

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122316\  
 Data File : BF091925.D  
 Acq On : 23 Dec 2016 15:55  
 Operator : UM/SJ  
 Sample : H6156-23  
 Misc :  
 ALS Vial : 10 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :

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-BF122116.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         | 4.899       | 243           | 246         | 252          | rBV      | 874829         | 1079990       | 16.86%          | 2.452%        |
| 2         | 5.379       | 285           | 288         | 290          | rBV      | 2339214        | 2472782       | 38.61%          | 5.613%        |
| 3         | 6.430       | 377           | 380         | 382          | rBV      | 1195150        | 1524669       | 23.81%          | 3.461%        |
| 4         | 6.522       | 385           | 388         | 391          | rBV      | 4196588        | 4259303       | 66.51%          | 9.669%        |
| 5         | 6.739       | 404           | 407         | 409          | rBV      | 1316118        | 1181352       | 18.45%          | 2.682%        |
| 6         | 6.899       | 418           | 421         | 423          | rVB      | 4272853        | 4494636       | 70.19%          | 10.203%       |
| 7         | 7.150       | 441           | 443         | 445          | rBV      | 70792          | 64859         | 1.01%           | 0.147%        |
| 8         | 7.310       | 454           | 457         | 459          | rBV      | 3540448        | 3877496       | 60.55%          | 8.802%        |
| 9         | 8.019       | 517           | 519         | 522          | rBV      | 1084874        | 1485627       | 23.20%          | 3.372%        |
| 10        | 9.105       | 611           | 614         | 616          | rBV      | 6297570        | 6403946       | 100.00%         | 14.537%       |
| 11        | 9.779       | 670           | 673         | 675          | rBV      | 1440089        | 1776079       | 27.73%          | 4.032%        |
| 12        | 10.568      | 739           | 742         | 745          | rBV      | 3633355        | 3847408       | 60.08%          | 8.734%        |
| 13        | 11.254      | 800           | 802         | 805          | rBV      | 1962490        | 1727268       | 26.97%          | 3.921%        |
| 14        | 12.671      | 923           | 926         | 928          | rBV      | 420304         | 368195        | 5.75%           | 0.836%        |
| 15        | 12.751      | 928           | 933         | 935          | rVB2     | 64946          | 108867        | 1.70%           | 0.247%        |
| 16        | 12.842      | 938           | 941         | 944          | rBV      | 5271101        | 6163259       | 96.24%          | 13.991%       |
| 17        | 13.368      | 985           | 987         | 989          | rBV2     | 216892         | 266031        | 4.15%           | 0.604%        |
| 18        | 13.882      | 1030          | 1032        | 1035         | rBV      | 1520697        | 1523339       | 23.79%          | 3.458%        |
| 19        | 14.362      | 1070          | 1074        | 1078         | rBV      | 51103          | 72015         | 1.12%           | 0.163%        |
| 20        | 14.660      | 1098          | 1100        | 1103         | rVB      | 71399          | 70991         | 1.11%           | 0.161%        |
| 21        | 15.277      | 1151          | 1154        | 1156         | rBV      | 867704         | 1194022       | 18.65%          | 2.710%        |
| 22        | 15.311      | 1156          | 1157        | 1162         | rVB      | 67528          | 89679         | 1.40%           | 0.204%        |

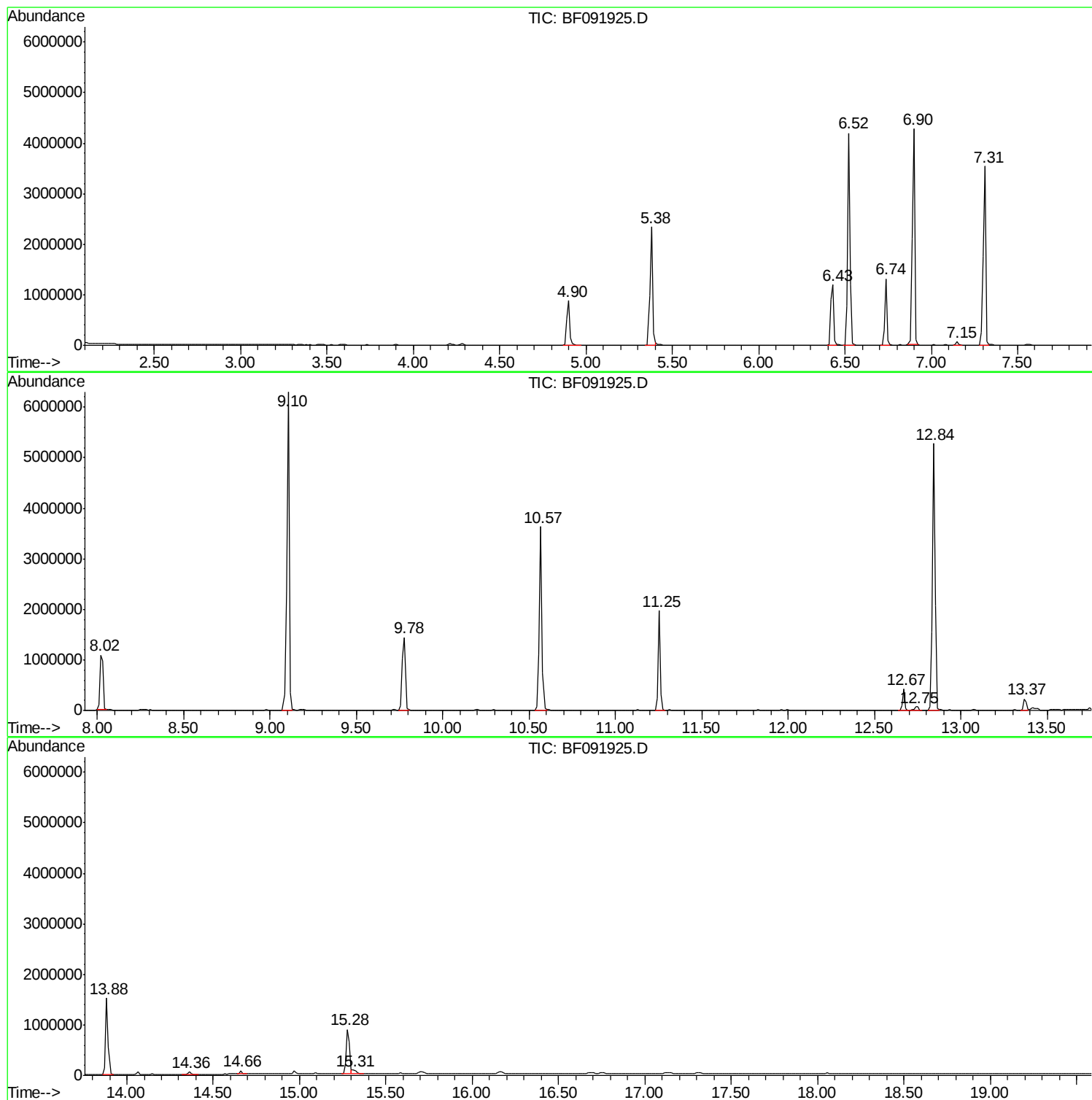
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ClientSampleId :

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF122116.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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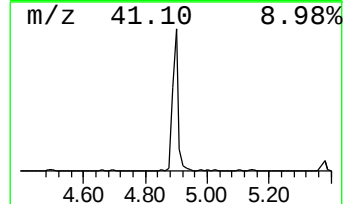
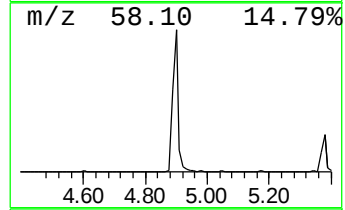
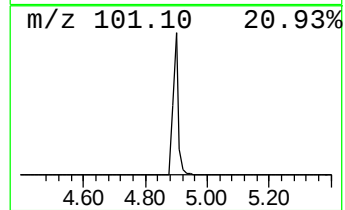
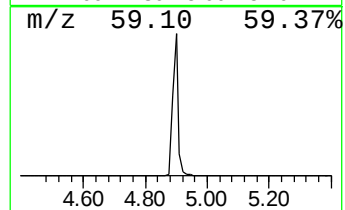
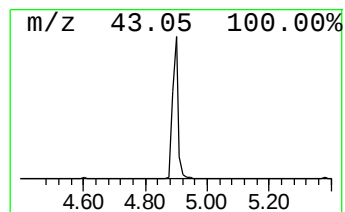
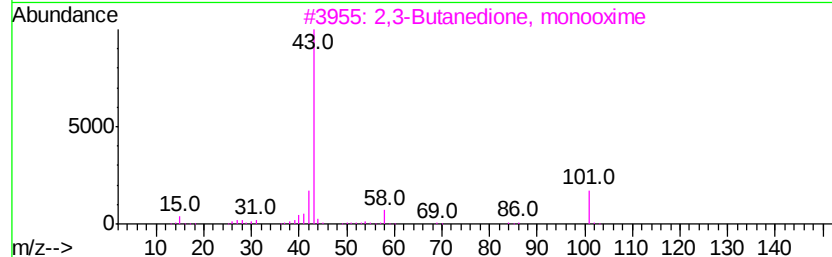
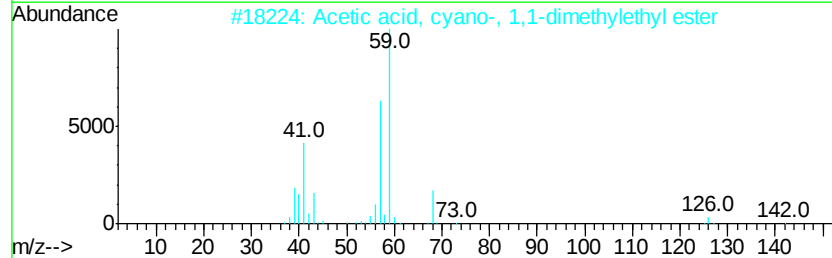
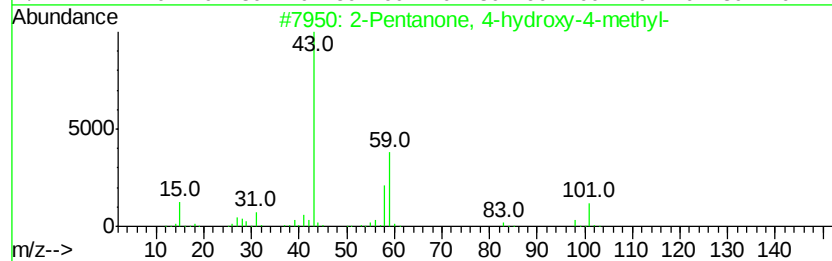
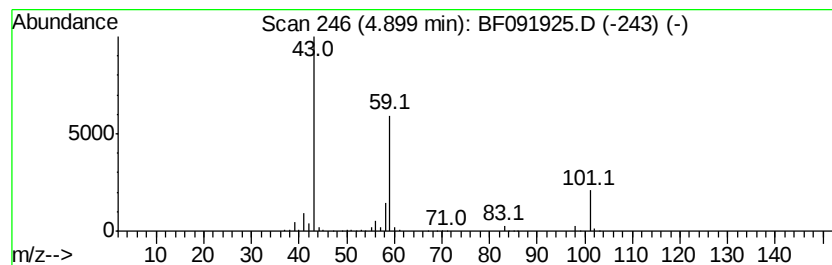
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 4.90 | 18.28 ng | 1079990 | 1,4-Dichlorobenzene-d4 | 6.74 |

| Hit# | of | Tentative ID                         | MW  | MolForm  | CAS#        | Qual |
|------|----|--------------------------------------|-----|----------|-------------|------|
| 1    | 5  | 2-Pentanone, 4-hydroxy-4-methyl-     | 116 | C6H12O2  | 000123-42-2 | 56   |
| 2    |    | Acetic acid, cyano-, 1,1-dimethyl... | 141 | C7H11NO2 | 001116-98-9 | 23   |
| 3    |    | 2,3-Butanedione, monooxime           | 101 | C4H7NO2  | 000057-71-6 | 9    |
| 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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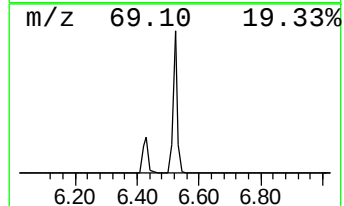
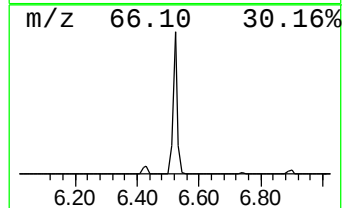
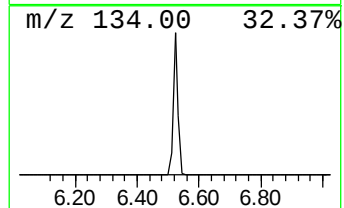
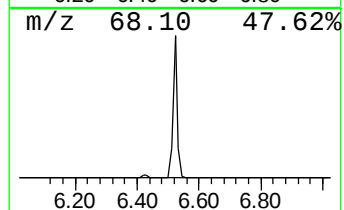
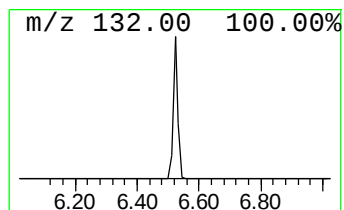
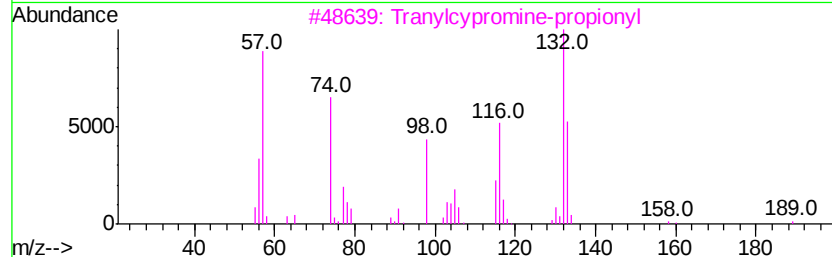
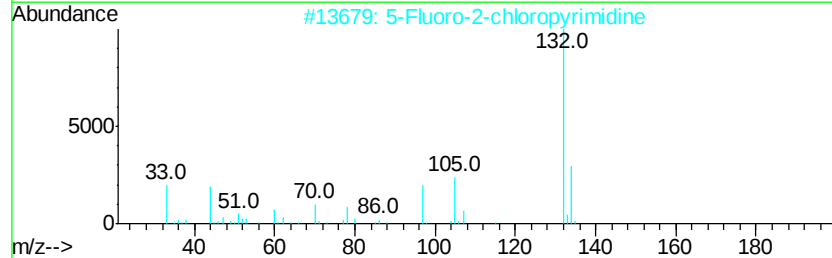
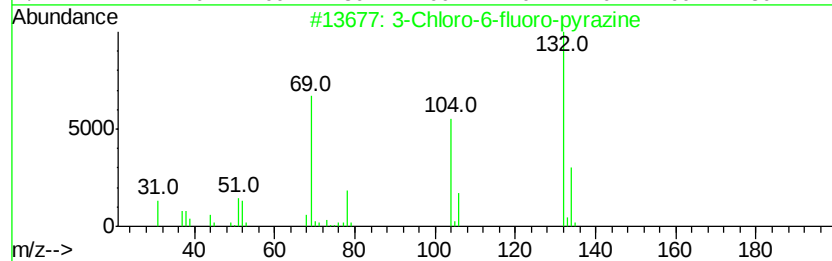
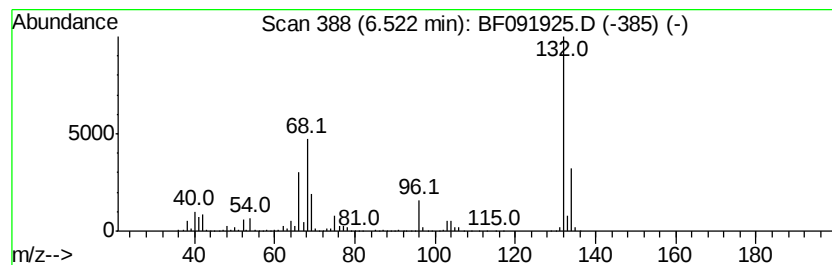
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 unknown6.52 Concentration Rank 2

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.52 | 72.11 ng | 4259300 | 1,4-Dichlorobenzene-d4 | 6.74 |

| Hit# | of | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|-------------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 3-Chloro-6-fluoro-pyrazine          | 132 | C4H2ClFN2 | 1000146-10-7 | 27   |
| 2    |    | 5-Fluoro-2-chloropyrimidine         | 132 | C4H2ClFN2 | 062802-42-0  | 12   |
| 3    |    | Tranvlcyproline-propionyl           | 189 | C12H15NO  | 1000123-86-3 | 10   |
| 4    |    | Benzene, 1,3,5-trifluoro-           | 132 | C6H3F3    | 000372-38-3  | 9    |
| 5    |    | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12    | 028749-81-7  | 9    |



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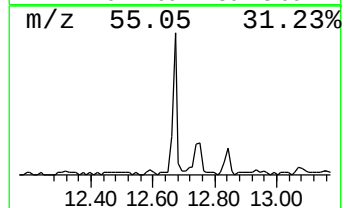
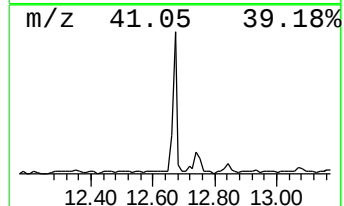
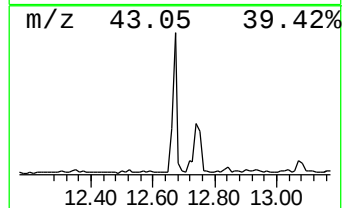
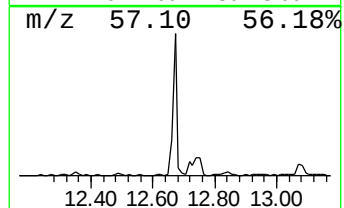
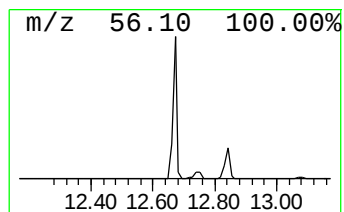
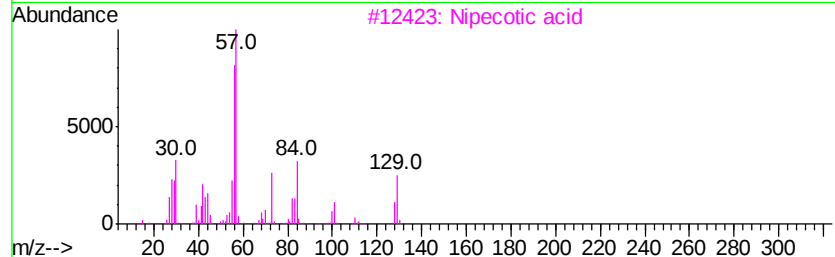
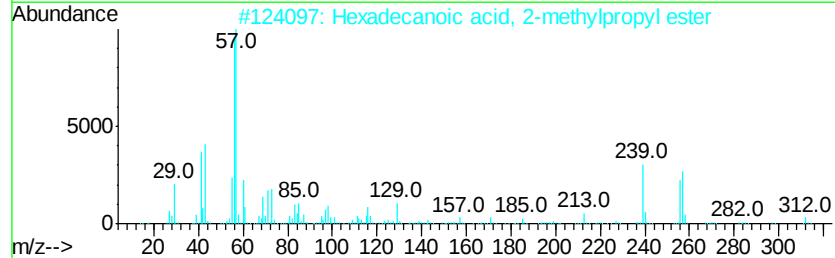
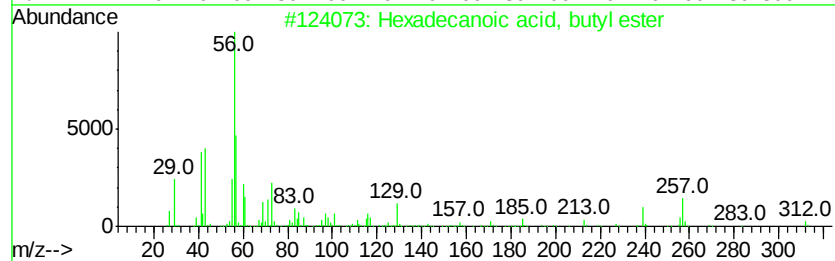
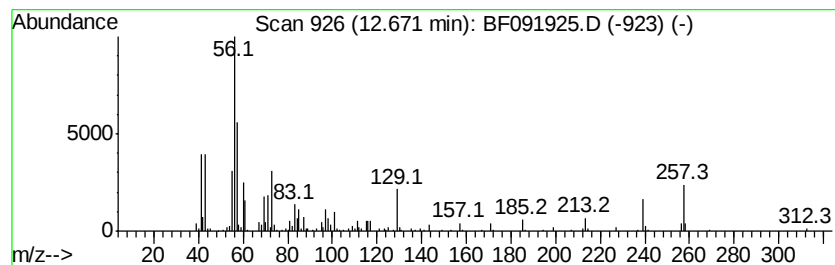
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TIC Integration Parameters: LSCINT.P

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Peak Number 4 Hexadecanoic acid, butyl ester Concentration Rank 4

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 12.67 | 4.83 ng | 368195 | Chrysene-d12     | 13.88 |

| Hit# | of | Tentative ID                         | MW  | MolForm  | CAS#        | Qual |
|------|----|--------------------------------------|-----|----------|-------------|------|
| 1    | 5  | Hexadecanoic acid, butyl ester       | 312 | C20H40O2 | 000111-06-8 | 91   |
| 2    |    | Hexadecanoic acid, 2-methylpropyl... | 312 | C20H40O2 | 000110-34-9 | 64   |
| 3    |    | Nipecotic acid                       | 129 | C6H11NO2 | 000498-95-3 | 47   |
| 4    |    | Cyclopropane, 1-(1-methylethyl)-...  | 210 | C15H30   | 041977-39-3 | 35   |
| 5    |    | 1,3-Pentanediol, 2,2,4-trimethyl-    | 146 | C8H18O2  | 000144-19-4 | 32   |



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Misc :  
ALS Vial : 10 Sample Multiplier: 1

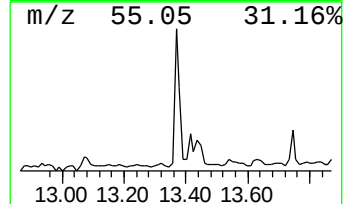
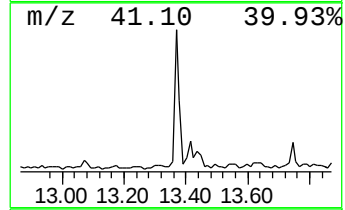
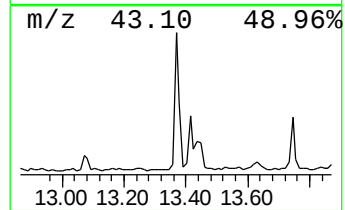
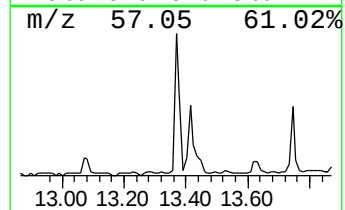
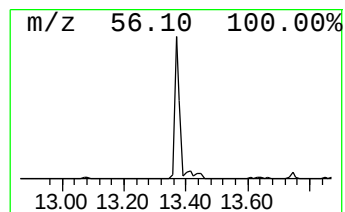
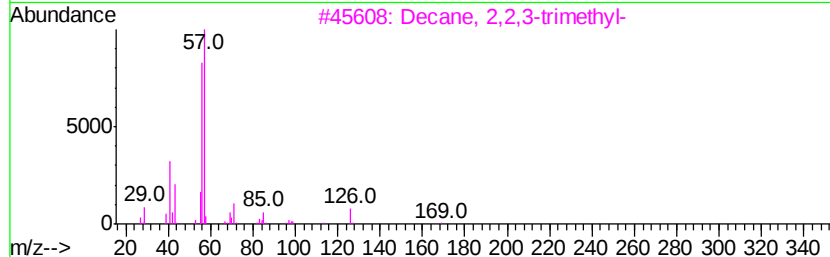
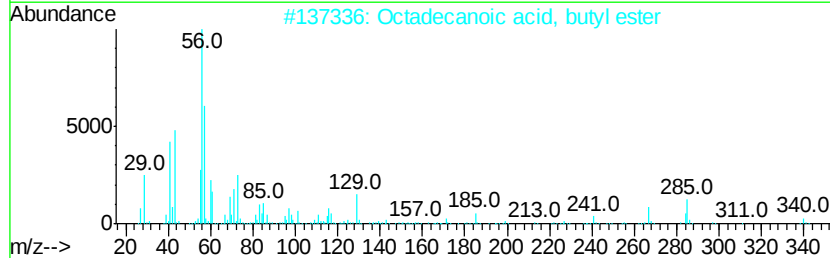
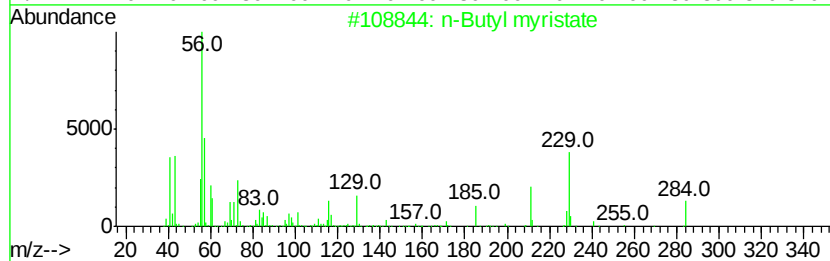
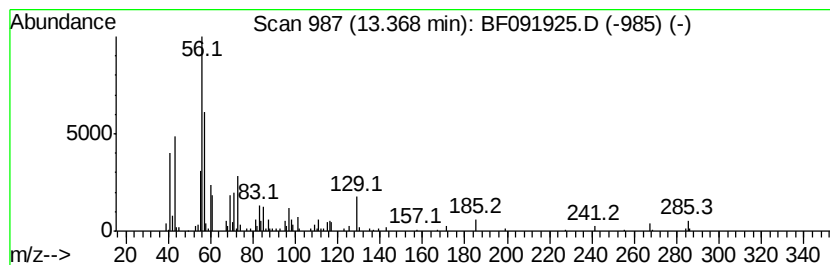
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ClientSampleId :

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\*\*\*\*\*  
Peak Number 5 n-Butyl myristate Concentration Rank 5

| R.T.      | EstConc                            | Area   | Relative to ISTD | R.T.        |      |
|-----------|------------------------------------|--------|------------------|-------------|------|
| 13.37     | 3.49 ng                            | 266031 | Chrysene-d12     | 13.88       |      |
| Hit# of 5 | Tentative ID                       | MW     | MolForm          | CAS#        | Qual |
| 1         | n-Butyl myristate                  | 284    | C18H36O2         | 000110-36-1 | 80   |
| 2         | Octadecanoic acid, butyl ester     | 340    | C22H44O2         | 000123-95-5 | 72   |
| 3         | Decane, 2,2,3-trimethyl-           | 184    | C13H28           | 062338-09-4 | 38   |
| 4         | Cyclobutane, 1,1-dimethyl-2-octyl- | 196    | C14H28           | 062338-30-1 | 38   |
| 5         | Hexane, 3,4-dimethyl-              | 114    | C8H18            | 000583-48-2 | 32   |



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| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |         |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|---------|------|
|                      |       |         |       |          | #                     | RT    | Resp    | Conc |
| 2-Pentanone, 4-hy... | 4.90  | 18.3    | ng    | 1079990  | 1                     | 6.74  | 1181350 | 20.0 |
| unknown6.52          | 6.52  | 72.1    | ng    | 4259300  | 1                     | 6.74  | 1181350 | 20.0 |
| Hexadecanoic acid... | 12.67 | 4.8     | ng    | 368195   | 5                     | 13.88 | 1523340 | 20.0 |
| n-Butyl myristate    | 13.37 | 3.5     | ng    | 266031   | 5                     | 13.88 | 1523340 | 20.0 |