

Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF092817\  
 Data File : BF098905.D  
 Acq On : 28 Sep 2017 13:41  
 Operator : SJ/JU  
 Sample : I5447-04  
 Misc :  
 ALS Vial : 8 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 SASP2P-ENV-115-5(5-10)

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-BF092317.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         | 2.228       | 20            | 24          | 32           | rVB      | 92982          | 136247        | 3.36%           | 0.404%        |
| 2         | 5.151       | 517           | 521         | 532          | rVB      | 521340         | 723720        | 17.83%          | 2.145%        |
| 3         | 5.540       | 581           | 587         | 590          | rBV      | 3415835        | 3605571       | 88.81%          | 10.684%       |
| 4         | 6.540       | 751           | 757         | 761          | rBV      | 3029702        | 3661751       | 90.20%          | 10.851%       |
| 5         | 6.687       | 777           | 782         | 785          | rBV      | 3624127        | 3660911       | 90.18%          | 10.848%       |
| 6         | 6.916       | 817           | 821         | 824          | rBV      | 1008721        | 814101        | 20.05%          | 2.412%        |
| 7         | 7.075       | 843           | 848         | 851          | rBV      | 3002143        | 2820423       | 69.47%          | 8.358%        |
| 8         | 7.481       | 911           | 917         | 919          | rBV      | 2155814        | 2362469       | 58.19%          | 7.001%        |
| 9         | 8.198       | 1034          | 1039        | 1042         | rBV      | 1188357        | 1096176       | 27.00%          | 3.248%        |
| 10        | 9.275       | 1216          | 1222        | 1225         | rBV      | 4052684        | 4059775       | 100.00%         | 12.030%       |
| 11        | 9.663       | 1283          | 1288        | 1291         | rBV      | 797820         | 682516        | 16.81%          | 2.022%        |
| 12        | 9.951       | 1333          | 1337        | 1341         | rBV      | 1394280        | 1201479       | 29.59%          | 3.560%        |
| 13        | 10.375      | 1406          | 1409        | 1412         | rVB      | 68692          | 53685         | 1.32%           | 0.159%        |
| 14        | 10.745      | 1463          | 1472        | 1475         | rBV      | 2266318        | 2317928       | 57.09%          | 6.869%        |
| 15        | 10.845      | 1486          | 1489        | 1494         | rBV      | 79991          | 75507         | 1.86%           | 0.224%        |
| 16        | 11.439      | 1586          | 1590        | 1593         | rBV      | 1475039        | 1189161       | 29.29%          | 3.524%        |
| 17        | 11.951      | 1673          | 1677        | 1687         | rBV2     | 120297         | 134914        | 3.32%           | 0.400%        |
| 18        | 12.739      | 1807          | 1811        | 1818         | rBV      | 46313          | 54603         | 1.34%           | 0.162%        |
| 19        | 13.027      | 1855          | 1860        | 1863         | rBV      | 3500308        | 3505111       | 86.34%          | 10.387%       |
| 20        | 13.904      | 2006          | 2009        | 2014         | rBV      | 160231         | 155140        | 3.82%           | 0.460%        |
| 21        | 14.074      | 2035          | 2038        | 2042         | rVB      | 826597         | 757670        | 18.66%          | 2.245%        |
| 22        | 15.568      | 2286          | 2292        | 2299         | rBV      | 534442         | 677527        | 16.69%          | 2.008%        |

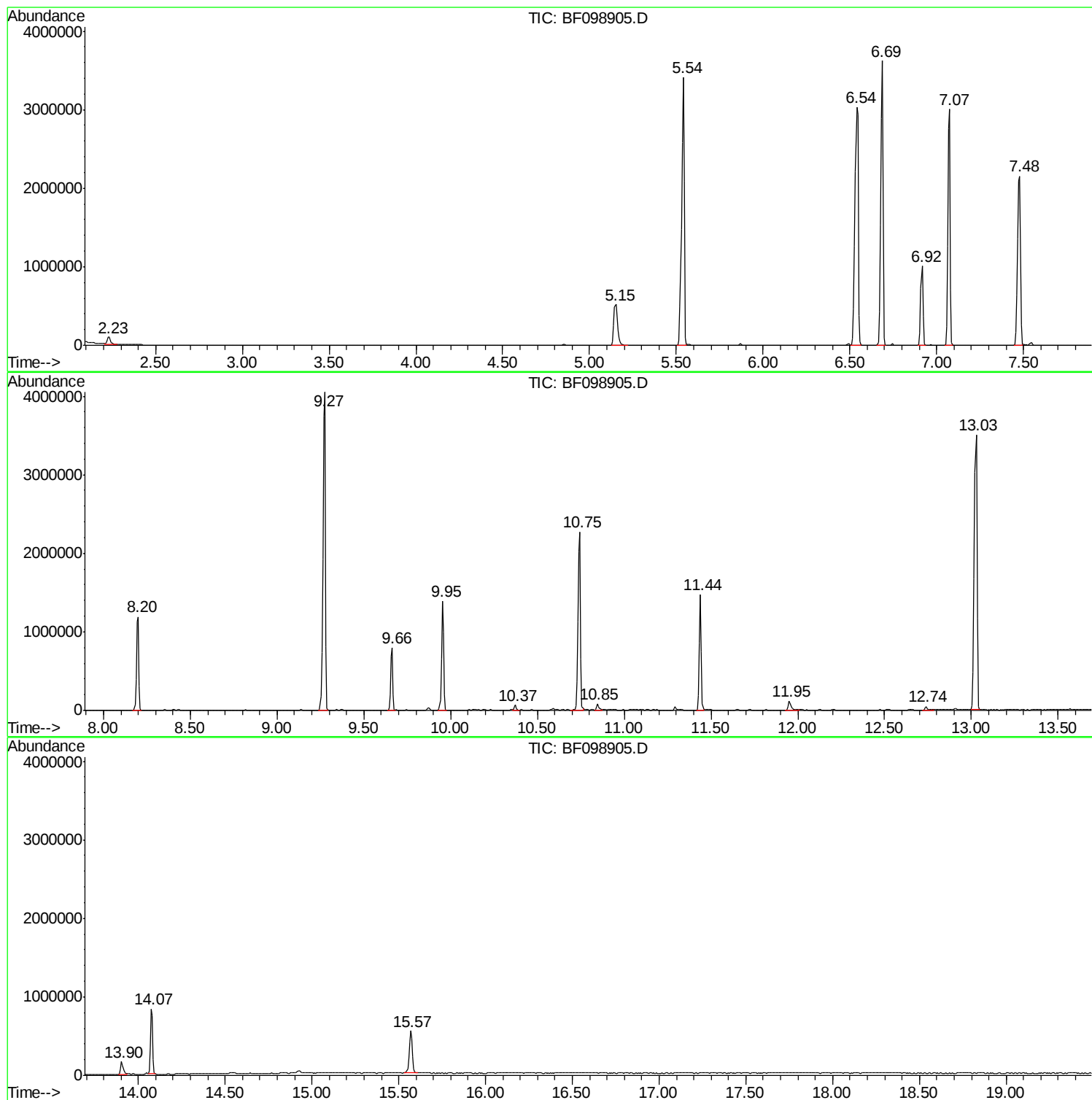
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Operator : SJ/JU  
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Misc :  
ALS Vial : 8 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
SASP2P-ENV-115-5(5-10)

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF092317.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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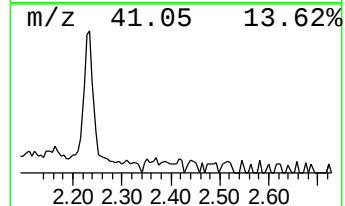
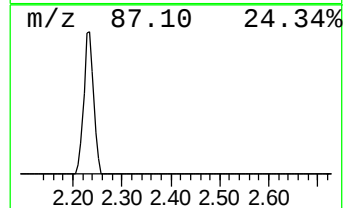
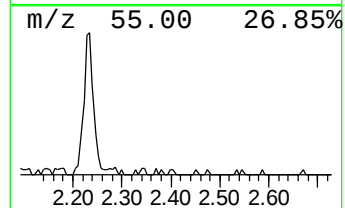
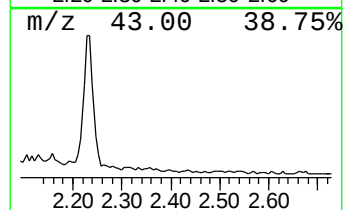
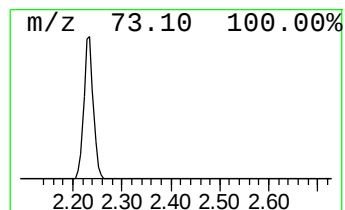
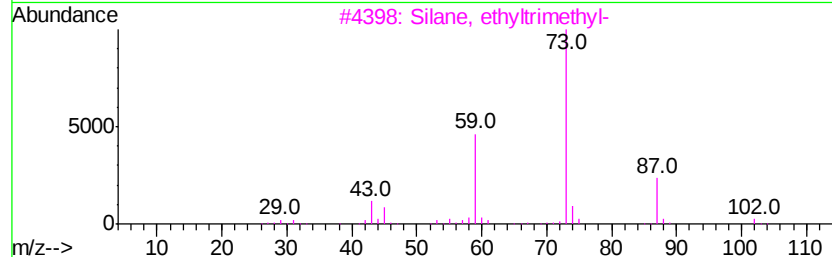
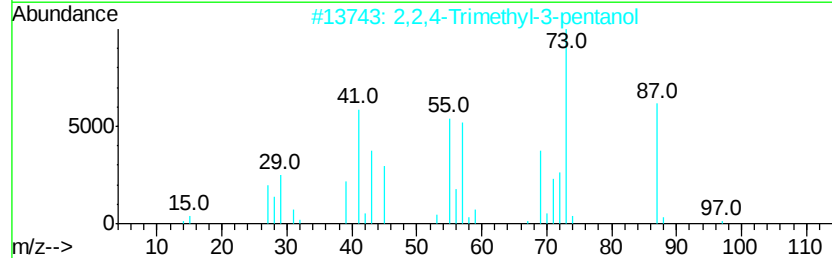
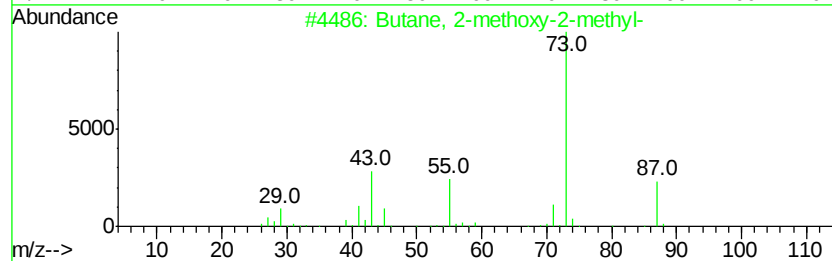
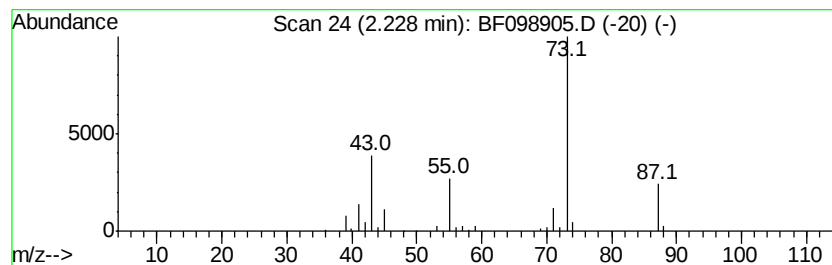
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TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

| R.T. | EstConc | Area   | Relative to ISTD       | R.T. |
|------|---------|--------|------------------------|------|
| 2.23 | 3.35 ng | 136247 | 1,4-Dichlorobenzene-d4 | 6.92 |

| Hit# | of | Tentative ID                | MW  | MolForm | CAS#        | Qual |
|------|----|-----------------------------|-----|---------|-------------|------|
| 1    | 5  | Butane, 2-methoxy-2-methyl- | 102 | C6H14O  | 000994-05-8 | 83   |
| 2    |    | 2,2,4-Trimethyl-3-pentanol  | 130 | C8H18O  | 005162-48-1 | 39   |
| 3    |    | Silane, ethyltrimethyl-     | 102 | C5H14Si | 003439-38-1 | 33   |
| 4    |    | 2-Methyl-5-hexen-3-ol       | 114 | C7H14O  | 032815-70-6 | 25   |
| 5    |    | 3-Hexanol, 2-methyl-        | 116 | C7H16O  | 000617-29-8 | 12   |



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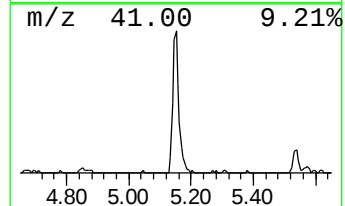
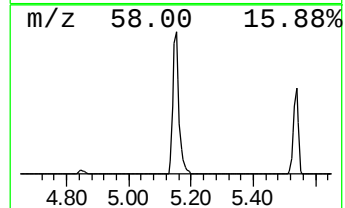
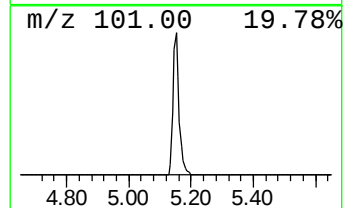
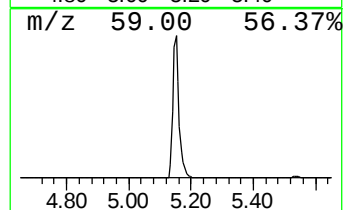
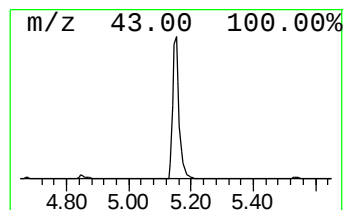
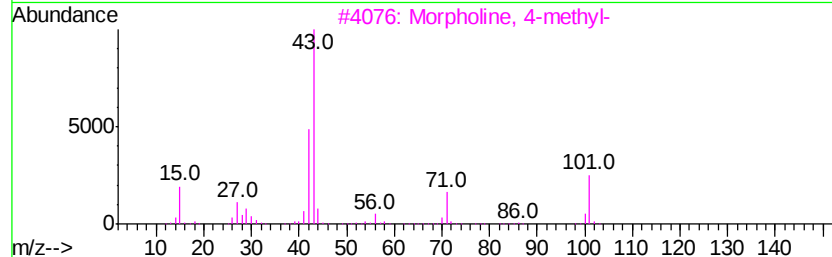
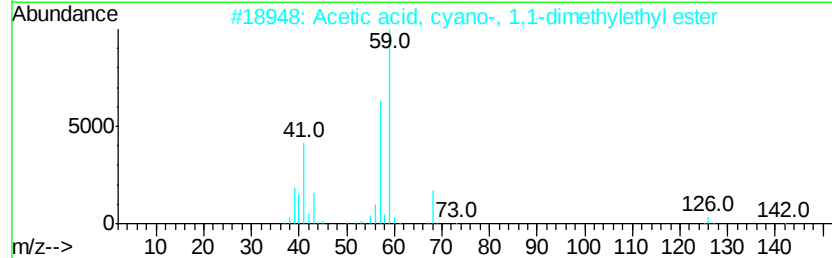
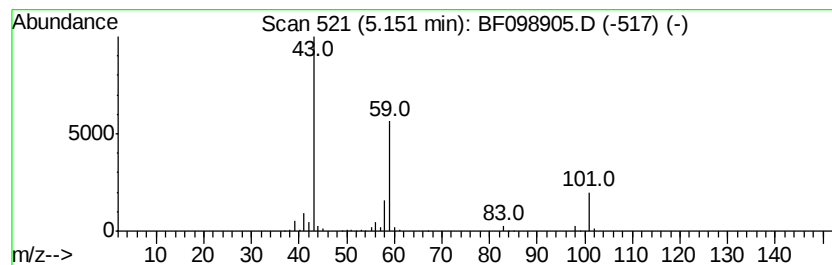
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T. | EstConc  | Area   | Relative to ISTD       | R.T. |
|------|----------|--------|------------------------|------|
| 5.15 | 17.78 ng | 723720 | 1,4-Dichlorobenzene-d4 | 6.92 |

| 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-dimethyl... | 141 | C7H11NO2 | 001116-98-9 | 17   |
| 3    |    | Morpholine, 4-methyl-                | 101 | C5H11NO  | 000109-02-4 | 9    |
| 4    |    | 2,3-Butanedione, monooxime           | 101 | C4H7NO2  | 000057-71-6 | 9    |
| 5    |    | Propane, 1-ethoxy-2-methyl-          | 102 | C6H14O   | 000627-02-1 | 9    |



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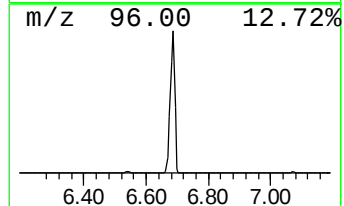
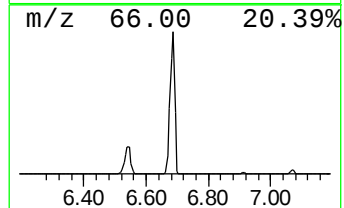
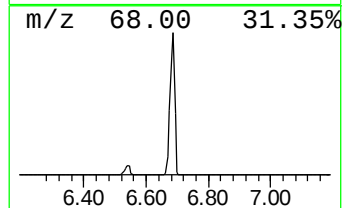
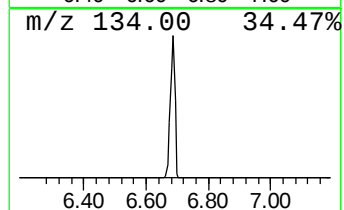
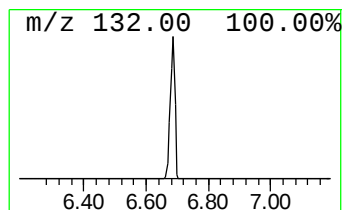
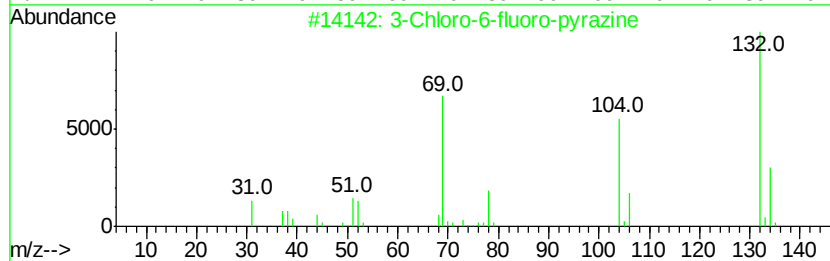
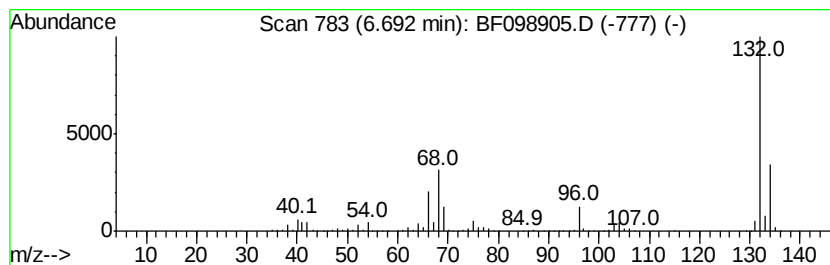
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 unknown6.69 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.69 | 89.94 ng | 3660910 | 1,4-Dichlorobenzene-d4 | 6.92 |

| Hit# | of | Tentative ID                     | MW  | MolForm   | CAS#         | Qual |
|------|----|----------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 3-Chloro-6-fluoro-pyrazine       | 132 | C4H2ClFN2 | 1000146-10-7 | 35   |
| 2    |    | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO   | 031357-76-3  | 17   |
| 3    |    | 5-Aminoindole                    | 132 | C8H8N2    | 005192-03-0  | 12   |
| 4    |    | Tranylcypromine-propionyl        | 189 | C12H15NO  | 1000123-86-3 | 12   |
| 5    |    | 1,3,5-Trifluorobenzene           | 132 | C6H3F3    | 000372-38-3  | 9    |



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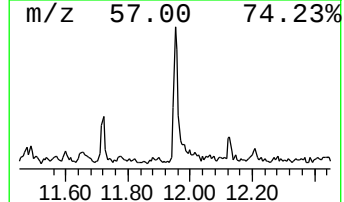
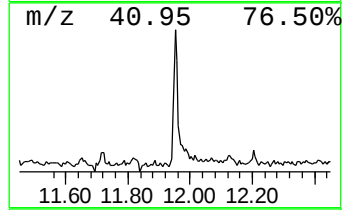
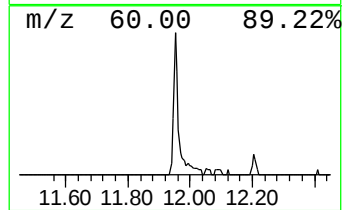
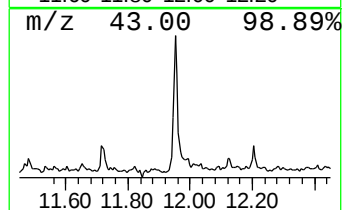
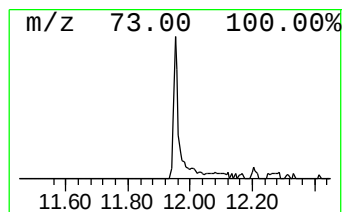
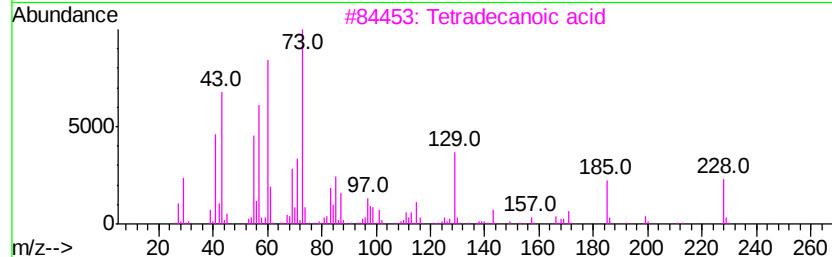
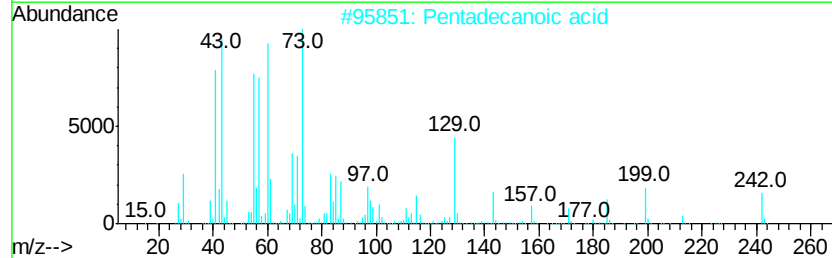
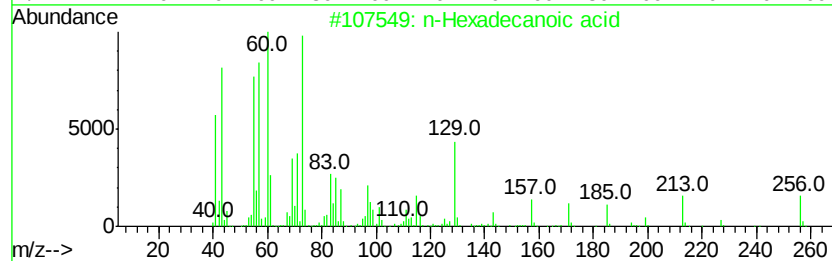
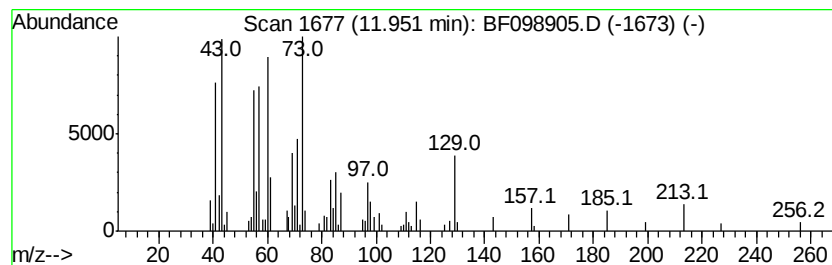
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 11.95 | 2.27 ng | 134914 | Phenanthrene-d10 | 11.44 |

| Hit# of | 5 | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|---------|---|-------------------------------------|-----|----------|--------------|------|
| 1       |   | n-Hexadecanoic acid                 | 256 | C16H32O2 | 000057-10-3  | 99   |
| 2       |   | Pentadecanoic acid                  | 242 | C15H30O2 | 001002-84-2  | 87   |
| 3       |   | Tetradecanoic acid                  | 228 | C14H28O2 | 000544-63-8  | 87   |
| 4       |   | n-Decanoic acid                     | 172 | C10H20O2 | 000334-48-5  | 58   |
| 5       |   | Oxalic acid, allyl pentadecyl ester | 340 | C20H36O4 | 1000309-24-3 | 15   |



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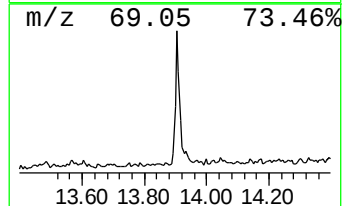
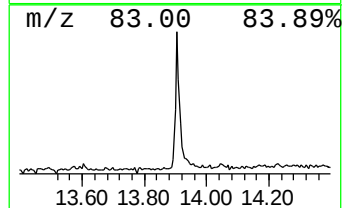
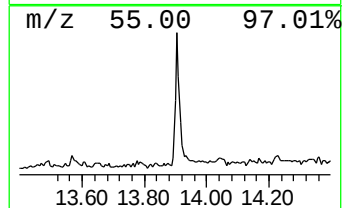
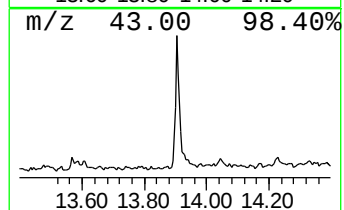
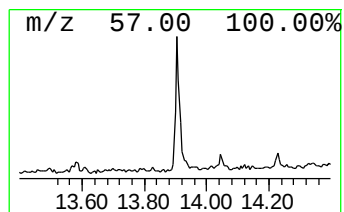
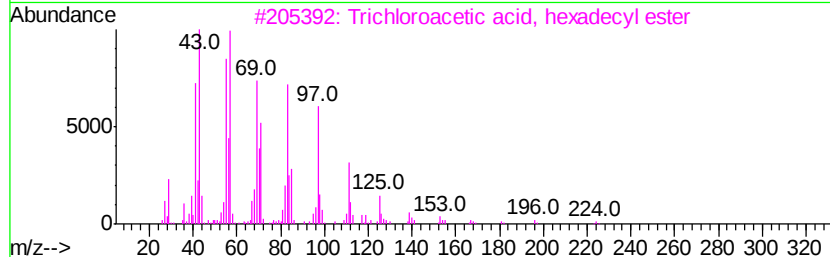
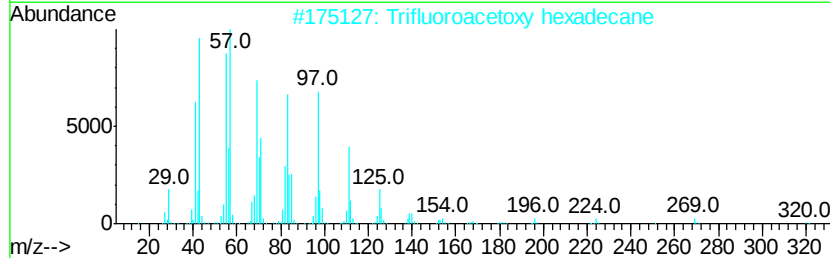
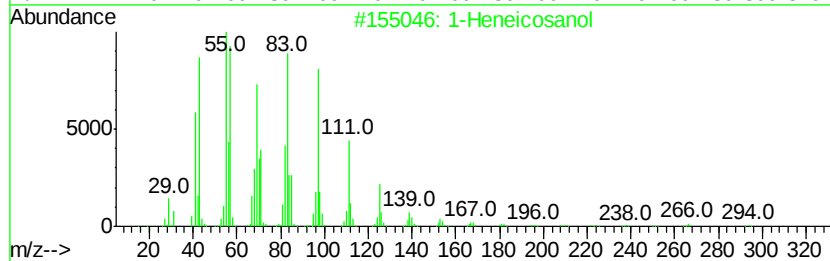
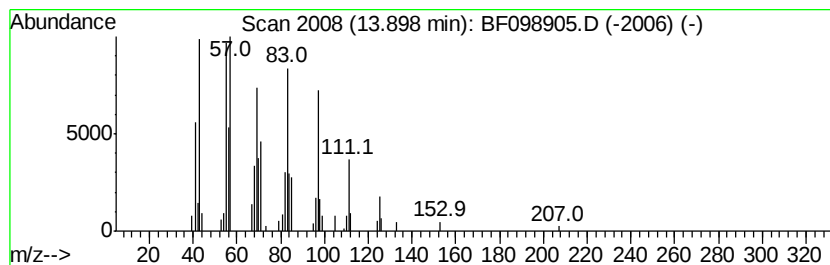
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\*\*\*\*\*  
Peak Number 6 1-Heneicosanol Concentration Rank 4

| R.T.    | EstConc | Area                                | Relative to ISTD | R.T.           |
|---------|---------|-------------------------------------|------------------|----------------|
| 13.90   | 4.10 ng | 155140                              | Chrysene-d12     | 14.07          |
| Hit# of | 5       | Tentative ID                        | MW MolForm       | CAS# Qual      |
| 1       |         | 1-Heneicosanol                      | 312 C21H44O      | 015594-90-8 95 |
| 2       |         | Trifluoroacetoxy hexadecane         | 338 C18H33F3O2   | 006222-03-3 95 |
| 3       |         | Trichloroacetic acid, hexadecyl ... | 386 C18H33Cl3O2  | 074339-54-1 94 |
| 4       |         | n-Tetracosanol-1                    | 354 C24H50O      | 000506-51-4 93 |
| 5       |         | Behenic alcohol                     | 326 C22H46O      | 000661-19-8 93 |



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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |         |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|---------|------|
|                      |       |         |       |          | #                     | RT    | Resp    | Conc |
| Butane, 2-methoxy... | 2.23  | 3.4     | ng    | 136247   | 1                     | 6.92  | 814101  | 20.0 |
| 2-Pentanone, 4-hy... | 5.15  | 17.8    | ng    | 723720   | 1                     | 6.92  | 814101  | 20.0 |
| unknown6.69          | 6.69  | 89.9    | ng    | 3660910  | 1                     | 6.92  | 814101  | 20.0 |
| n-Hexadecanoic acid  | 11.95 | 2.3     | ng    | 134914   | 4                     | 11.44 | 1189160 | 20.0 |
| 1-Heneicosanol       | 13.90 | 4.1     | ng    | 155140   | 5                     | 14.07 | 757670  | 20.0 |