          | rBV      | 1121972        | 1646425       | 24.38%          | 2.815%        |
| 14        | 10.179      | 732           | 743         | 745          | rBV3     | 53656          | 105663        | 1.56%           | 0.181%        |
| 15        | 10.533      | 771           | 774         | 776          | rBV      | 3727886        | 4266231       | 63.18%          | 7.293%        |
| 16        | 10.659      | 783           | 785         | 791          | rVB      | 89406          | 158186        | 2.34%           | 0.270%        |
| 17        | 11.105      | 822           | 824         | 825          | rBV      | 73628          | 75441         | 1.12%           | 0.129%        |
| 18        | 11.219      | 832           | 834         | 838          | rBV      | 1881378        | 1668996       | 24.71%          | 2.853%        |
| 19        | 12.808      | 970           | 973         | 976          | rBV      | 4759998        | 5259096       | 77.88%          | 8.991%        |
| 20        | 13.711      | 1049          | 1052        | 1060         | rBV      | 204443         | 260288        | 3.85%           | 0.445%        |
| 21        | 13.848      | 1062          | 1064        | 1067         | rBV      | 1161948        | 1298881       | 19.23%          | 2.220%        |
| 22        | 15.242      | 1183          | 1186        | 1196         | rBV      | 739585         | 968955        | 14.35%          | 1.656%        |

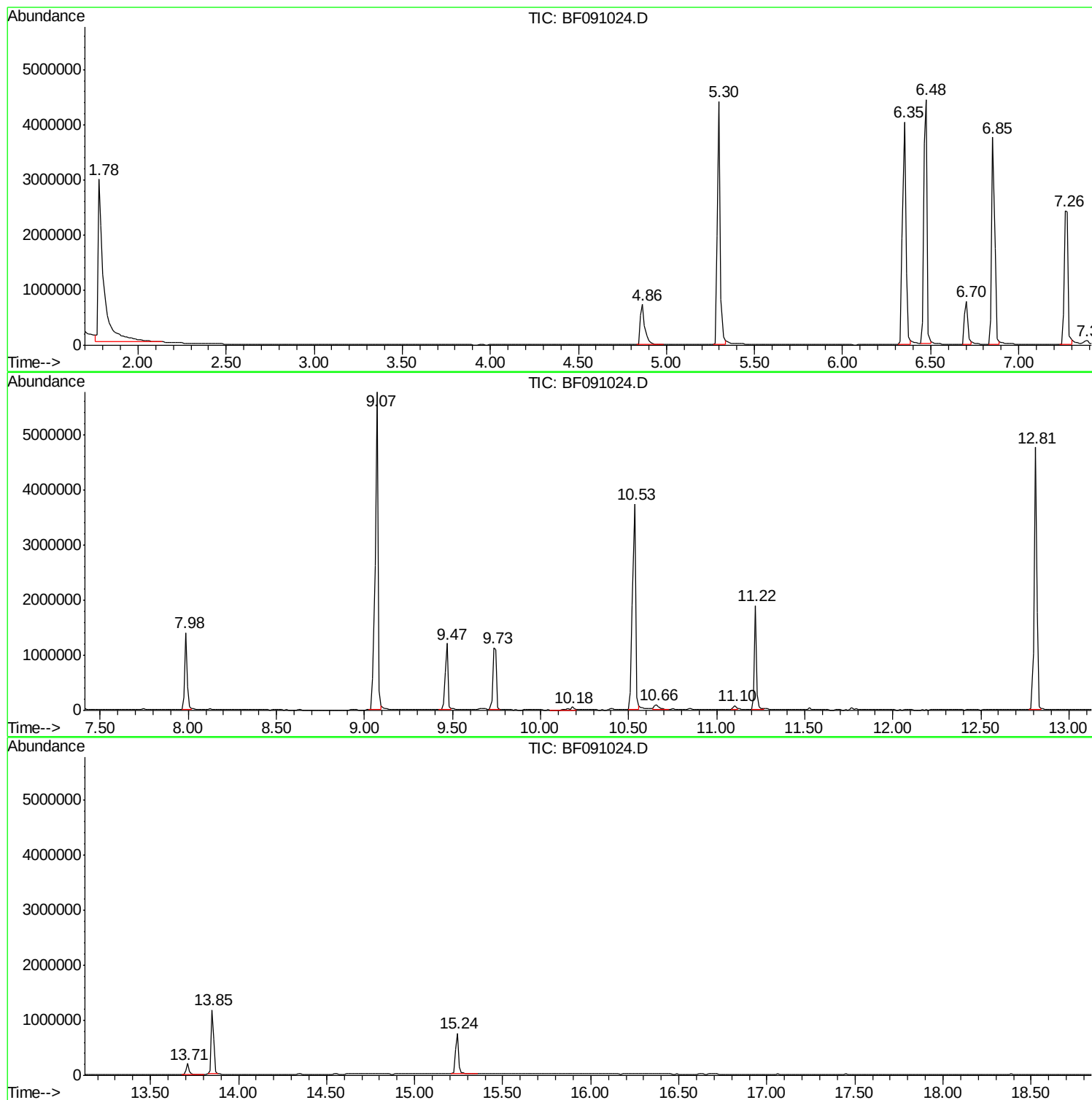
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BNA\_F  
ClientSampleId :  
SB-103-21.5-22.0

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF110316.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P



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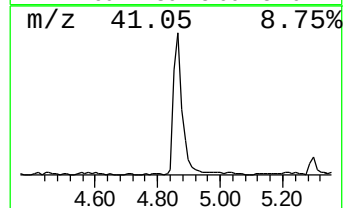
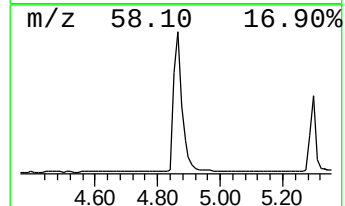
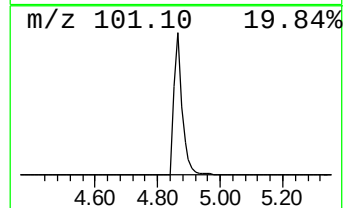
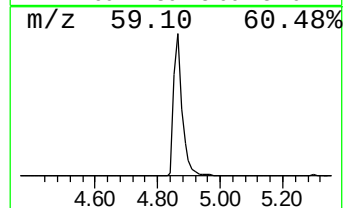
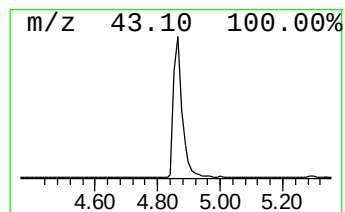
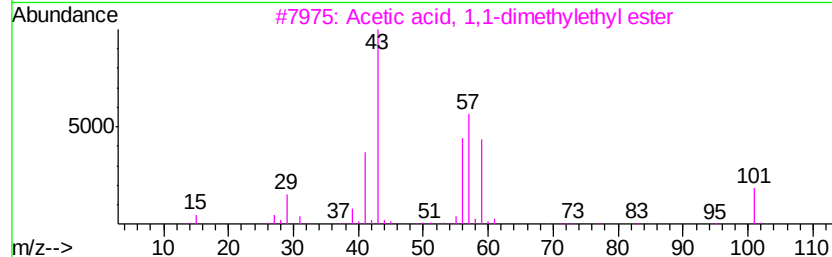
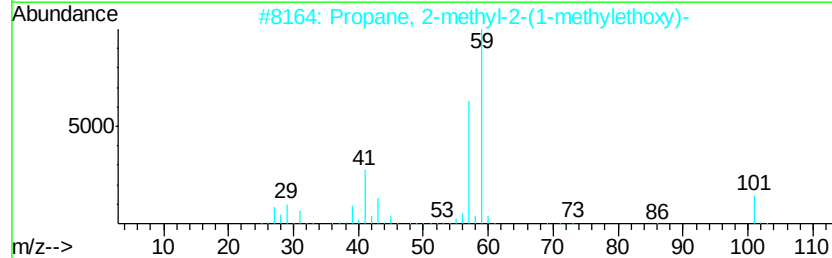
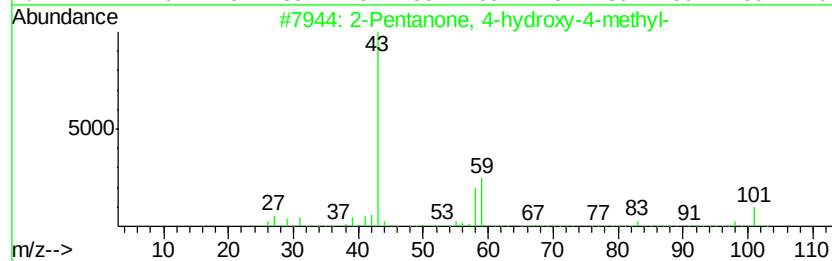
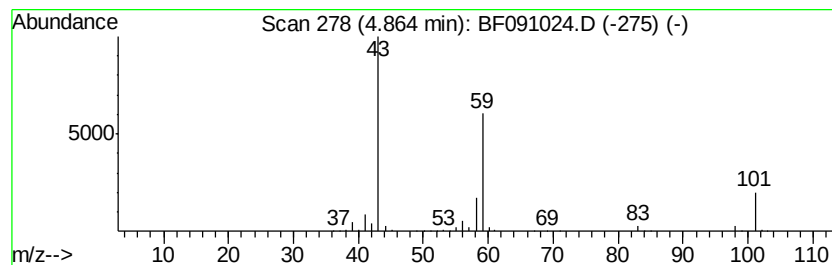
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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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. |
|------|----------|---------|------------------------|------|
| 4.86 | 26.08 ng | 1322840 | 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 | 64   |
| 2    |    | Propane, 2-methyl-2-(1-methyleth... | 116 | C7H16O   | 017348-59-3 | 42   |
| 3    |    | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2  | 000540-88-5 | 39   |
| 4    |    | 3-Hexanol, 4-methyl-                | 116 | C7H16O   | 000615-29-2 | 28   |
| 5    |    | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 23   |



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ClientSampled :  
SB-103-21.5-22.0

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF110316.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

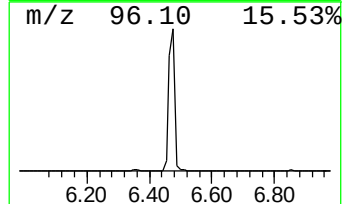
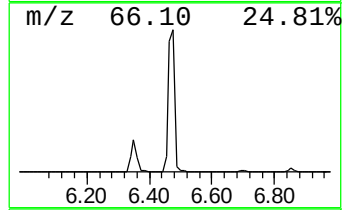
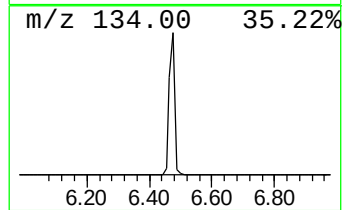
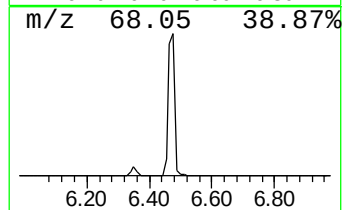
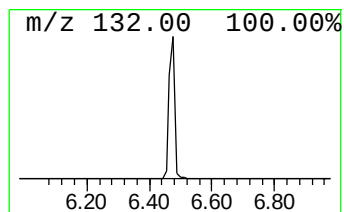
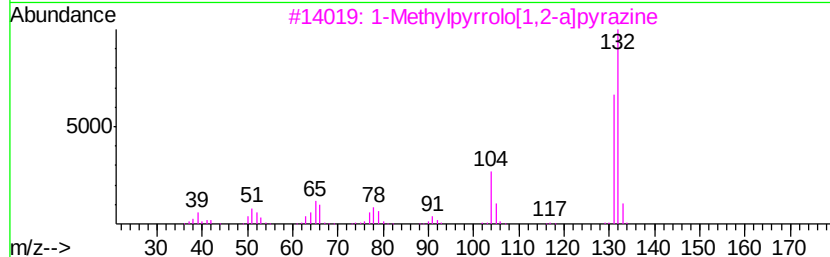
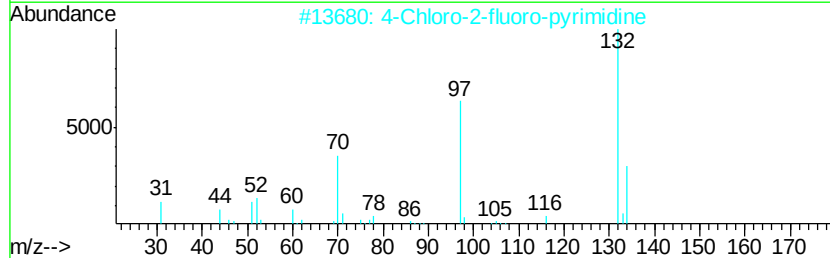
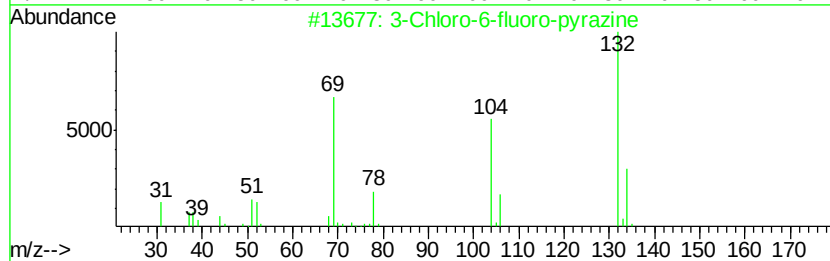
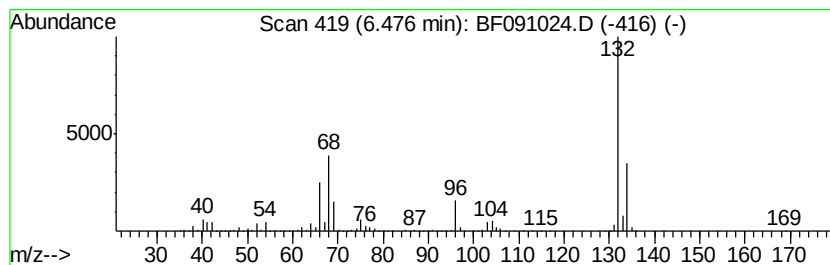
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 unknown6.48 Concentration Rank 2

| R.T. | EstConc   | Area    | Relative to ISTD       | R.T. |
|------|-----------|---------|------------------------|------|
| 6.48 | 116.41 ng | 5905170 | 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 | 16   |
| 2    |    | 4-Chloro-2-fluoro-pyrimidine     | 132 | C4H2ClFN2 | 051422-00-5  | 9    |
| 3    |    | 1-Methylpyrrolo[1,2-a]pyrazine   | 132 | C8H8N2    | 064608-59-9  | 9    |
| 4    |    | Imidazole, 4,5-dicyano-1-methyl- | 132 | C6H4N4    | 019485-35-9  | 9    |
| 5    |    | 4-Methylpyrrolo[1,2-a]pyrazine   | 132 | C8H8N2    | 064608-60-2  | 9    |



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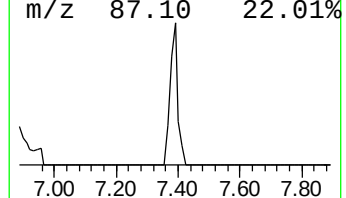
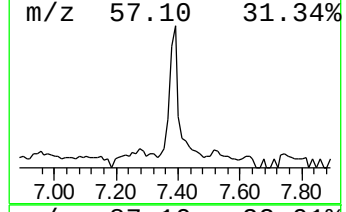
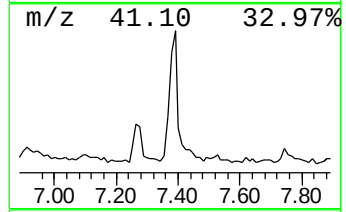
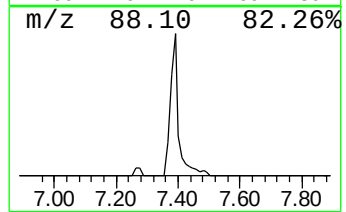
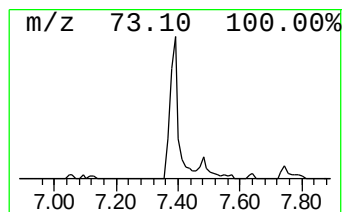
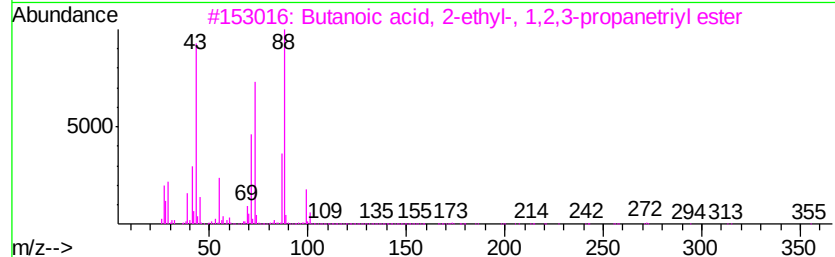
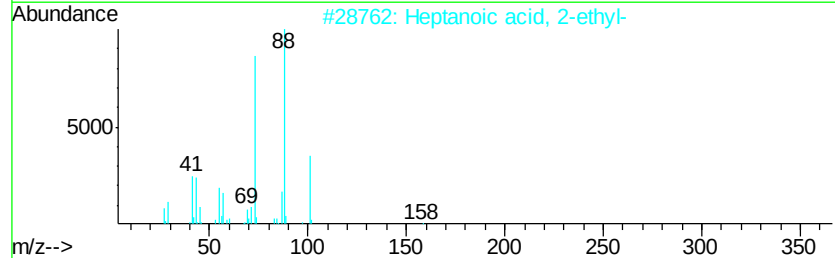
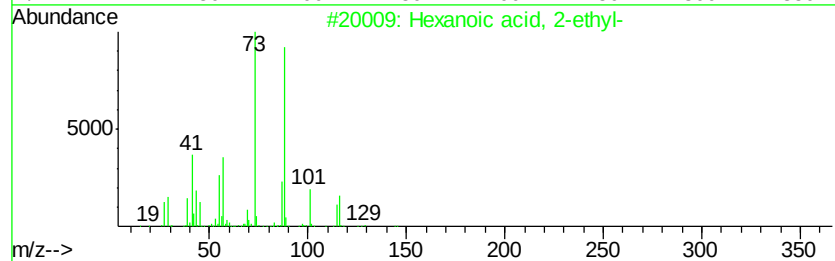
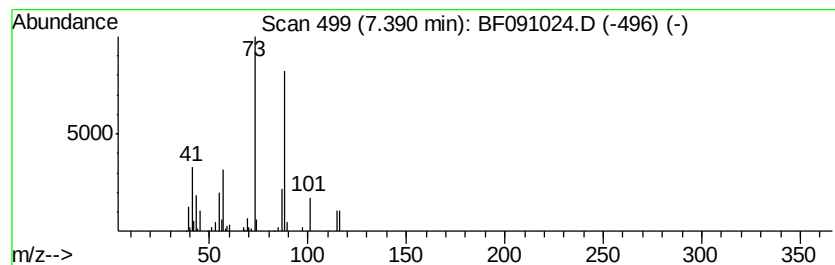
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 Hexanoic acid, 2-ethyl- Concentration Rank 6

| R.T. | EstConc | Area   | Relative to ISTD | R.T. |
|------|---------|--------|------------------|------|
| 7.39 | 2.05 ng | 150753 | Naphthalene-d8   | 7.98 |

| Hit# | of | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|-------------------------------------|-----|----------|-------------|------|
| 1    | 5  | Hexanoic acid, 2-ethyl-             | 144 | C8H16O2  | 000149-57-5 | 83   |
| 2    |    | Heptanoic acid, 2-ethyl-            | 158 | C9H18O2  | 003274-29-1 | 53   |
| 3    |    | Butanoic acid, 2-ethyl-, 1,2,3-p... | 386 | C21H38O6 | 056554-54-2 | 53   |
| 4    |    | 1,4-Dioxane                         | 88  | C4H8O2   | 000123-91-1 | 43   |
| 5    |    | Hydroxypivalic acid                 | 118 | C5H10O3  | 004835-90-9 | 36   |



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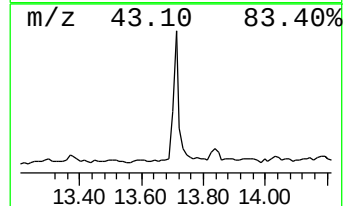
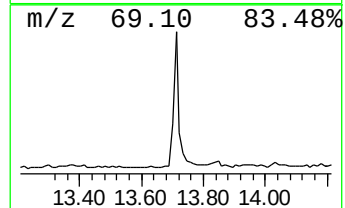
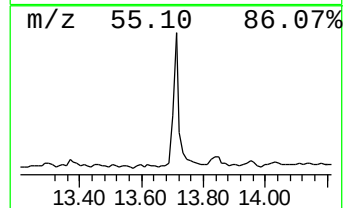
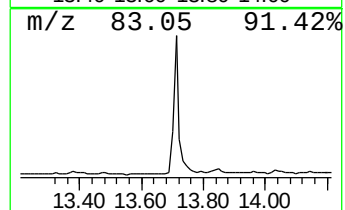
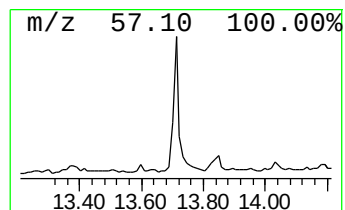
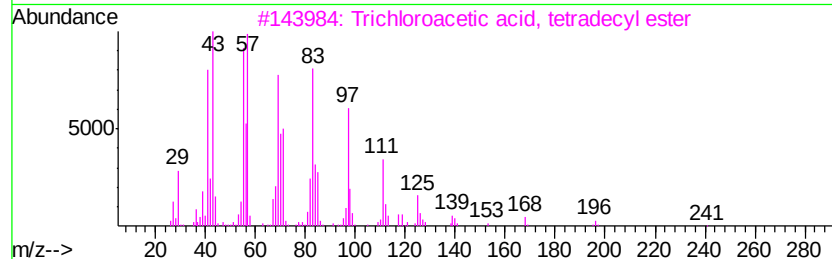
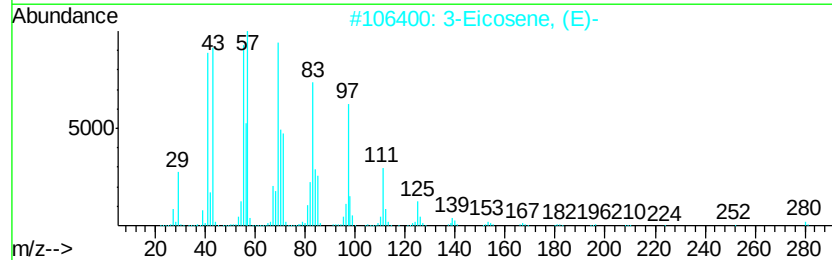
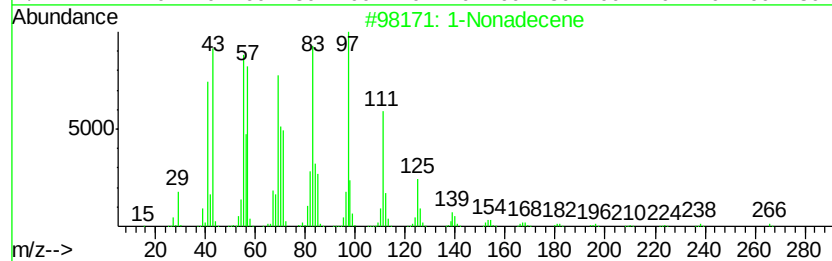
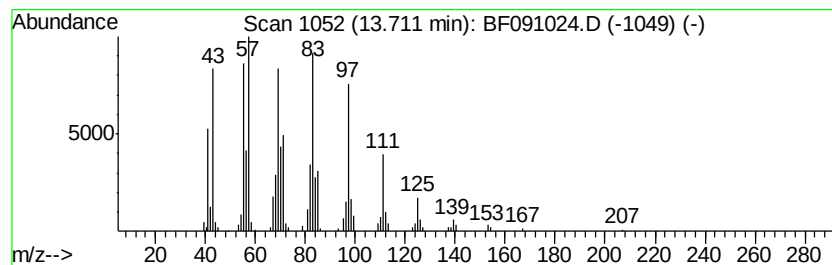
Instrument :  
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ClientSampleId :  
SB-103-21.5-22.0

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\*\*\*\*\*  
Peak Number 6 1-Nonadecene Concentration Rank 5

| R.T.      | EstConc                             | Area   | Relative to ISTD | R.T.         |      |
|-----------|-------------------------------------|--------|------------------|--------------|------|
| 13.71     | 4.01 ng                             | 260288 | Chrysene-d12     | 13.85        |      |
| Hit# of 5 | Tentative ID                        | MW     | MolForm          | CAS#         | Qual |
| 1         | 1-Nonadecene                        | 266    | C19H38           | 018435-45-5  | 91   |
| 2         | 3-Eicosene, (E)-                    | 280    | C20H40           | 074685-33-9  | 91   |
| 3         | Trichloroacetic acid, tetradecyl... | 358    | C16H29Cl3O2      | 074339-52-9  | 90   |
| 4         | Trichloroacetic acid, pentadecyl... | 372    | C17H31Cl3O2      | 074339-53-0  | 90   |
| 5         | 3-Chloropropionic acid, heptadec... | 346    | C20H39ClO2       | 1000283-05-1 | 90   |



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| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |         |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|---------|------|
|                      |       |         |       |          | #                     | RT    | Resp    | Conc |
| 2-Pentanone, 4-hy... | 4.86  | 26.1    | ng    | 1322840  | 1                     | 6.70  | 1014570 | 20.0 |
| unknown6.48          | 6.48  | 116.4   | ng    | 5905170  | 1                     | 6.70  | 1014570 | 20.0 |
| Hexanoic acid, 2-... | 7.39  | 2.0     | ng    | 150753   | 2                     | 7.98  | 1467230 | 20.0 |
| 1-Nonadecene         | 13.71 | 4.0     | ng    | 260288   | 5                     | 13.85 | 1298880 | 20.0 |