

Data Path : Z:\SVOASRV\HPCHEM1\BNA\_F\DATA\BF053119\  
 Data File : BF114734.D  
 Acq On : 1 Jun 2019 3:40  
 Operator : HP/JU  
 Sample : K3104-04  
 Misc :  
 ALS Vial : 19 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 SUMP

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:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF052919.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         | 3.657       | 263           | 267         | 278          | rVB2     | 58073          | 118277        | 1.10%           | 0.177%        |
| 2         | 4.881       | 468           | 475         | 485          | rVB2     | 169818         | 240842        | 2.24%           | 0.361%        |
| 3         | 5.304       | 542           | 547         | 550          | rBV      | 3288979        | 3192827       | 29.70%          | 4.787%        |
| 4         | 6.322       | 716           | 720         | 723          | rBV      | 2684160        | 2105430       | 19.59%          | 3.157%        |
| 5         | 6.463       | 739           | 744         | 747          | rBV      | 6455332        | 5826117       | 54.20%          | 8.735%        |
| 6         | 6.692       | 780           | 783         | 787          | rBV      | 2700061        | 2407985       | 22.40%          | 3.610%        |
| 7         | 6.857       | 806           | 811         | 814          | rBV      | 7873971        | 7849621       | 73.02%          | 11.769%       |
| 8         | 7.257       | 873           | 879         | 882          | rBV      | 5765953        | 6311341       | 58.71%          | 9.462%        |
| 9         | 7.975       | 997           | 1001        | 1004         | rBV      | 3633955        | 2979389       | 27.71%          | 4.467%        |
| 10        | 9.051       | 1178          | 1184        | 1187         | rBV      | 10148231       | 10750124      | 100.00%         | 16.117%       |
| 11        | 9.439       | 1246          | 1250        | 1256         | rBV      | 814615         | 676753        | 6.30%           | 1.015%        |
| 12        | 9.722       | 1293          | 1298        | 1306         | rBV      | 3646635        | 3224310       | 29.99%          | 4.834%        |
| 13        | 10.504      | 1426          | 1431        | 1434         | rBV      | 4435430        | 4280392       | 39.82%          | 6.417%        |
| 14        | 11.192      | 1544          | 1548        | 1552         | rBV      | 3352255        | 2876970       | 26.76%          | 4.313%        |
| 15        | 11.733      | 1637          | 1640        | 1650         | rBV      | 376824         | 469358        | 4.37%           | 0.704%        |
| 16        | 12.515      | 1770          | 1773        | 1783         | rBV      | 158495         | 207226        | 1.93%           | 0.311%        |
| 17        | 12.780      | 1813          | 1818        | 1821         | rBV      | 8441817        | 8612158       | 80.11%          | 12.912%       |
| 18        | 13.680      | 1967          | 1971        | 1977         | rBV2     | 189604         | 244963        | 2.28%           | 0.367%        |
| 19        | 13.815      | 1989          | 1994        | 1997         | rBV      | 2282394        | 2209877       | 20.56%          | 3.313%        |
| 20        | 14.915      | 2178          | 2181        | 2186         | rVB      | 107951         | 114936        | 1.07%           | 0.172%        |
| 21        | 15.198      | 2224          | 2229        | 2236         | rBV      | 1657462        | 1878170       | 17.47%          | 2.816%        |
| 22        | 15.262      | 2237          | 2240        | 2245         | rVB      | 108830         | 122132        | 1.14%           | 0.183%        |

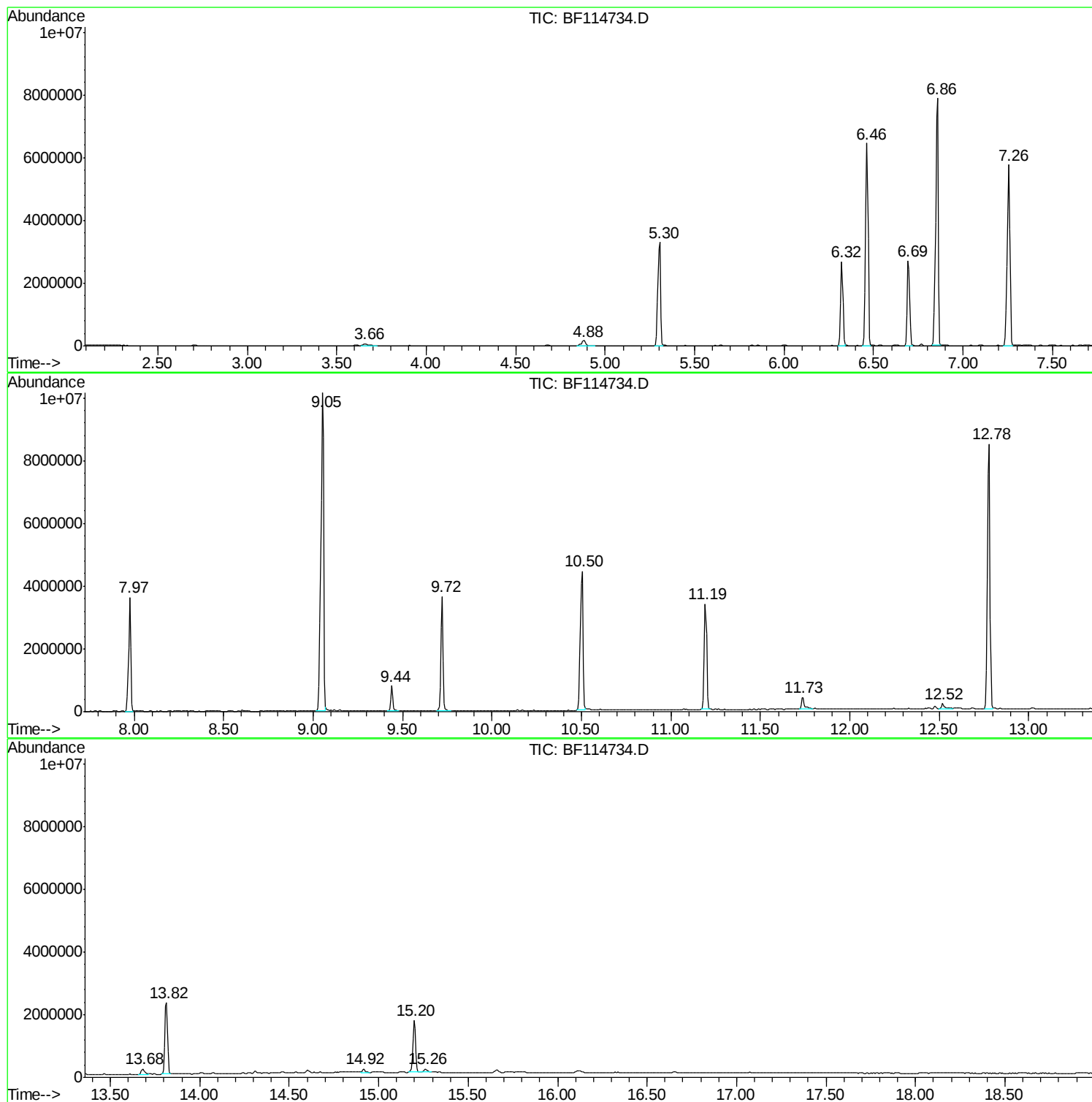
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF052919.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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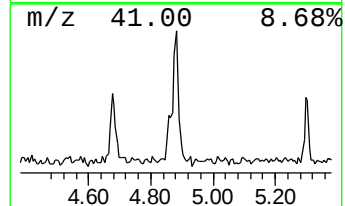
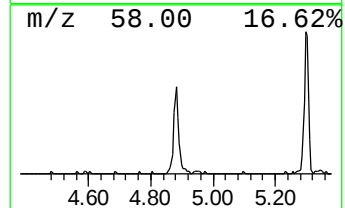
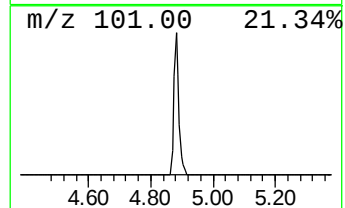
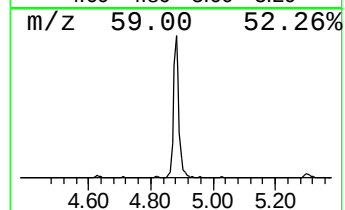
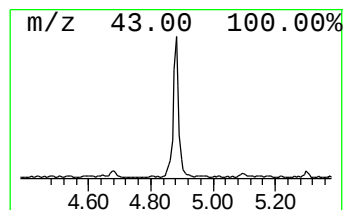
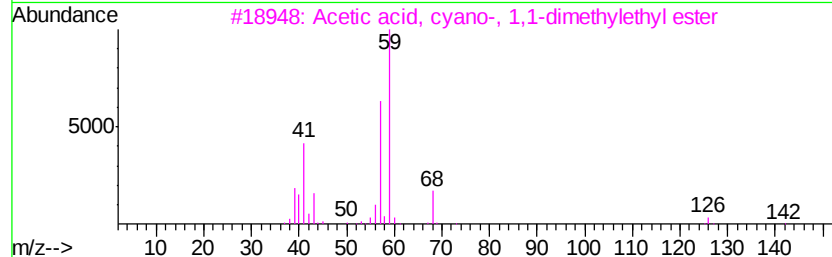
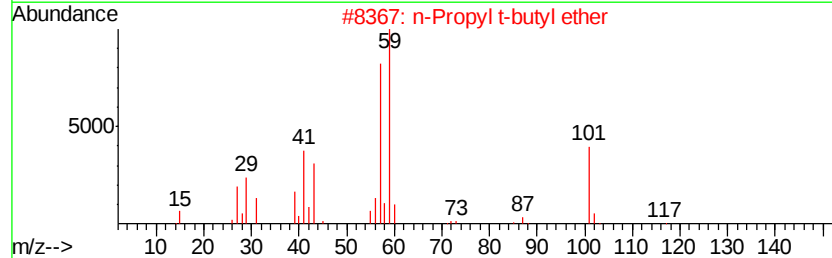
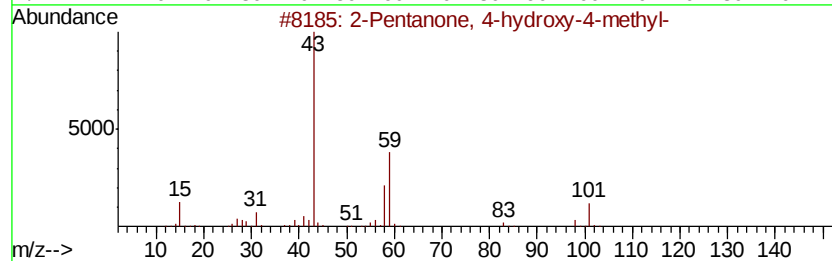
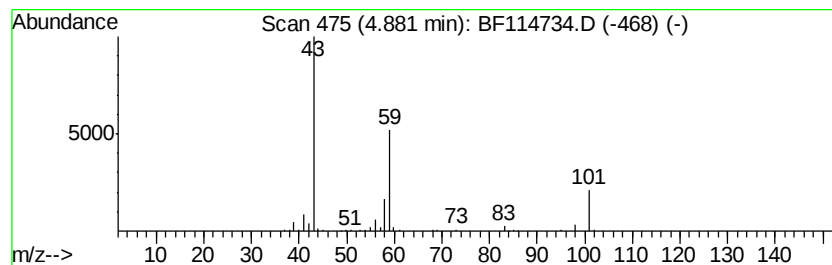
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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 5

| R.T. | EstConc | Area   | Relative to ISTD       | R.T. |
|------|---------|--------|------------------------|------|
| 4.88 | 2.00 ng | 240842 | 1,4-Dichlorobenzene-d4 | 6.69 |

| Hit# | of | 5 | Tentative ID                         | MW  | MolForm  | CAS#         | Qual |
|------|----|---|--------------------------------------|-----|----------|--------------|------|
| 1    |    |   | 2-Pentanone, 4-hydroxy-4-methyl-     | 116 | C6H12O2  | 000123-42-2  | 45   |
| 2    |    |   | n-Propyl t-butyl ether               | 116 | C7H16O   | 1000334-81-9 | 33   |
| 3    |    |   | Acetic acid, cyano-, 1,1-dimethyl... | 141 | C7H11NO2 | 001116-98-9  | 23   |
| 4    |    |   | 3-Hydroxy-3-methyl-2-butanone        | 102 | C5H10O2  | 000115-22-0  | 17   |
| 5    |    |   | Morpholine, 4-methyl-                | 101 | C5H11NO  | 000109-02-4  | 9    |



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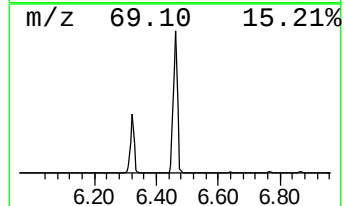
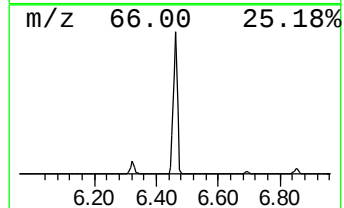
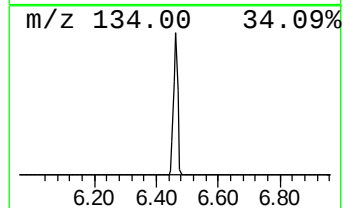
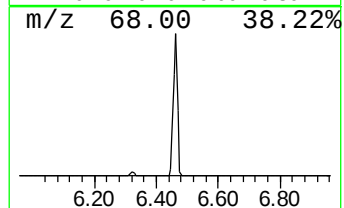
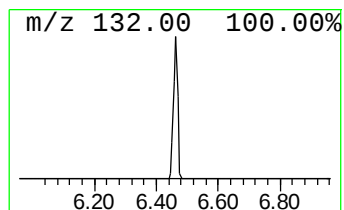
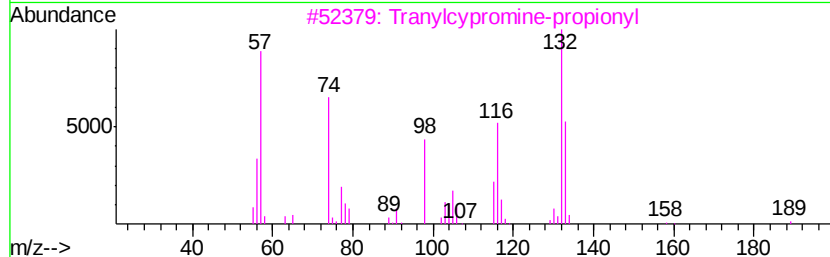
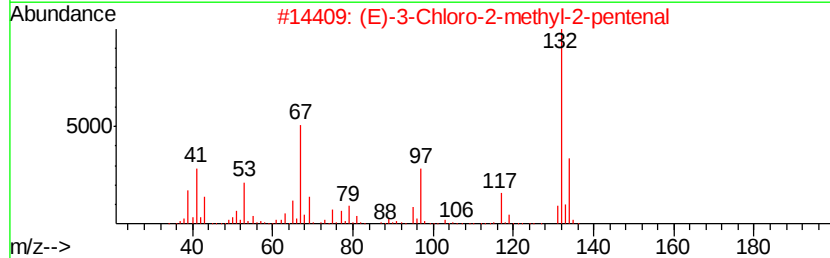
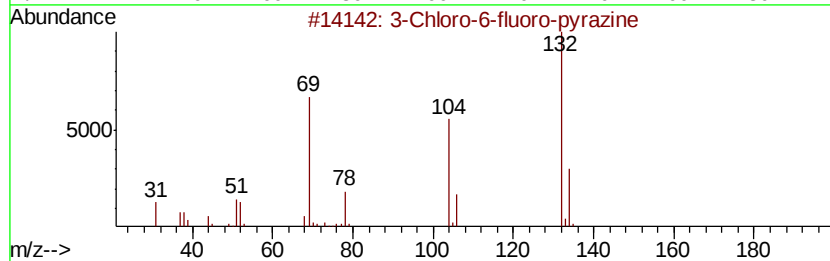
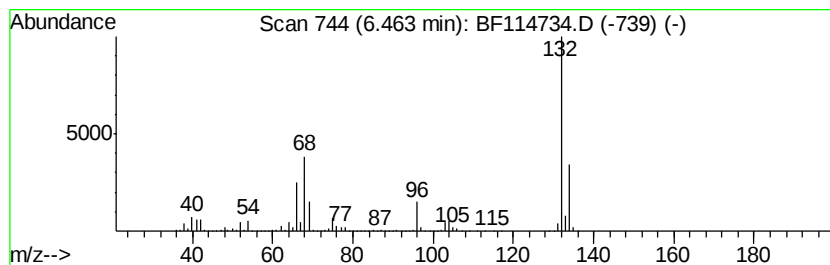
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TIC Integration Parameters: LSCINT.P

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Peak Number 2 unknown6.46 Concentration Rank 2

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.46 | 48.39 ng | 5826120 | 1,4-Dichlorobenzene-d4 | 6.69 |

| 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  | 16   |
| 3    |    | Tranvlcypropine-propionyl           | 189 | C12H15NO  | 1000123-86-3 | 12   |
| 4    |    | 5-Aminoindole                       | 132 | C8H8N2    | 005192-03-0  | 12   |
| 5    |    | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12    | 028749-81-7  | 9    |



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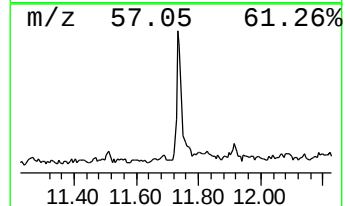
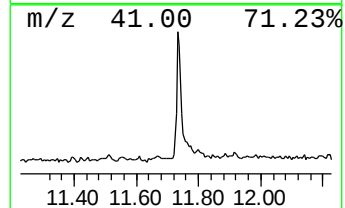
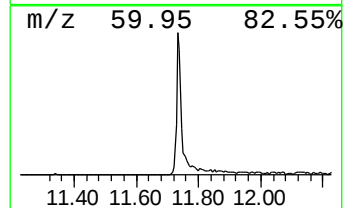
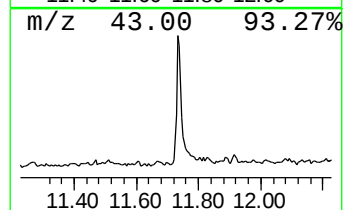
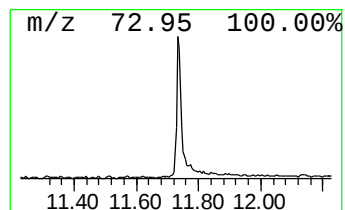
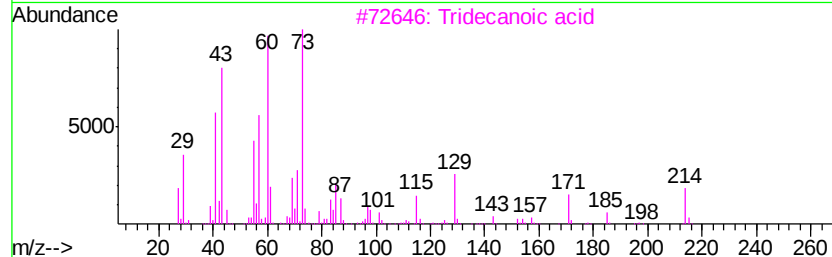
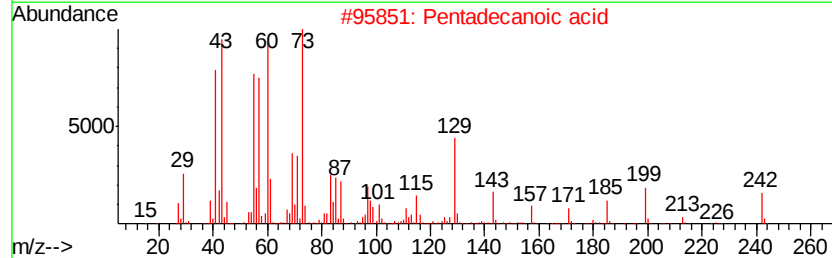
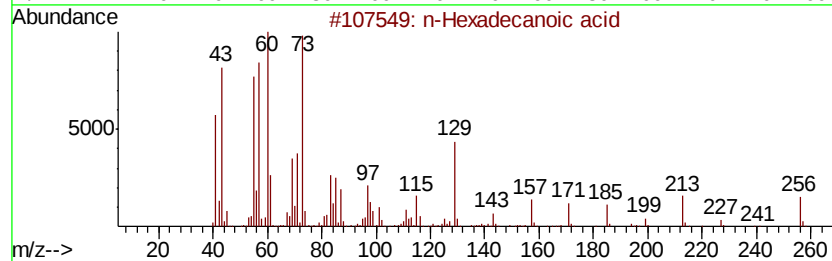
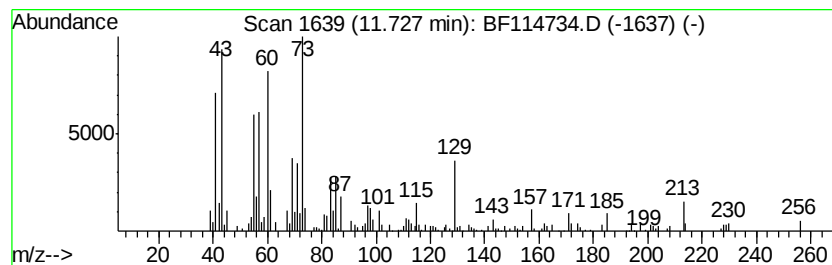
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 11.73 | 3.26 ng | 469358 | Phenanthrene-d10 | 11.19 |

| 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  | 94   |
| 3       |   | Tridecanoic acid                    | 214 | C13H26O2  | 000638-53-9  | 93   |
| 4       |   | n-Decanoic acid                     | 172 | C10H20O2  | 000334-48-5  | 68   |
| 5       |   | Sulfurous acid, octadecyl 2-prop... | 376 | C21H44O3S | 1000309-12-7 | 20   |



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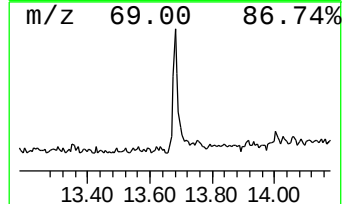
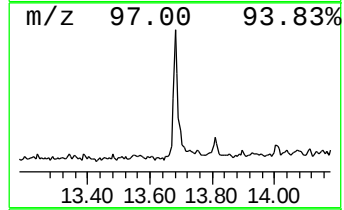
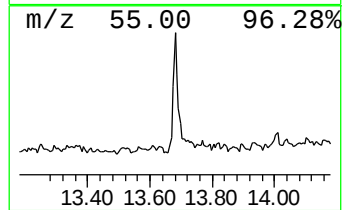
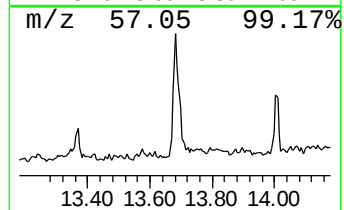
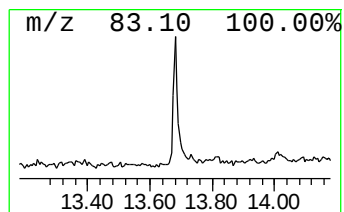
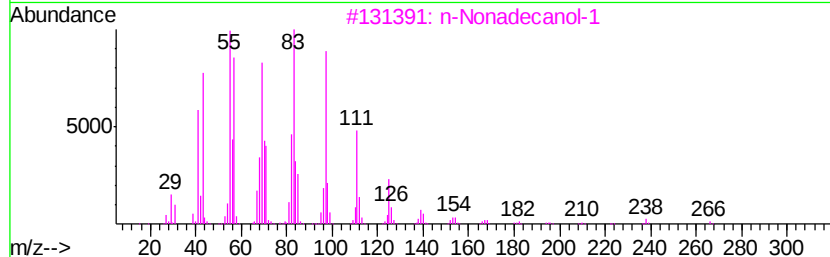
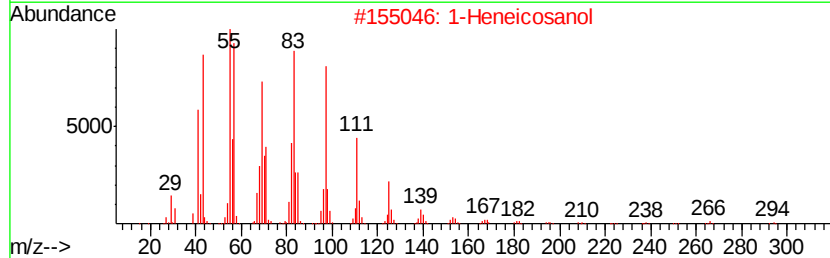
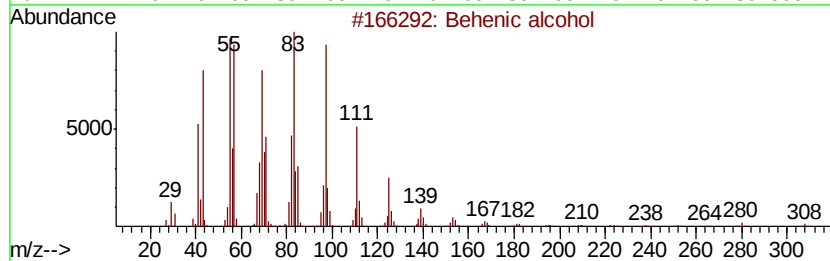
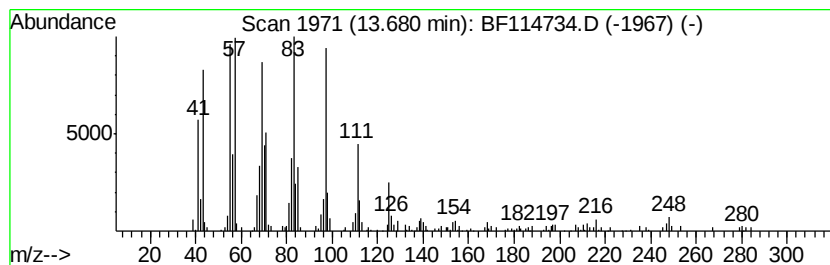
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Peak Number 5 Behenic alcohol Concentration Rank 4

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 13.68 | 2.22 ng | 244963 | Chrysene-d12     | 13.82 |

| Hit# of | 5 | Tentative ID     | MW  | MolForm | CAS#        | Qual |
|---------|---|------------------|-----|---------|-------------|------|
| 1       |   | Behenic alcohol  | 326 | C22H46O | 000661-19-8 | 95   |
| 2       |   | 1-Heneicosanol   | 312 | C21H44O | 015594-90-8 | 95   |
| 3       |   | n-Nonadecanol-1  | 284 | C19H40O | 001454-84-8 | 94   |
| 4       |   | 3-Eicosene, (E)- | 280 | C20H40  | 074685-33-9 | 93   |
| 5       |   | n-Tetracosanol-1 | 354 | C24H50O | 000506-51-4 | 91   |



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| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |         |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|---------|------|
|                      |       |         |       |          | #                     | RT    | Resp    | Conc |
| 2-Pentanone, 4-hy... | 4.88  | 2.0     | ng    | 240842   | 1                     | 6.69  | 2407990 | 20.0 |
| unknown6.46          | 6.46  | 48.4    | ng    | 5826120  | 1                     | 6.69  | 2407990 | 20.0 |
| n-Hexadecanoic acid  | 11.73 | 3.3     | ng    | 469358   | 4                     | 11.19 | 2876970 | 20.0 |
| Behenic alcohol      | 13.68 | 2.2     | ng    | 244963   | 5                     | 13.82 | 2209880 | 20.0 |