

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012218\  
 Data File : BF102300.D  
 Acq On : 22 Jan 2018 15:36  
 Operator : SJ/JU  
 Sample : J1228-23  
 Misc :  
 ALS Vial : 5 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 COMP-2

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         | 4.916       | 475           | 481         | 489          | rBV      | 167095         | 250507        | 6.95%           | 0.812%        |
| 2         | 5.328       | 545           | 551         | 554          | rBV      | 3042829        | 3208658       | 89.00%          | 10.399%       |
| 3         | 6.357       | 720           | 726         | 743          | rBV      | 2975409        | 3393644       | 94.13%          | 10.999%       |
| 4         | 6.487       | 743           | 748         | 751          | rBV      | 3237531        | 3325694       | 92.24%          | 10.778%       |
| 5         | 6.710       | 783           | 786         | 795          | rBV      | 948015         | 839168        | 23.28%          | 2.720%        |
| 6         | 6.869       | 809           | 813         | 816          | rBV      | 2871762        | 2564396       | 71.13%          | 8.311%        |
| 7         | 7.281       | 878           | 883         | 886          | rBV      | 2151730        | 2103785       | 58.35%          | 6.818%        |
| 8         | 7.992       | 1000          | 1004        | 1013         | rBV      | 1185720        | 1154952       | 32.03%          | 3.743%        |
| 9         | 9.075       | 1182          | 1188        | 1191         | rBV      | 3781330        | 3605380       | 100.00%         | 11.685%       |
| 10        | 9.469       | 1251          | 1255        | 1258         | rBV      | 353061         | 319870        | 8.87%           | 1.037%        |
| 11        | 9.681       | 1287          | 1291        | 1295         | rBV      | 79198          | 67615         | 1.88%           | 0.219%        |
| 12        | 9.745       | 1298          | 1302        | 1312         | rVB      | 1354074        | 1253909       | 34.78%          | 4.064%        |
| 13        | 10.181      | 1372          | 1376        | 1378         | rVB2     | 80578          | 76921         | 2.13%           | 0.249%        |
| 14        | 10.463      | 1419          | 1424        | 1426         | rBV      | 78756          | 75599         | 2.10%           | 0.245%        |
| 15        | 10.539      | 1430          | 1437        | 1440         | rBV      | 2018277        | 2048827       | 56.83%          | 6.640%        |
| 16        | 10.651      | 1453          | 1456        | 1461         | rBV      | 72502          | 78959         | 2.19%           | 0.256%        |
| 17        | 11.233      | 1551          | 1555        | 1557         | rBV      | 1273949        | 1160665       | 32.19%          | 3.762%        |
| 18        | 11.251      | 1557          | 1558        | 1562         | rVB      | 97474          | 64296         | 1.78%           | 0.208%        |
| 19        | 11.763      | 1642          | 1645        | 1649         | rBV2     | 53582          | 52995         | 1.47%           | 0.172%        |
| 20        | 12.439      | 1754          | 1760        | 1763         | rBV      | 95377          | 83719         | 2.32%           | 0.271%        |
| 21        | 12.669      | 1796          | 1799        | 1801         | rVB      | 73990          | 58731         | 1.63%           | 0.190%        |
| 22        | 12.716      | 1805          | 1807        | 1812         | rVB3     | 41872          | 44040         | 1.22%           | 0.143%        |
| 23        | 12.816      | 1820          | 1824        | 1828         | rBV      | 2696727        | 2781002       | 77.13%          | 9.013%        |
| 24        | 13.710      | 1973          | 1976        | 1981         | rBV      | 283428         | 277228        | 7.69%           | 0.898%        |
| 25        | 13.863      | 1997          | 2002        | 2006         | rBV      | 848345         | 909724        | 25.23%          | 2.948%        |
| 26        | 14.616      | 2127          | 2130        | 2136         | rBV      | 203528         | 242042        | 6.71%           | 0.784%        |
| 27        | 15.292      | 2240          | 2245        | 2252         | rVB      | 611981         | 813004        | 22.55%          | 2.635%        |

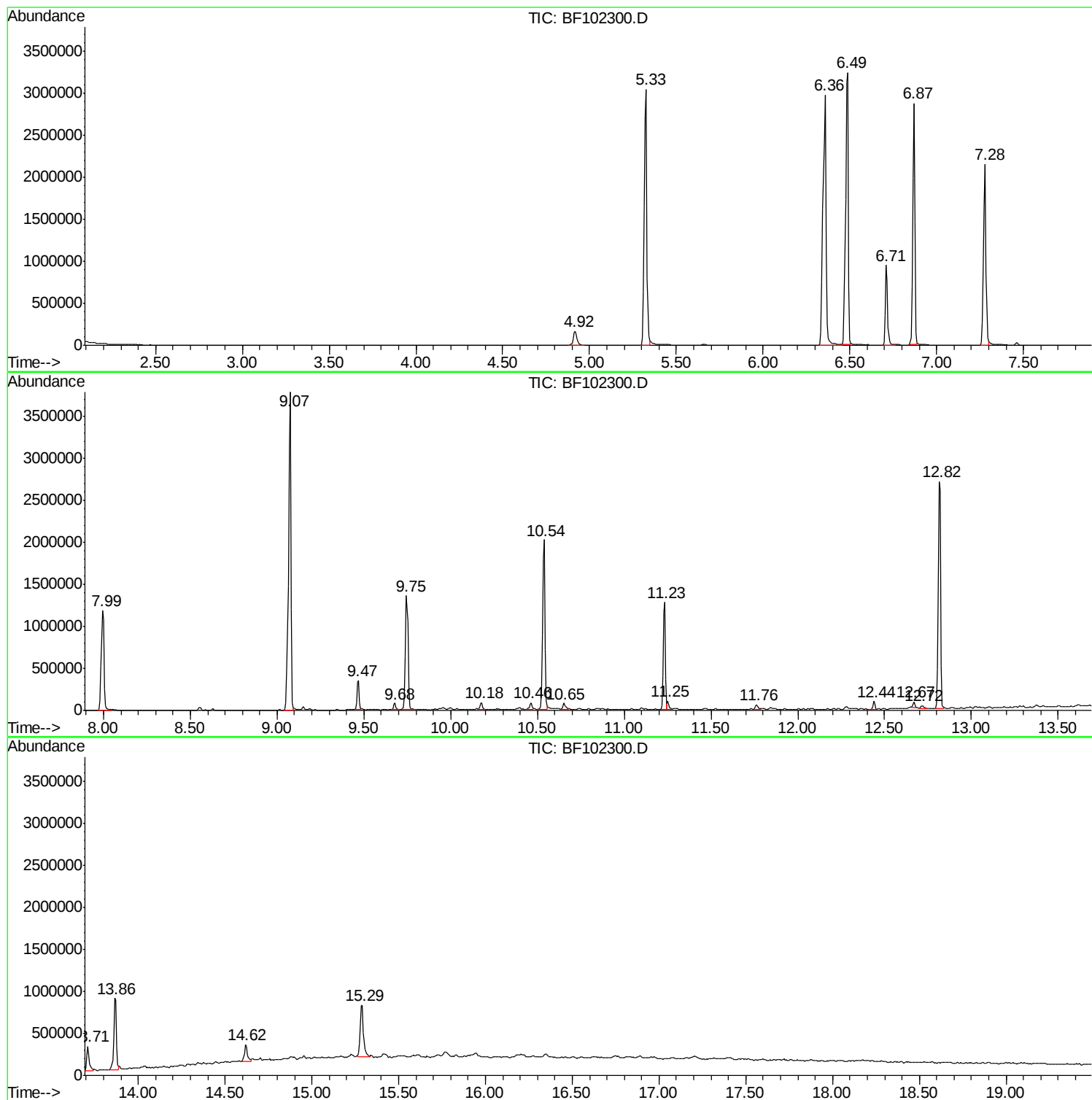
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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF012218.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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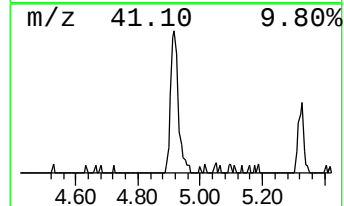
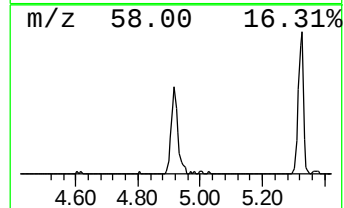
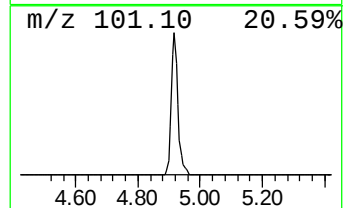
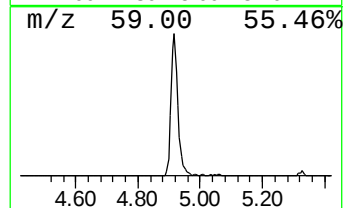
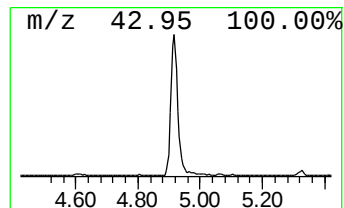
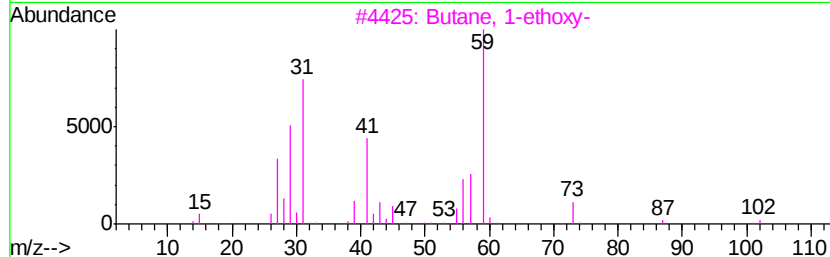
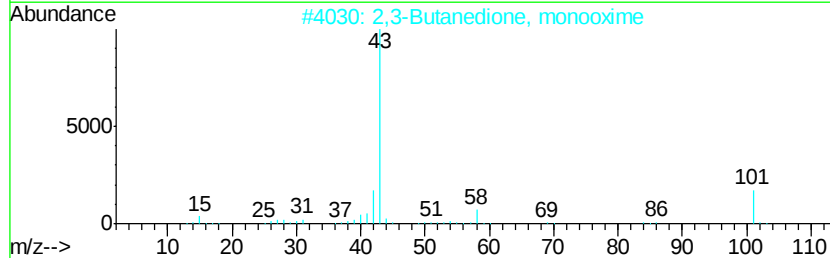
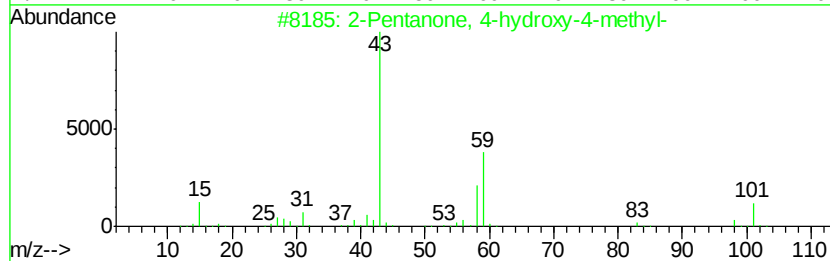
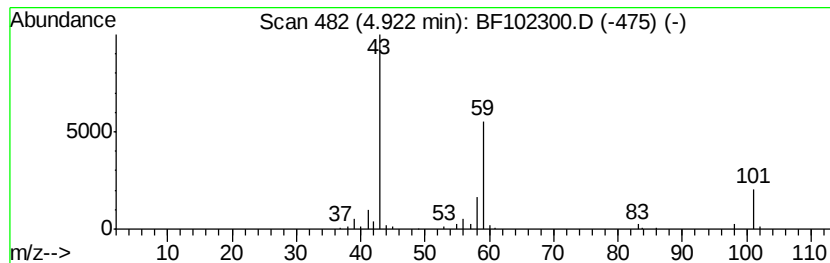
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF012218.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

| R.T. | EstConc | Area   | Relative to ISTD       | R.T. |
|------|---------|--------|------------------------|------|
| 4.92 | 5.97 ng | 250507 | 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 | 72   |
| 2    |    |   | 2,3-Butanedione, monooxime         | 101 | C4H7NO2 | 000057-71-6 | 9    |
| 3    |    |   | Butane, 1-ethoxy-                  | 102 | C6H14O  | 000628-81-9 | 9    |
| 4    |    |   | Morpholine, 4-methyl-              | 101 | C5H11NO | 000109-02-4 | 9    |
| 5    |    |   | (+)-4-Amino-4,5-dihydro-2(3H)-f... | 101 | C4H7NO2 | 016504-58-8 | 9    |



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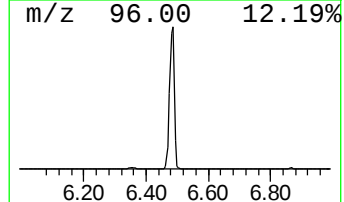
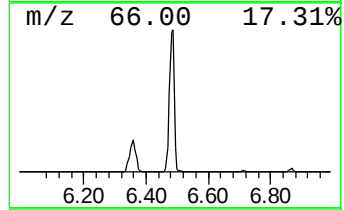
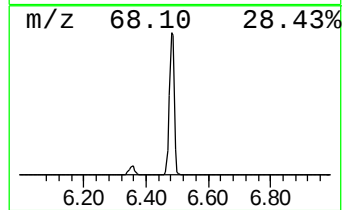
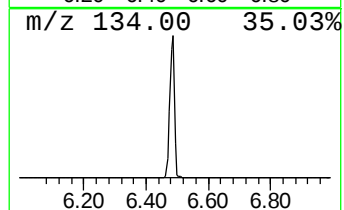
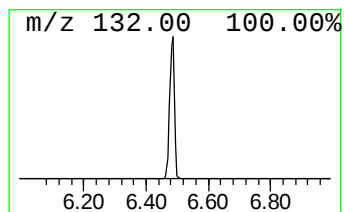
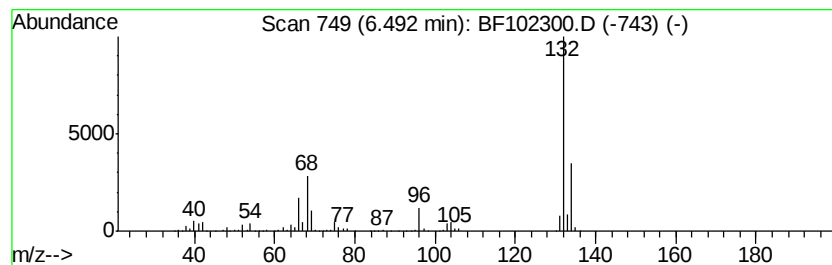
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF012218.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 2 unknown6.49 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.49 | 79.26 ng | 3325690 | 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 | 35   |
| 2    |    | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO   | 031357-76-3  | 17   |
| 3    |    | Tranvlcyproline-propionyl        | 189 | C12H15NO  | 1000123-86-3 | 12   |
| 4    |    | 1,3,5-Trifluorobenzene           | 132 | C6H3F3    | 000372-38-3  | 9    |
| 5    |    | 5-Fluoro-2-chloropyrimidine      | 132 | C4H2ClFN2 | 062802-42-0  | 9    |



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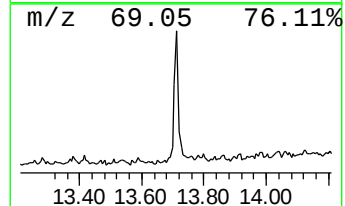
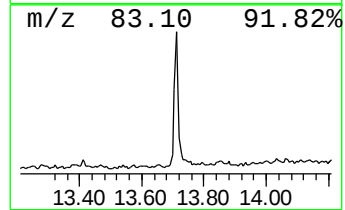
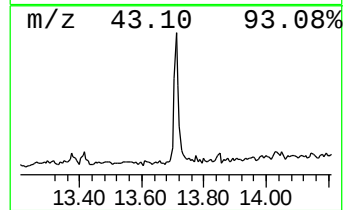
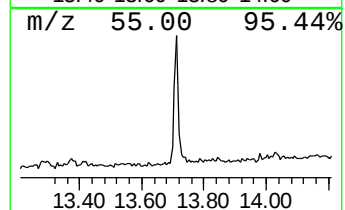
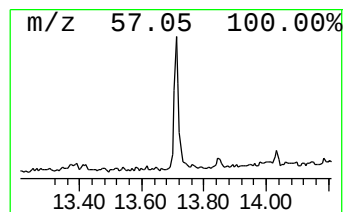
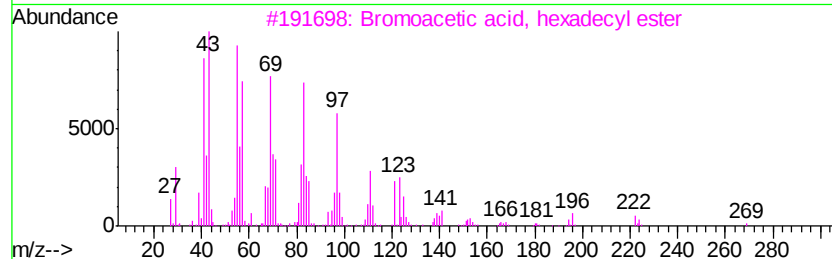
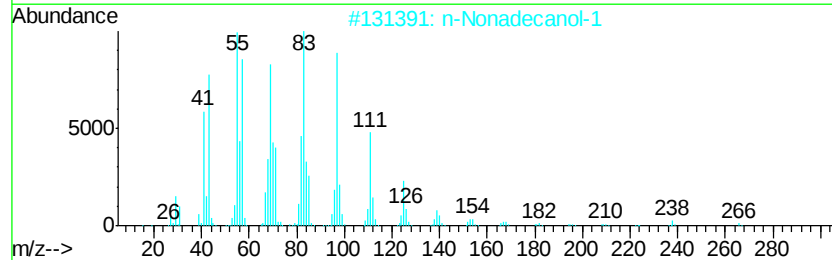
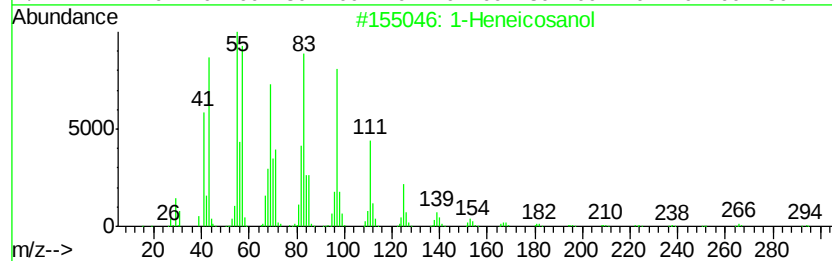
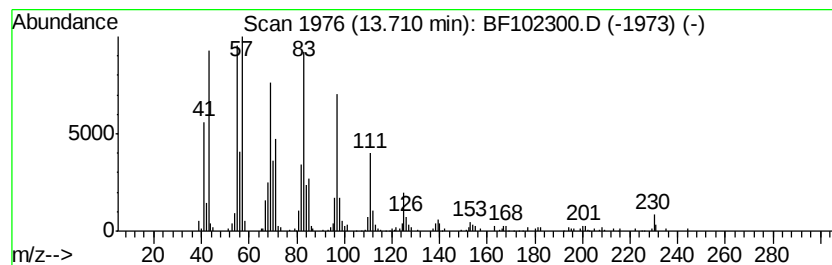
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 1-Heneicosanol Concentration Rank 3

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 13.71 | 6.09 ng | 277228 | Chrysene-d12     | 13.87 |

| Hit# | of | Tentative ID                      | MW  | MolForm    | CAS#         | Qual |
|------|----|-----------------------------------|-----|------------|--------------|------|
| 1    | 5  | 1-Heneicosanol                    | 312 | C21H44O    | 015594-90-8  | 93   |
| 2    |    | n-Nonadecanol-1                   | 284 | C19H40O    | 001454-84-8  | 93   |
| 3    |    | Bromoacetic acid, hexadecyl ester | 362 | C18H35BrO2 | 005454-48-8  | 93   |
| 4    |    | 1-Heptacosanol                    | 396 | C27H56O    | 002004-39-9  | 91   |
| 5    |    | Heptadecyl trifluoroacetate       | 352 | C19H35F3O2 | 1000351-87-0 | 91   |



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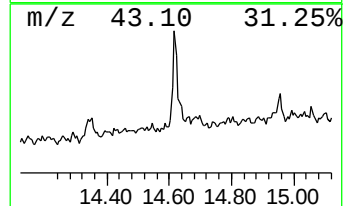
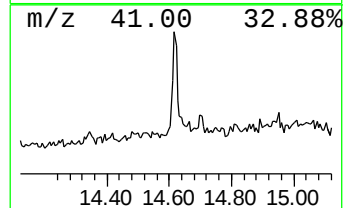
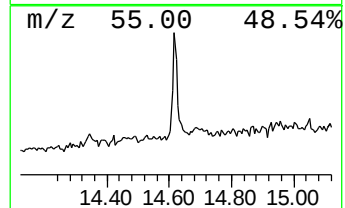
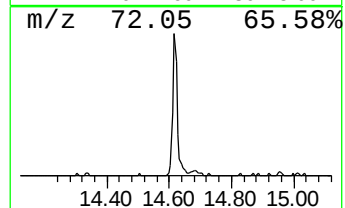
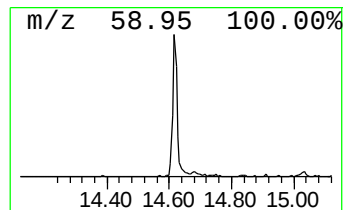
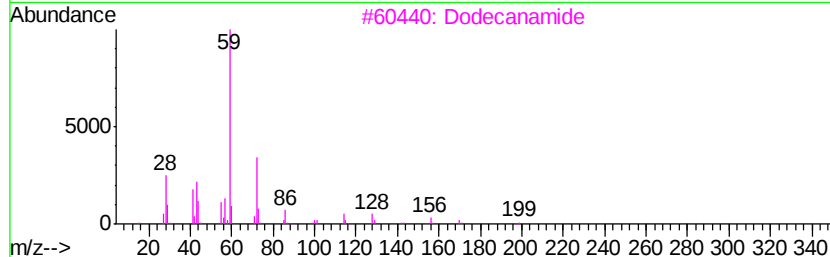
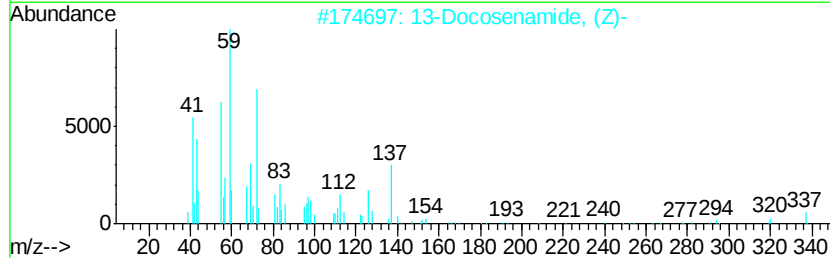
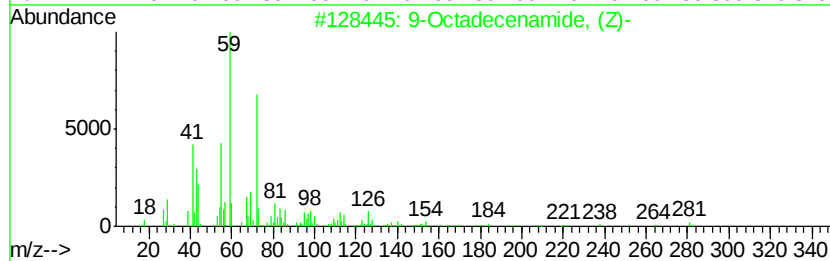
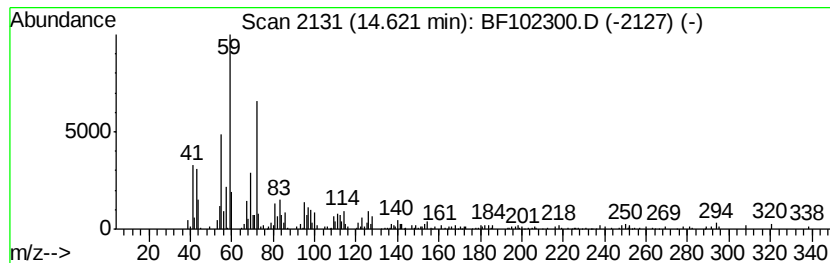
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 14.62 | 5.95 ng | 242042 | Perylene-d12     | 15.29 |

| Hit# | of | Tentative ID           | MW  | MolForm  | CAS#        | Qual |
|------|----|------------------------|-----|----------|-------------|------|
| 1    | 5  | 9-Octadecenamide, (Z)- | 281 | C18H35NO | 000301-02-0 | 95   |
| 2    |    | 13-Docosenamide, (Z)-  | 337 | C22H43NO | 000112-84-5 | 90   |
| 3    |    | Dodecanamide           | 199 | C12H25NO | 001120-16-7 | 70   |
| 4    |    | Octanamide             | 143 | C8H17NO  | 000629-01-6 | 53   |
| 5    |    | Hexadecanamide         | 255 | C16H33NO | 000629-54-9 | 53   |



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| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                      |       |         |       |          | #                     | RT    | Resp   | Conc |
| 2-Pentanone, 4-hy... | 4.92  | 6.0     | ng    | 250507   | 1                     | 6.71  | 839168 | 20.0 |
| unknown6.49          | 6.49  | 79.3    | ng    | 3325690  | 1                     | 6.71  | 839168 | 20.0 |
| 1-Heneicosanol       | 13.71 | 6.1     | ng    | 277228   | 5                     | 13.87 | 909724 | 20.0 |
| 9-Octadecenamide,... | 14.62 | 6.0     | ng    | 242042   | 6                     | 15.29 | 813004 | 20.0 |