

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080717\  
 Data File : BF097437.D  
 Acq On : 7 Aug 2017 18:58  
 Operator : SJ/JU  
 Sample : I4623-02  
 Misc :  
 ALS Vial : 13 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 TEC-BS

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF072517.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         | 4.522       | 461           | 465         | 477          | rBV      | 84393          | 136466        | 11.72%          | 1.187%        |
| 2         | 5.004       | 544           | 547         | 571          | rBV      | 606254         | 910990        | 78.24%          | 7.924%        |
| 3         | 6.081       | 727           | 730         | 745          | rBV      | 887415         | 1098914       | 94.38%          | 9.558%        |
| 4         | 6.187       | 745           | 748         | 757          | rVB      | 988453         | 1061798       | 91.19%          | 9.235%        |
| 5         | 6.410       | 783           | 786         | 796          | rBV      | 618209         | 554291        | 47.60%          | 4.821%        |
| 6         | 6.563       | 809           | 812         | 822          | rBV      | 606655         | 578383        | 49.67%          | 5.031%        |
| 7         | 6.981       | 880           | 883         | 899          | rBV      | 802168         | 795143        | 68.29%          | 6.916%        |
| 8         | 7.145       | 908           | 911         | 920          | rVB3     | 11024          | 17676         | 1.52%           | 0.154%        |
| 9         | 7.692       | 1001          | 1004        | 1010         | rBV      | 848242         | 717697        | 61.64%          | 6.242%        |
| 10        | 8.769       | 1184          | 1187        | 1191         | rBV      | 1323874        | 1164383       | 100.00%         | 10.127%       |
| 11        | 8.910       | 1207          | 1211        | 1215         | rVB      | 24295          | 22087         | 1.90%           | 0.192%        |
| 12        | 9.175       | 1253          | 1256        | 1265         | rBV      | 218192         | 177576        | 15.25%          | 1.545%        |
| 13        | 9.433       | 1297          | 1300        | 1310         | rVB      | 711117         | 679317        | 58.34%          | 5.908%        |
| 14        | 9.892       | 1375          | 1378        | 1381         | rVB      | 30206          | 23645         | 2.03%           | 0.206%        |
| 15        | 10.045      | 1398          | 1404        | 1411         | rBV3     | 8026           | 14275         | 1.23%           | 0.124%        |
| 16        | 10.222      | 1431          | 1434        | 1447         | rBV      | 675285         | 685158        | 58.84%          | 5.959%        |
| 17        | 10.363      | 1455          | 1458        | 1465         | rBV      | 40947          | 45935         | 3.95%           | 0.400%        |
| 18        | 10.804      | 1529          | 1533        | 1536         | rBV      | 20471          | 18380         | 1.58%           | 0.160%        |
| 19        | 10.910      | 1547          | 1551        | 1560         | rBV      | 614065         | 538239        | 46.23%          | 4.681%        |
| 20        | 11.127      | 1584          | 1588        | 1595         | rBV2     | 9008           | 14592         | 1.25%           | 0.127%        |
| 21        | 11.469      | 1641          | 1646        | 1649         | rBV      | 39613          | 37607         | 3.23%           | 0.327%        |
| 22        | 12.245      | 1776          | 1778        | 1781         | rBV      | 12277          | 13254         | 1.14%           | 0.115%        |
| 23        | 12.333      | 1790          | 1793        | 1797         | rVB3     | 16346          | 14969         | 1.29%           | 0.130%        |
| 24        | 12.492      | 1816          | 1820        | 1823         | rBV      | 1050723        | 990623        | 85.08%          | 8.616%        |
| 25        | 13.063      | 1913          | 1917        | 1922         | rBV2     | 15898          | 19277         | 1.66%           | 0.168%        |
| 26        | 13.427      | 1974          | 1979        | 1990         | rBV2     | 41212          | 96007         | 8.25%           | 0.835%        |
| 27        | 13.533      | 1993          | 1997        | 2004         | rBV      | 587470         | 543052        | 46.64%          | 4.723%        |
| 28        | 14.610      | 2176          | 2180        | 2184         | rBV5     | 12072          | 22841         | 1.96%           | 0.199%        |
| 29        | 14.780      | 2204          | 2209        | 2210         | rBV4     | 10904          | 18699         | 1.61%           | 0.163%        |
| 30        | 14.868      | 2220          | 2224        | 2229         | rBV      | 431143         | 466503        | 40.06%          | 4.057%        |
| 31        | 15.245      | 2285          | 2288        | 2294         | rVB4     | 12335          | 19536         | 1.68%           | 0.170%        |

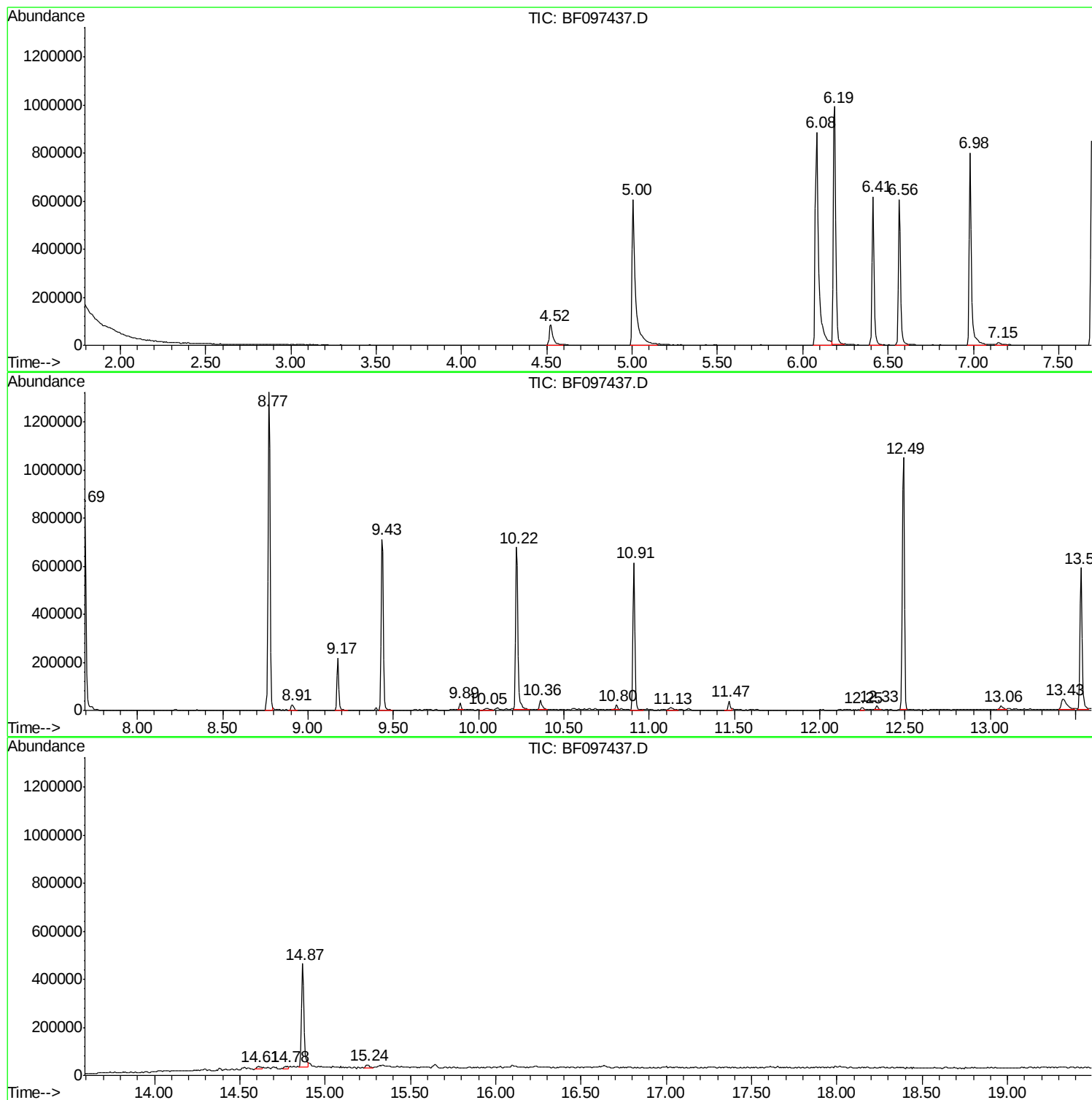
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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF072517.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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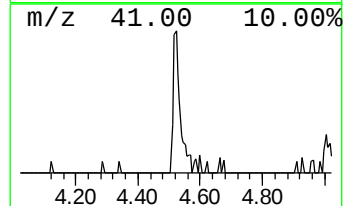
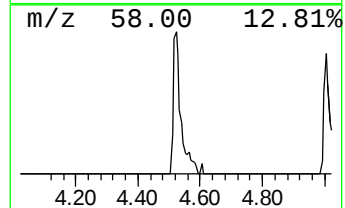
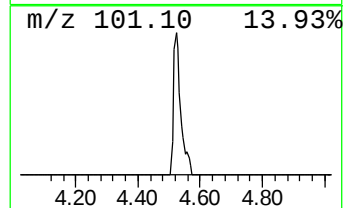
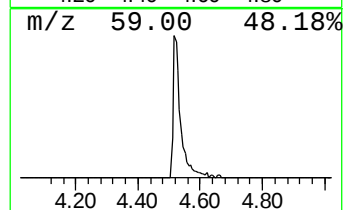
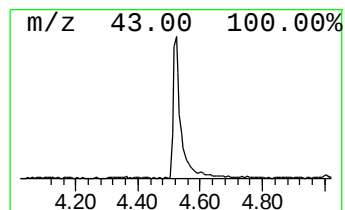
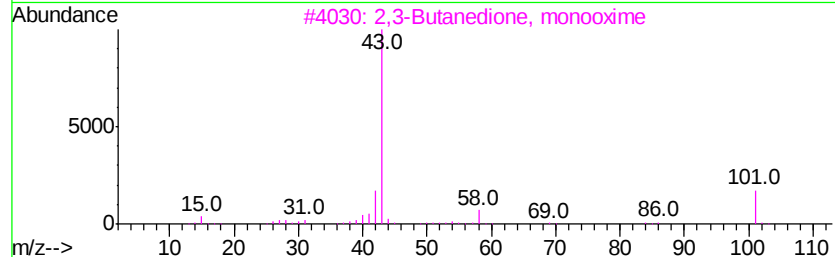
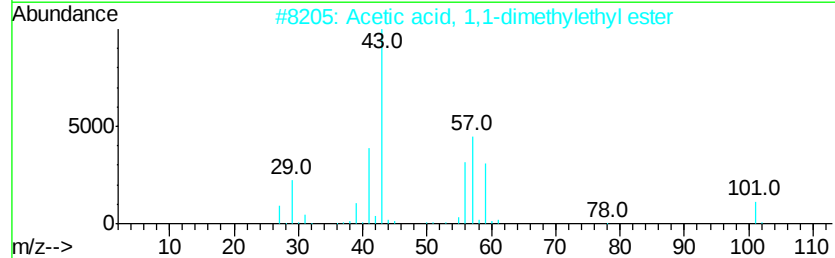
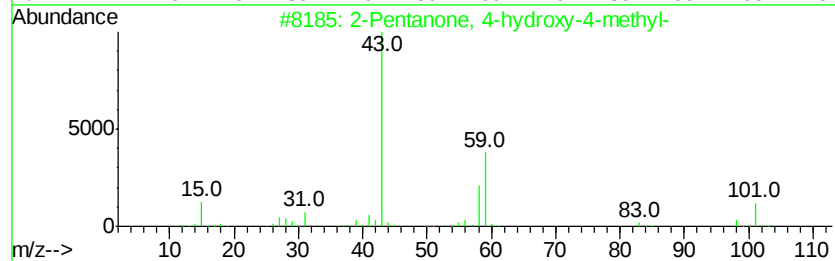
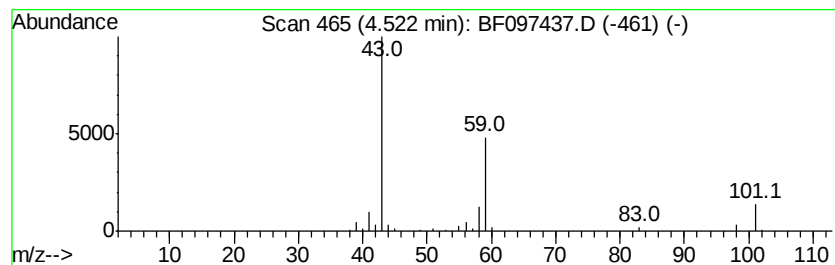
Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF072517.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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 3

| R.T. | EstConc | Area   | Relative to ISTD       | R.T. |
|------|---------|--------|------------------------|------|
| 4.52 | 4.92 ng | 136466 | 1,4-Dichlorobenzene-d4 | 6.41 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm   | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|-----------|-------------|------|
| 1    |    |   | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2   | 000123-42-2 | 56   |
| 2    |    |   | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2   | 000540-88-5 | 28   |
| 3    |    |   | 2,3-Butanedione, monooxime          | 101 | C4H7NO2   | 000057-71-6 | 9    |
| 4    |    |   | 1,3,4-Oxadiazole, 2-(acetyloxy)-... | 172 | C7H12N2O3 | 066398-57-0 | 9    |
| 5    |    |   | Butanoic acid, 4-amino-3-hydroxy... | 119 | C4H9NO3   | 000924-49-2 | 9    |



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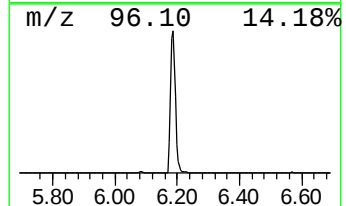
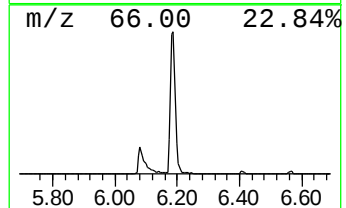
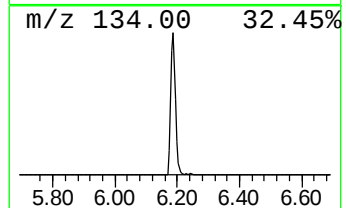
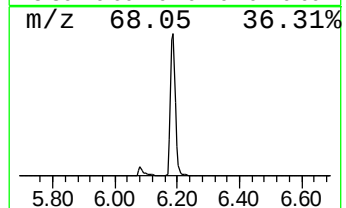
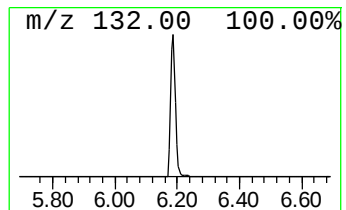
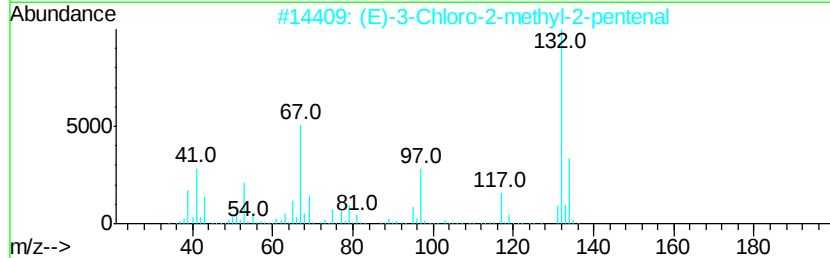
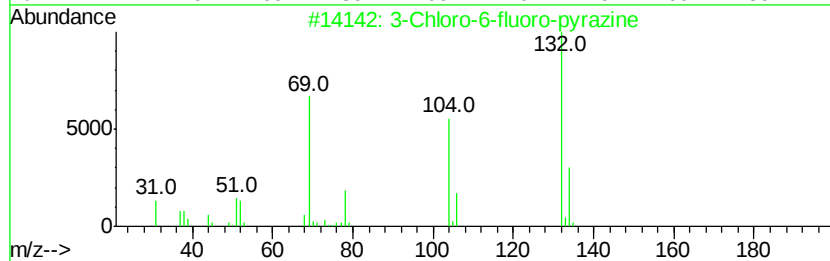
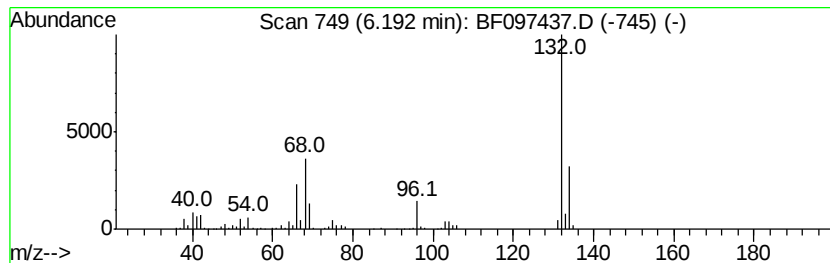
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Peak Number 2 unknown6.19 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.19 | 38.31 ng | 1061800 | 1,4-Dichlorobenzene-d4 | 6.41 |

| 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    |    | Tranvlcypropine-propionyl        | 189 | C12H15NO  | 1000123-86-3 | 12   |
| 4    |    | 5-Aminoindole                    | 132 | C8H8N2    | 005192-03-0  | 12   |
| 5    |    | 4-Methylpyrrolo[1,2-a]pyrazine   | 132 | C8H8N2    | 064608-60-2  | 9    |



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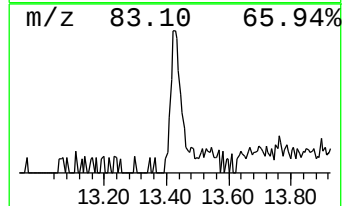
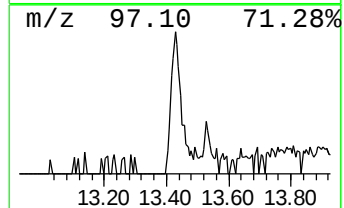
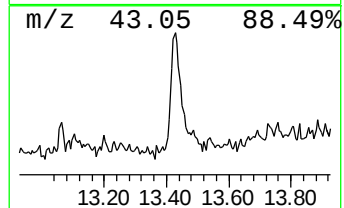
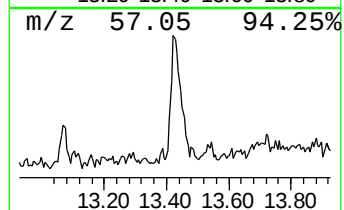
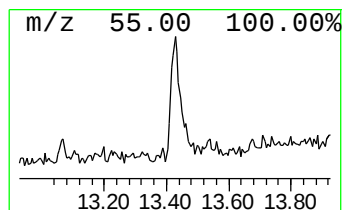
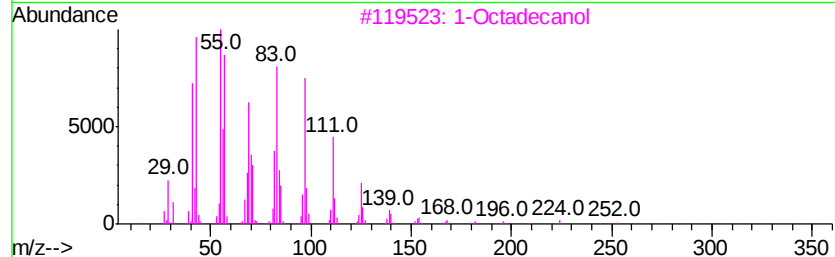
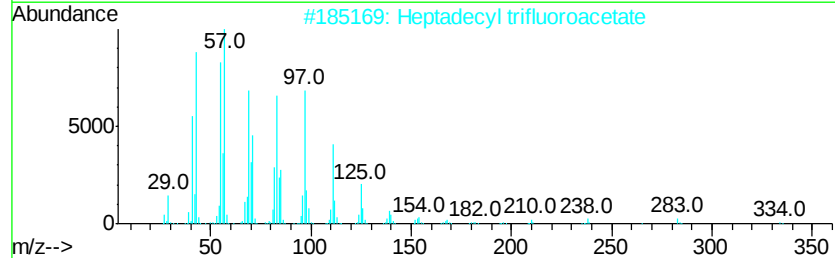
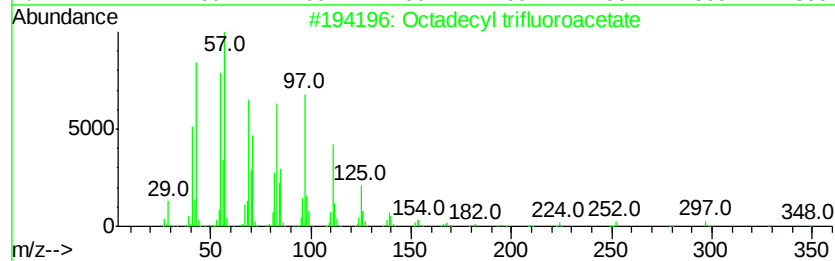
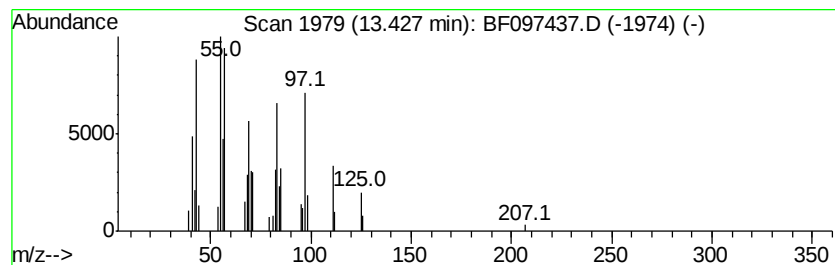
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Peak Number 4 Octadecyl trifluoroacetate Concentration Rank 4

| R.T.  | EstConc | Area  | Relative to ISTD | R.T.  |
|-------|---------|-------|------------------|-------|
| 13.43 | 3.54 ng | 96007 | Chrysene-d12     | 13.53 |

| Hit# | of | 5 | Tentative ID                       | MW  | MolForm    | CAS#         | Qual |
|------|----|---|------------------------------------|-----|------------|--------------|------|
| 1    |    |   | Octadecyl trifluoroacetate         | 366 | C20H37F3O2 | 079392-43-1  | 91   |
| 2    |    |   | Heptadecyl trifluoroacetate        | 352 | C19H35F3O2 | 1000351-87-0 | 91   |
| 3    |    |   | 1-Octadecanol                      | 270 | C18H38O    | 000112-92-5  | 91   |
| 4    |    |   | Bromoacetic acid, tetradecyl ester | 334 | C16H31BrO2 | 018992-01-3  | 90   |
| 5    |    |   | n-Heptadecanol-1                   | 256 | C17H36O    | 001454-85-9  | 90   |



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| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                      |       |         |       |          | #                     | RT    | Resp   | Conc |
| 2-Pentanone, 4-hy... | 4.52  | 4.9     | ng    | 136466   | 1                     | 6.41  | 554291 | 20.0 |
| unknown6.19          | 6.19  | 38.3    | ng    | 1061800  | 1                     | 6.41  | 554291 | 20.0 |
| Octadecyl trifluo... | 13.43 | 3.5     | ng    | 96007    | 5                     | 13.53 | 543052 | 20.0 |