

Data Path : Z:\HPCHEM1\BNA F\DATA\BF022317\  
 Data File : BF093142.D  
 Acq On : 24 Feb 2017 10:39  
 Operator : SJ/MA  
 Sample : I1947-01  
 Misc :  
 ALS Vial : 38 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 022117-PRRT-E-D-M

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-BF013017.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         | 4.990       | 252           | 254         | 266          | rBV      | 299721         | 454957        | 11.86%          | 2.004%        |
| 2         | 5.424       | 291           | 292         | 301          | rVB      | 716224         | 1061201       | 27.67%          | 4.673%        |
| 3         | 6.476       | 382           | 384         | 393          | rBV      | 665808         | 701244        | 18.28%          | 3.088%        |
| 4         | 6.601       | 393           | 395         | 398          | rBV      | 1769695        | 1966189       | 51.26%          | 8.659%        |
| 5         | 6.841       | 413           | 416         | 418          | rBV      | 935997         | 877672        | 22.88%          | 3.865%        |
| 6         | 7.002       | 427           | 430         | 432          | rBV      | 2619751        | 3008487       | 78.44%          | 13.249%       |
| 7         | 7.413       | 463           | 466         | 468          | rBV      | 2563442        | 2473784       | 64.50%          | 10.894%       |
| 8         | 8.133       | 526           | 529         | 531          | rBV      | 1045893        | 1057705       | 27.58%          | 4.658%        |
| 9         | 9.207       | 620           | 623         | 625          | rBV      | 4199322        | 3835544       | 100.00%         | 16.891%       |
| 10        | 9.882       | 679           | 682         | 684          | rBV      | 1090829        | 982707        | 25.62%          | 4.328%        |
| 11        | 10.670      | 748           | 751         | 753          | rBV      | 866712         | 1058195       | 27.59%          | 4.660%        |
| 12        | 10.785      | 759           | 761         | 768          | rVB      | 32738          | 48098         | 1.25%           | 0.212%        |
| 13        | 11.356      | 809           | 811         | 814          | rBV2     | 591852         | 758024        | 19.76%          | 3.338%        |
| 14        | 12.762      | 932           | 934         | 937          | rBV      | 77826          | 83161         | 2.17%           | 0.366%        |
| 15        | 12.945      | 947           | 950         | 953          | rBV      | 2600699        | 2451306       | 63.91%          | 10.795%       |
| 16        | 13.471      | 994           | 996         | 998          | rBV      | 70179          | 58186         | 1.52%           | 0.256%        |
| 17        | 13.996      | 1040          | 1042        | 1045         | rBV      | 873727         | 774211        | 20.19%          | 3.409%        |
| 18        | 15.425      | 1164          | 1167        | 1173         | rBV      | 589635         | 725965        | 18.93%          | 3.197%        |
| 19        | 15.848      | 1201          | 1204        | 1210         | rVB      | 29542          | 51278         | 1.34%           | 0.226%        |
| 20        | 16.317      | 1242          | 1245        | 1248         | rVB2     | 29256          | 50967         | 1.33%           | 0.224%        |
| 21        | 16.865      | 1290          | 1293        | 1297         | rBV2     | 25720          | 59238         | 1.54%           | 0.261%        |
| 22        | 17.528      | 1346          | 1351        | 1356         | rVB      | 24265          | 66624         | 1.74%           | 0.293%        |
| 23        | 18.305      | 1414          | 1419        | 1423         | rVB5     | 15847          | 49854         | 1.30%           | 0.220%        |
| 24        | 19.231      | 1495          | 1500        | 1506         | rVB6     | 13314          | 53506         | 1.40%           | 0.236%        |

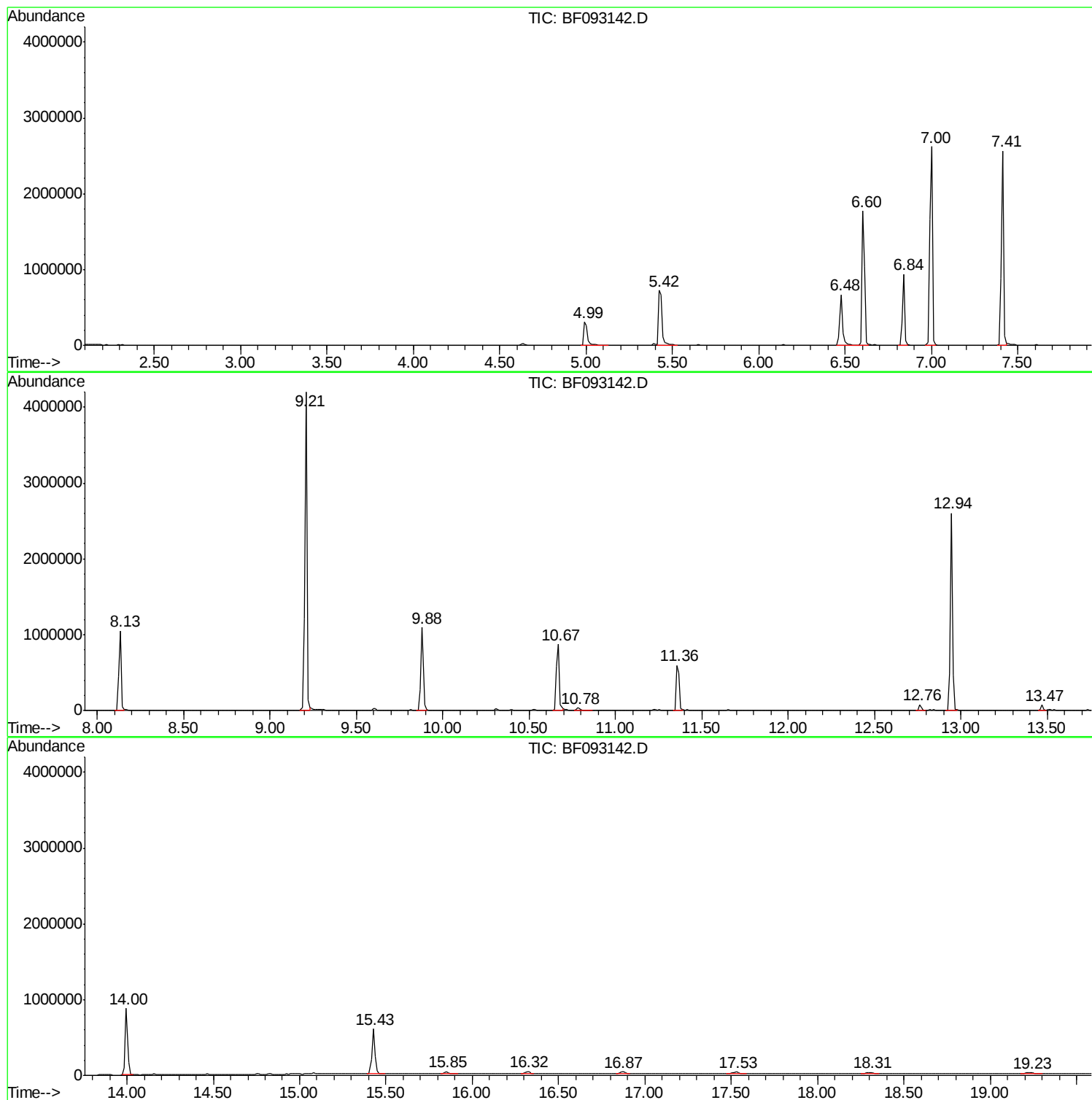
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022117-PRRT-E-D-M

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF013017.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P



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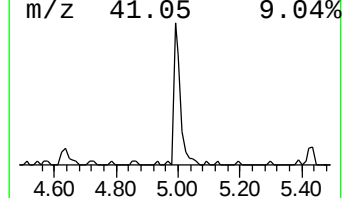
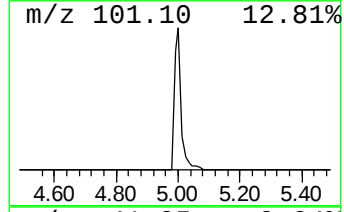
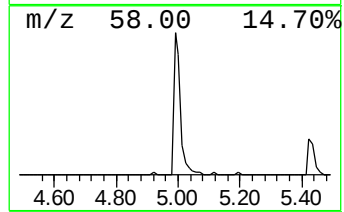
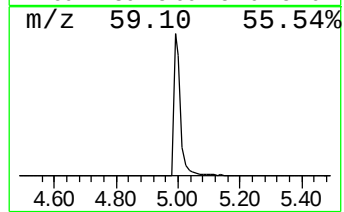
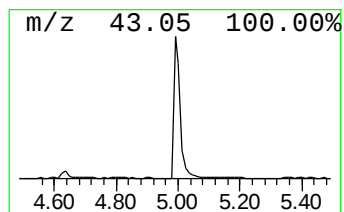
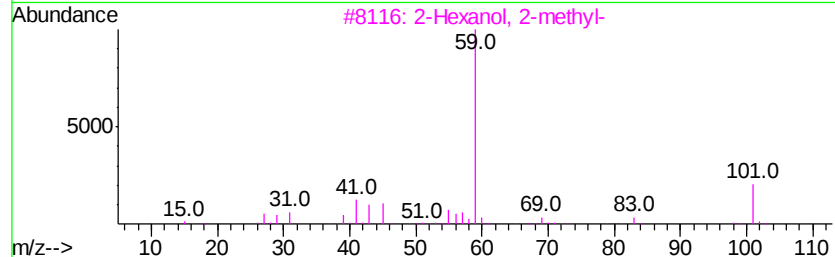
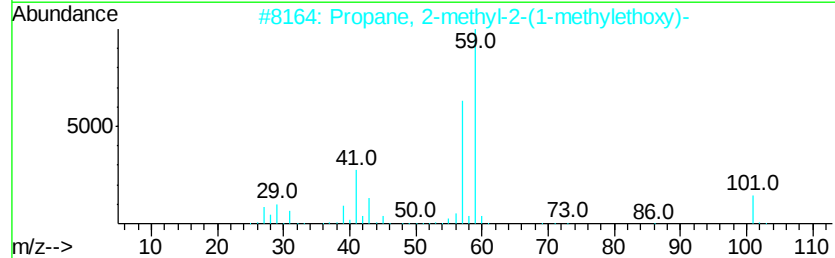
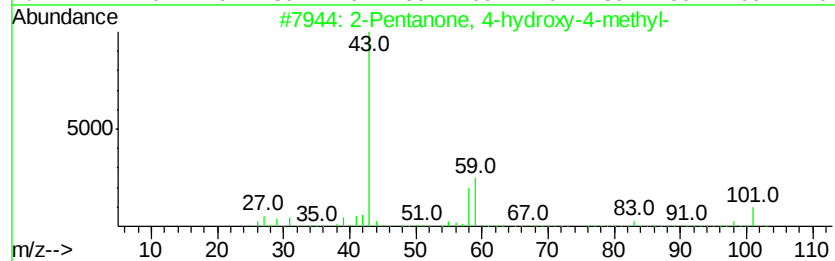
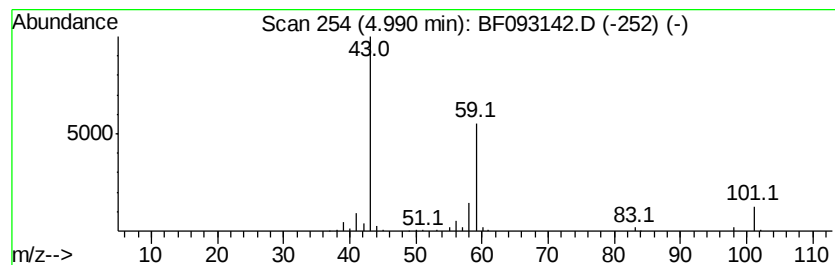
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TIC Integration Parameters: LSCINT.P

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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. |
|------|----------|--------|------------------------|------|
| 4.99 | 10.37 ng | 454957 | 1,4-Dichlorobenzene-d4 | 6.84 |

| Hit# | of | Tentative ID                          | MW  | MolForm | CAS#        | Qual |
|------|----|---------------------------------------|-----|---------|-------------|------|
| 1    | 5  | 2-Pentanone, 4-hydroxy-4-methyl-      | 116 | C6H12O2 | 000123-42-2 | 59   |
| 2    |    | Propane, 2-methyl-2-(1-methylethoxy)- | 116 | C7H16O  | 017348-59-3 | 42   |
| 3    |    | 2-Hexanol, 2-methyl-                  | 116 | C7H16O  | 000625-23-0 | 33   |
| 4    |    | 3-Heptanol, 4-methyl-                 | 130 | C8H18O  | 014979-39-6 | 33   |
| 5    |    | 3-Hexanol                             | 102 | C6H14O  | 000623-37-0 | 33   |



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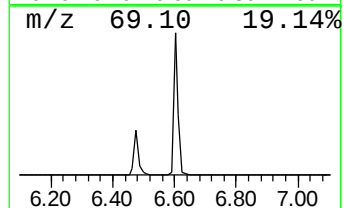
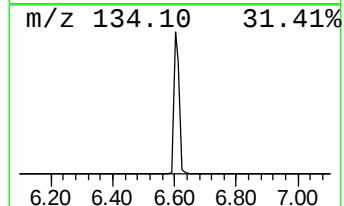
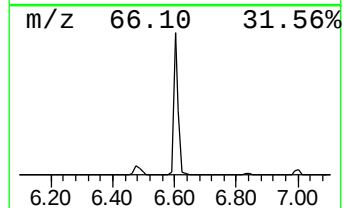
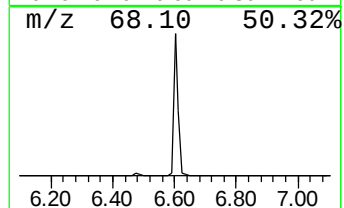
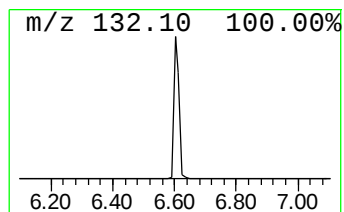
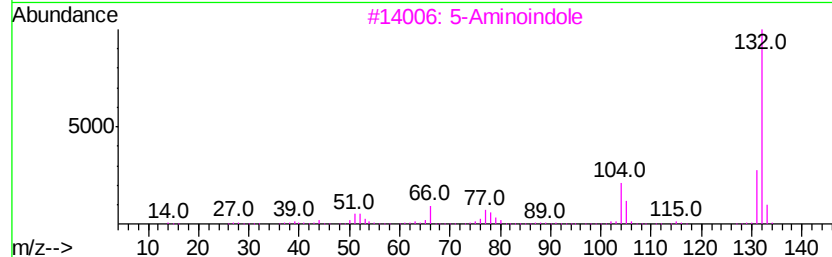
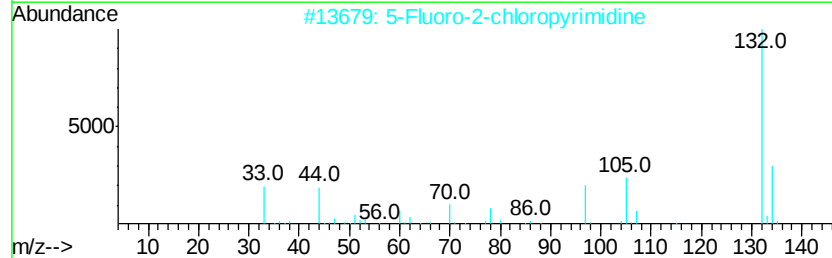
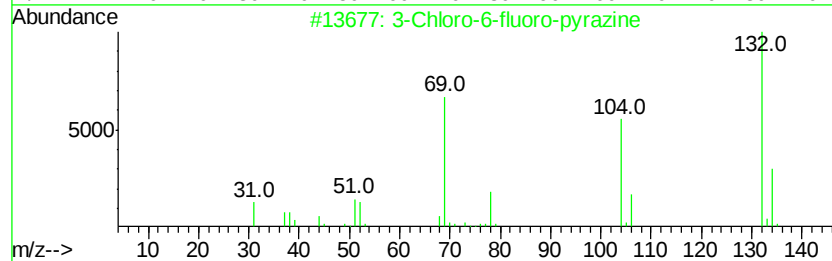
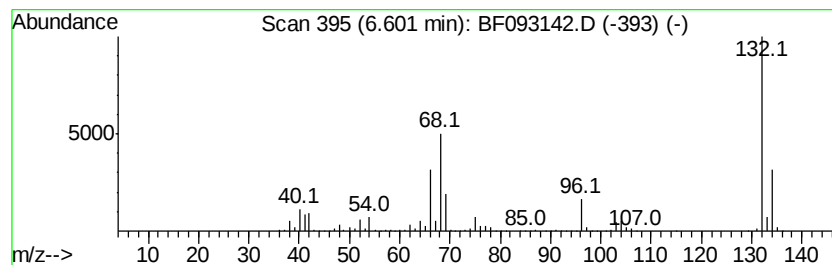
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Peak Number 2 unknown6.60 Concentration Rank 2

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.60 | 44.80 ng | 1966190 | 1,4-Dichlorobenzene-d4 | 6.84 |

| Hit# | of | Tentative ID                | MW  | MolForm   | CAS#         | Qual |
|------|----|-----------------------------|-----|-----------|--------------|------|
| 1    | 5  | 3-Chloro-6-fluoro-pyrazine  | 132 | C4H2ClFN2 | 1000146-10-7 | 27   |
| 2    |    | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0  | 12   |
| 3    |    | 5-Aminoindole               | 132 | C8H8N2    | 005192-03-0  | 12   |
| 4    |    | Tranylcypromine-propionyl   | 189 | C12H15NO  | 1000123-86-3 | 10   |
| 5    |    | 2-Cyclohexen-1-one          | 96  | C6H8O     | 000930-68-7  | 10   |



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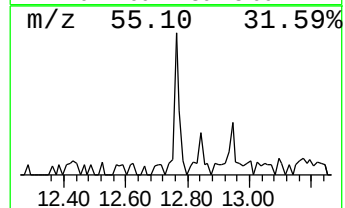
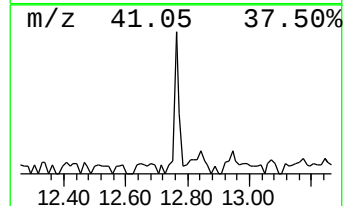
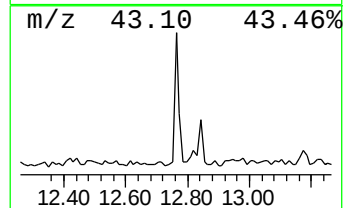
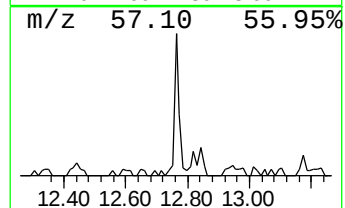
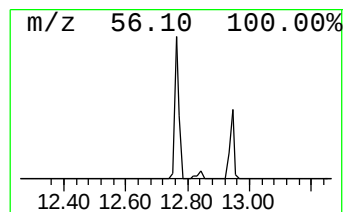
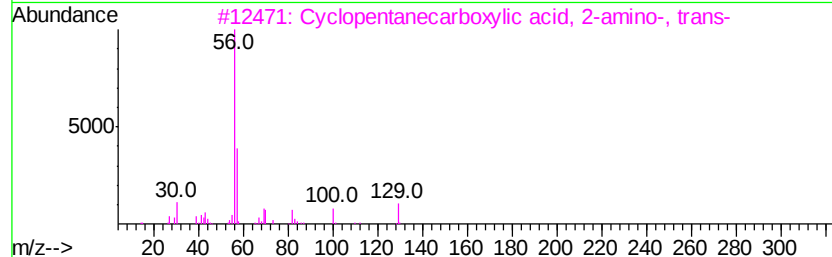
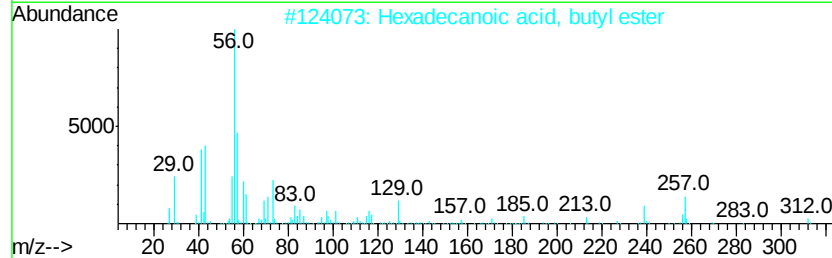
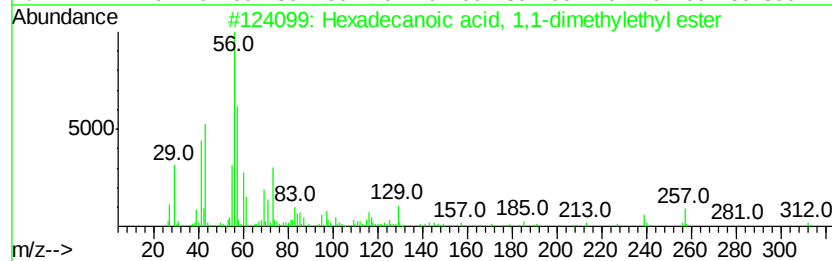
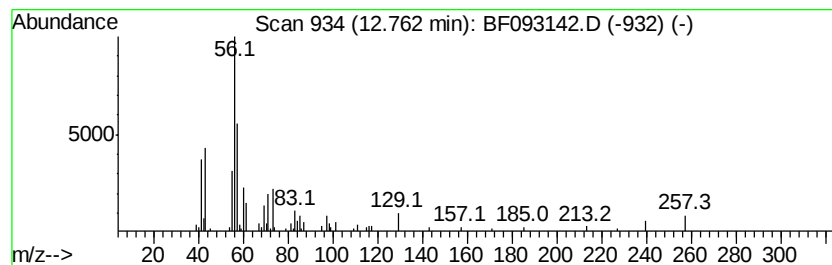
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Peak Number 4 Hexadecanoic acid, 1,1-dime... Concentration Rank 4

| R.T.  | EstConc | Area  | Relative to ISTD | R.T.  |
|-------|---------|-------|------------------|-------|
| 12.76 | 2.15 ng | 83161 | Chrysene-d12     | 14.00 |

| Hit# | of | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|-------------------------------------|-----|----------|-------------|------|
| 1    | 5  | Hexadecanoic acid, 1,1-dimethyle... | 312 | C20H40O2 | 031158-91-5 | 72   |
| 2    |    | Hexadecanoic acid, butyl ester      | 312 | C20H40O2 | 000111-06-8 | 43   |
| 3    |    | Cyclopentanecarboxylic acid, 2-a... | 129 | C6H11NO2 | 040482-05-1 | 38   |
| 4    |    | Cyclopentanecarboxylic acid, 2-a... | 129 | C6H11NO2 | 037910-65-9 | 38   |
| 5    |    | Decane, 2,2,3-trimethyl-            | 184 | C13H28   | 062338-09-4 | 37   |



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| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                      |       |         |       |          | #                     | RT    | Resp   | Conc |
| 2-Pentanone, 4-hy... | 4.99  | 10.4    | ng    | 454957   | 1                     | 6.84  | 877672 | 20.0 |
| unknown6.60          | 6.60  | 44.8    | ng    | 1966190  | 1                     | 6.84  | 877672 | 20.0 |
| Hexadecanoic acid... | 12.76 | 2.1     | ng    | 83161    | 5                     | 14.00 | 774211 | 20.0 |