

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012218\  
 Data File : BF102305.D  
 Acq On : 22 Jan 2018 17:58  
 Operator : SJ/JU  
 Sample : J1228-24  
 Misc :  
 ALS Vial : 10 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 COMP-3

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-BF012218.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         | 4.904       | 474           | 479         | 487          | rBV      | 142624         | 203902        | 6.86%           | 0.769%        |
| 2         | 5.322       | 545           | 550         | 553          | rBV      | 2716080        | 2577052       | 86.72%          | 9.724%        |
| 3         | 6.357       | 720           | 726         | 743          | rBV      | 2401483        | 2818311       | 94.84%          | 10.635%       |
| 4         | 6.481       | 743           | 747         | 751          | rBV      | 2853663        | 2737571       | 92.13%          | 10.330%       |
| 5         | 6.710       | 783           | 786         | 795          | rBV      | 828603         | 744086        | 25.04%          | 2.808%        |
| 6         | 6.869       | 809           | 813         | 816          | rBV      | 2407968        | 2098830       | 70.63%          | 7.920%        |
| 7         | 7.281       | 878           | 883         | 886          | rBV      | 1777532        | 1673620       | 56.32%          | 6.315%        |
| 8         | 7.992       | 1000          | 1004        | 1021         | rVB      | 1084657        | 1033962       | 34.79%          | 3.902%        |
| 9         | 9.075       | 1183          | 1188        | 1191         | rBV      | 3083642        | 2971583       | 100.00%         | 11.213%       |
| 10        | 9.469       | 1251          | 1255        | 1262         | rVB      | 247539         | 229261        | 7.72%           | 0.865%        |
| 11        | 9.681       | 1287          | 1291        | 1294         | rBV      | 63996          | 51175         | 1.72%           | 0.193%        |
| 12        | 9.745       | 1298          | 1302        | 1307         | rVV      | 1109066        | 1094120       | 36.82%          | 4.129%        |
| 13        | 10.180      | 1372          | 1376        | 1378         | rBV2     | 55500          | 46576         | 1.57%           | 0.176%        |
| 14        | 10.463      | 1420          | 1424        | 1430         | rVB      | 72984          | 65357         | 2.20%           | 0.247%        |
| 15        | 10.539      | 1432          | 1437        | 1447         | rVV      | 1732638        | 1721593       | 57.94%          | 6.496%        |
| 16        | 10.651      | 1453          | 1456        | 1465         | rVB      | 39855          | 49588         | 1.67%           | 0.187%        |
| 17        | 11.233      | 1551          | 1555        | 1558         | rBV      | 1182945        | 1075901       | 36.21%          | 4.060%        |
| 18        | 12.280      | 1730          | 1733        | 1736         | rBV      | 42851          | 40778         | 1.37%           | 0.154%        |
| 19        | 12.439      | 1757          | 1760        | 1765         | rVB      | 64476          | 62163         | 2.09%           | 0.235%        |
| 20        | 12.669      | 1796          | 1799        | 1801         | rBV      | 110521         | 89485         | 3.01%           | 0.338%        |
| 21        | 12.716      | 1805          | 1807        | 1813         | rVB3     | 40125          | 48562         | 1.63%           | 0.183%        |
| 22        | 12.821      | 1820          | 1825        | 1828         | rBV      | 2765873        | 2689765       | 90.52%          | 10.150%       |
| 23        | 12.886      | 1833          | 1836        | 1843         | rBV5     | 22947          | 31422         | 1.06%           | 0.119%        |
| 24        | 12.980      | 1848          | 1852        | 1854         | rBV5     | 20735          | 33009         | 1.11%           | 0.125%        |
| 25        | 13.104      | 1870          | 1873        | 1877         | rVB      | 30949          | 33755         | 1.14%           | 0.127%        |
| 26        | 13.710      | 1973          | 1976        | 1980         | rBV2     | 136413         | 144664        | 4.87%           | 0.546%        |
| 27        | 13.868      | 1998          | 2003        | 2006         | rBV      | 1078360        | 1008930       | 33.95%          | 3.807%        |
| 28        | 13.892      | 2006          | 2007        | 2013         | rVB      | 49612          | 36161         | 1.22%           | 0.136%        |
| 29        | 14.615      | 2127          | 2130        | 2136         | rVB      | 138338         | 157910        | 5.31%           | 0.596%        |
| 30        | 15.227      | 2231          | 2234        | 2240         | rVB      | 41691          | 45786         | 1.54%           | 0.173%        |
| 31        | 15.292      | 2240          | 2245        | 2254         | rBV      | 663988         | 886119        | 29.82%          | 3.344%        |

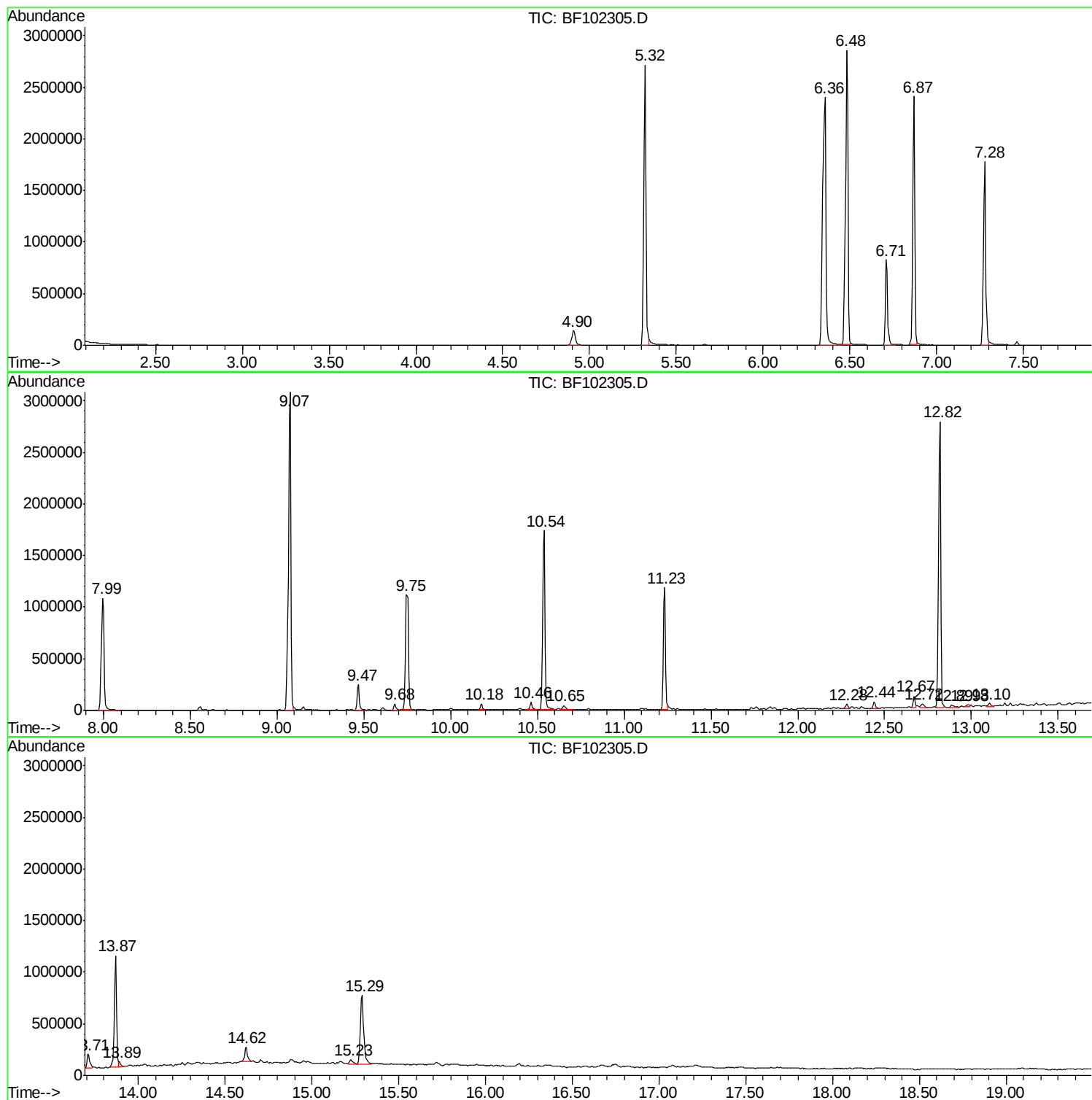
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Misc :  
ALS Vial : 10 Sample Multiplier: 1

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BNA\_F  
ClientSampleId :  
COMP-3

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF012218.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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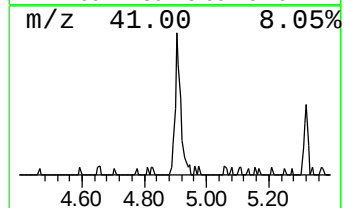
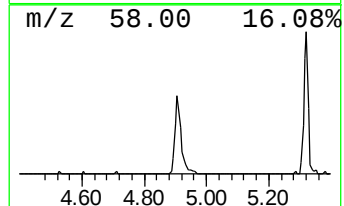
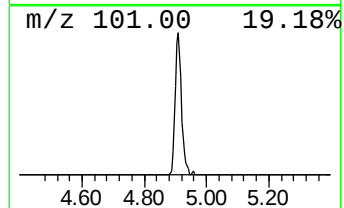
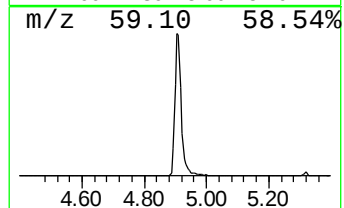
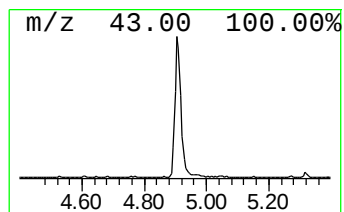
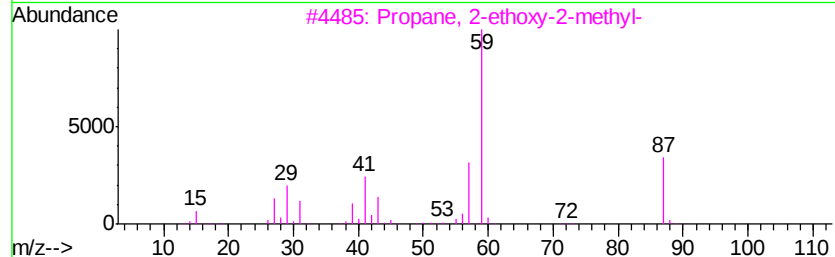
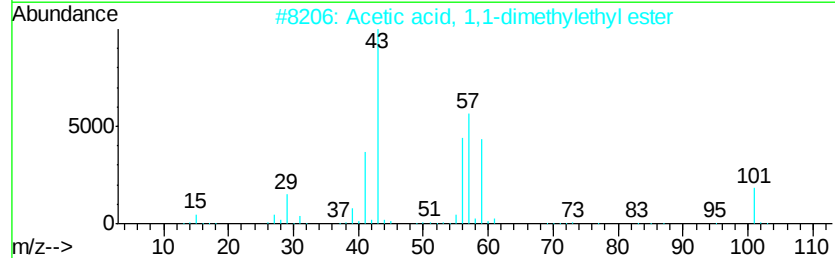
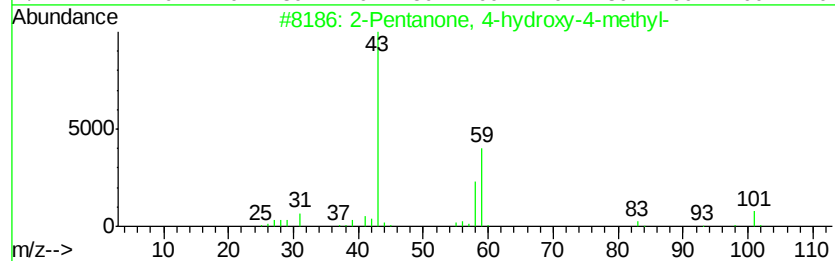
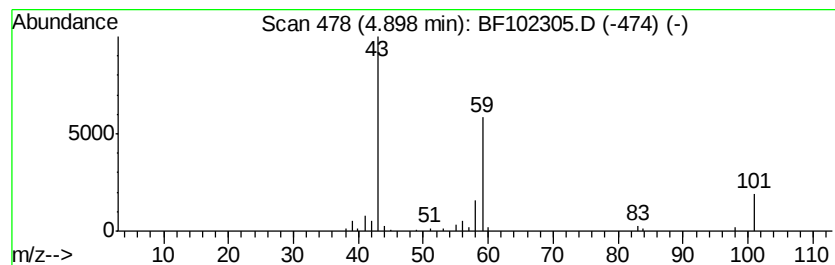
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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

| R.T. | EstConc | Area   | Relative to ISTD       | R.T. |
|------|---------|--------|------------------------|------|
| 4.90 | 5.48 ng | 203902 | 1,4-Dichlorobenzene-d4 | 6.71 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|---------|-------------|------|
| 1    |    |   | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2 | 000123-42-2 | 45   |
| 2    |    |   | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 39   |
| 3    |    |   | Propane, 2-ethoxy-2-methyl-         | 102 | C6H14O  | 000637-92-3 | 9    |
| 4    |    |   | 2-Hexanol, 2-methyl-                | 116 | C7H16O  | 000625-23-0 | 9    |
| 5    |    |   | Propane, 1-ethoxy-2-methyl-         | 102 | C6H14O  | 000627-02-1 | 9    |



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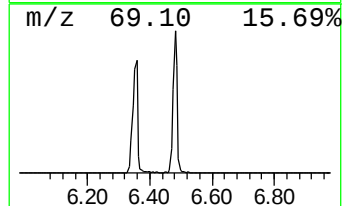
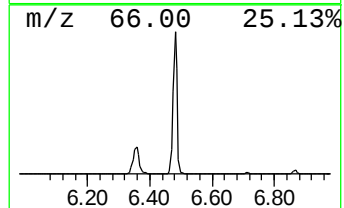
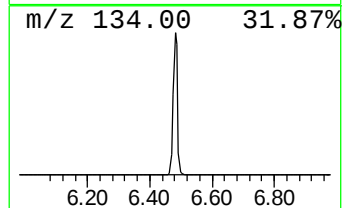
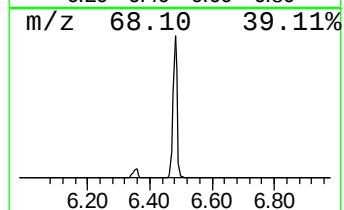
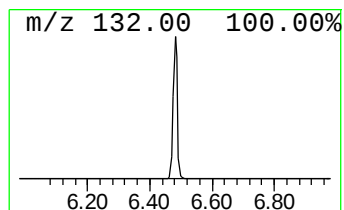
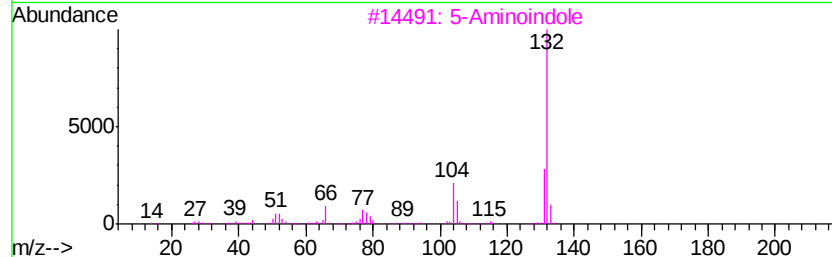
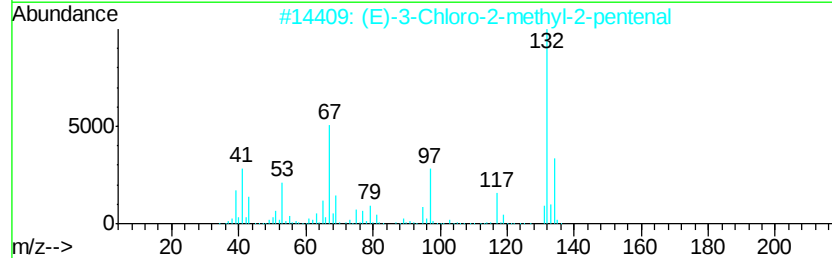
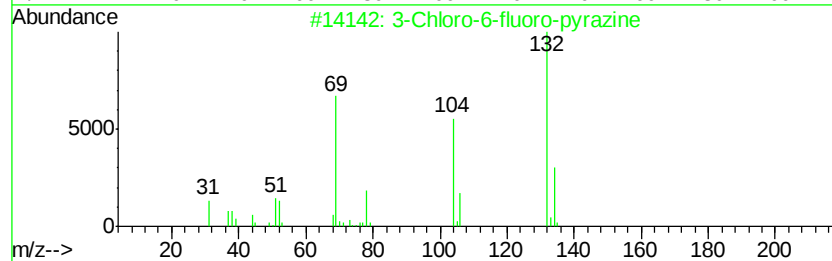
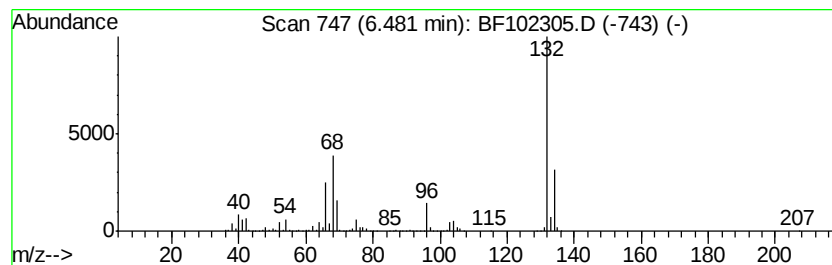
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF012218.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 2 unknown6.48 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.48 | 73.58 ng | 2737570 | 1,4-Dichlorobenzene-d4 | 6.71 |

| 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  | 27   |
| 3    |    | 5-Aminoindole                       | 132 | C8H8N2    | 005192-03-0  | 12   |
| 4    |    | Tranylcypromine-propionyl           | 189 | C12H15NO  | 1000123-86-3 | 10   |
| 5    |    | 2H-Cyclopenta[d]pyridazine, 2-me... | 132 | C8H8N2    | 022291-85-6  | 9    |



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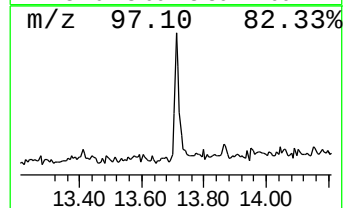
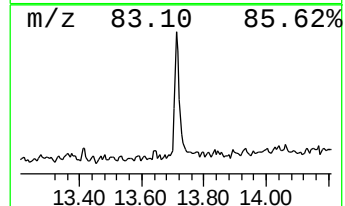
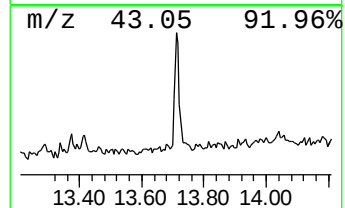
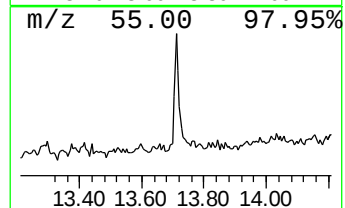
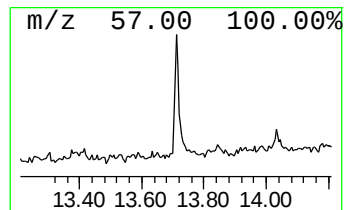
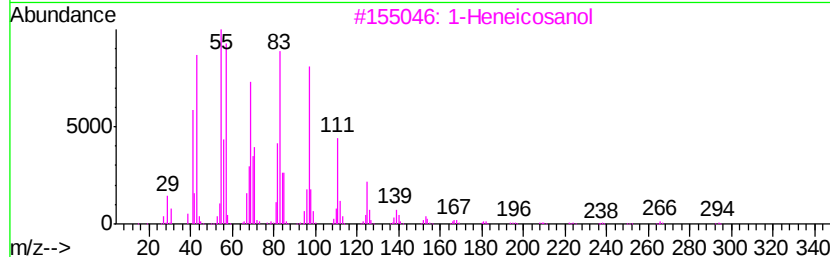
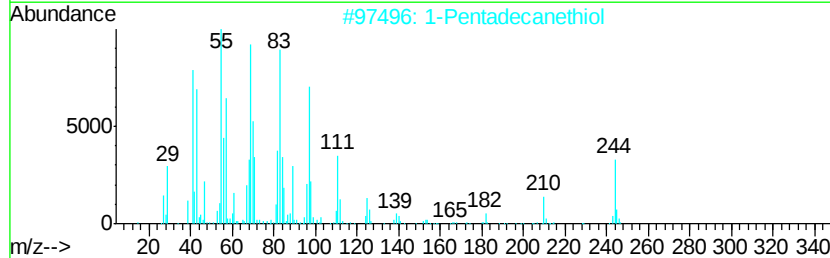
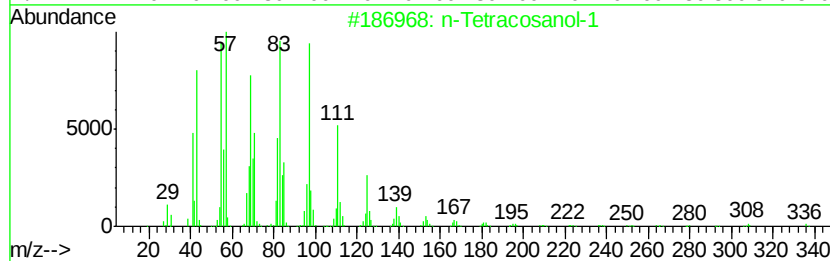
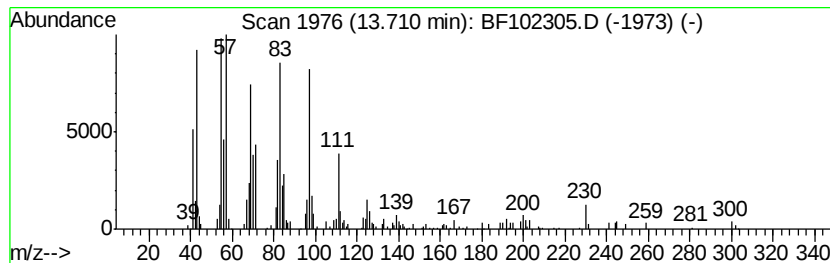
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 n-Tetracosanol-1 Concentration Rank 5

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 13.71 | 2.87 ng | 144664 | Chrysene-d12     | 13.87 |

| Hit# | of | Tentative ID       | MW  | MolForm | CAS#        | Qual |
|------|----|--------------------|-----|---------|-------------|------|
| 1    | 5  | n-Tetracosanol-1   | 354 | C24H50O | 000506-51-4 | 94   |
| 2    |    | 1-Pentadecanethiol | 244 | C15H32S | 025276-70-4 | 93   |
| 3    |    | 1-Heneicosanol     | 312 | C21H44O | 015594-90-8 | 91   |
| 4    |    | 1-Nonadecene       | 266 | C19H38  | 018435-45-5 | 91   |
| 5    |    | 1-Docosene         | 308 | C22H44  | 001599-67-3 | 90   |



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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF012218.M  
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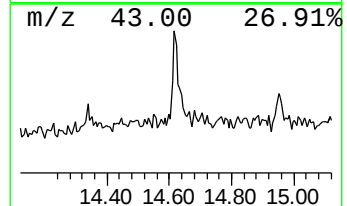
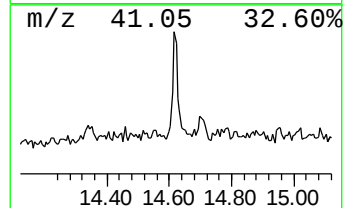
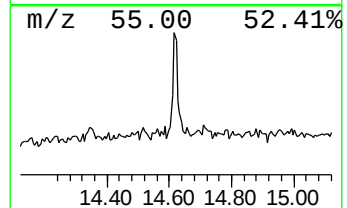
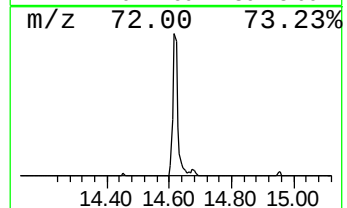
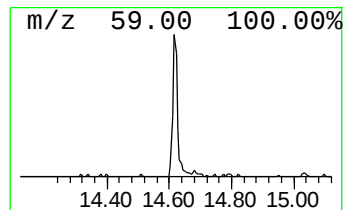
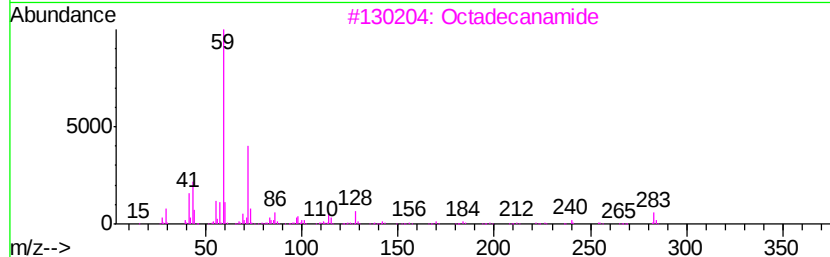
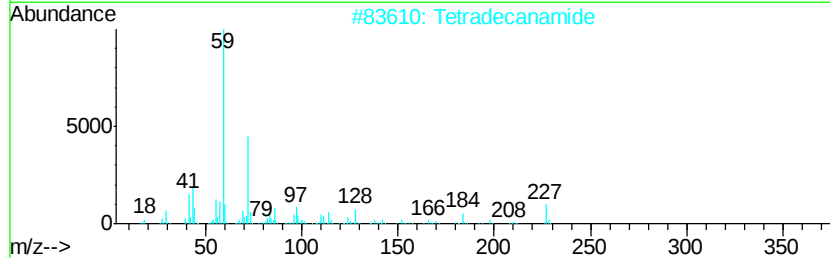
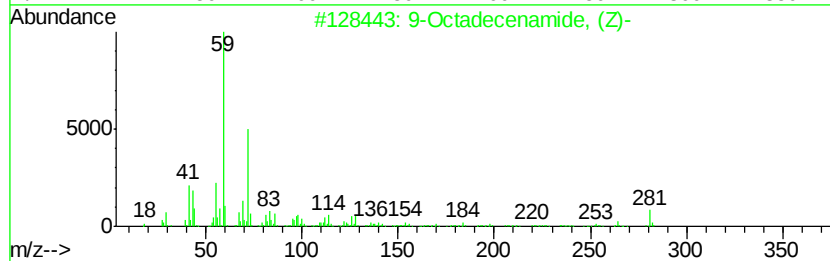
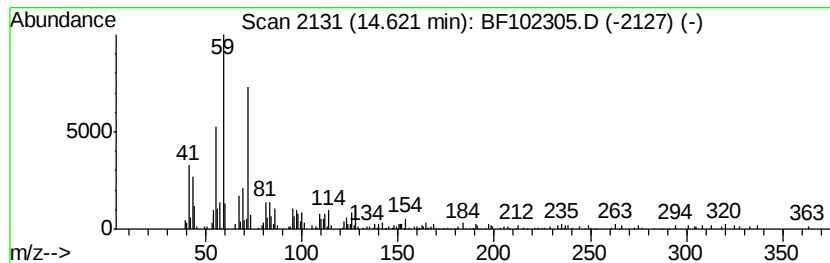
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 4

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 14.62 | 3.56 ng | 157910 | Perylene-d12     | 15.29 |

| Hit# of | 5 | Tentative ID           | MW  | MolForm  | CAS#        | Qual |
|---------|---|------------------------|-----|----------|-------------|------|
| 1       |   | 9-Octadecenamide, (Z)- | 281 | C18H35NO | 000301-02-0 | 87   |
| 2       |   | Tetradecanamide        | 227 | C14H29NO | 000638-58-4 | 78   |
| 3       |   | Octadecanamide         | 283 | C18H37NO | 000124-26-5 | 78   |
| 4       |   | Dodecanamide           | 199 | C12H25NO | 001120-16-7 | 76   |
| 5       |   | Octanamide             | 143 | C8H17NO  | 000629-01-6 | 59   |



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

| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |         |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|---------|------|
|                      |       |         |       |          | #                     | RT    | Resp    | Conc |
| 2-Pentanone, 4-hy... | 4.90  | 5.5     | ng    | 203902   | 1                     | 6.71  | 744086  | 20.0 |
| unknown6.48          | 6.48  | 73.6    | ng    | 2737570  | 1                     | 6.71  | 744086  | 20.0 |
| n-Tetracosanol-1     | 13.71 | 2.9     | ng    | 144664   | 5                     | 13.87 | 1008930 | 20.0 |
| 9-Octadecenamide,... | 14.62 | 3.6     | ng    | 157910   | 6                     | 15.29 | 886119  | 20.0 |