

Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF120816\  
 Data File : BF091519.D  
 Acq On : 8 Dec 2016 22:57  
 Operator : UM/SJ  
 Sample : H5917-02  
 Misc :  
 ALS Vial : 12 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 URSMW-08

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-BF112916.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         | 4.996       | 234           | 237         | 244          | rVB      | 480870         | 635286        | 10.27%          | 1.496%        |
| 2         | 5.419       | 271           | 274         | 276          | rBV      | 2445839        | 2175722       | 35.17%          | 5.123%        |
| 3         | 6.447       | 362           | 364         | 367          | rBV      | 1225009        | 1419580       | 22.95%          | 3.343%        |
| 4         | 6.584       | 373           | 376         | 379          | rBV      | 3439594        | 3524181       | 56.97%          | 8.298%        |
| 5         | 6.813       | 394           | 396         | 399          | rBV      | 1408111        | 1475571       | 23.85%          | 3.474%        |
| 6         | 6.973       | 407           | 410         | 413          | rVB      | 3448905        | 3198498       | 51.70%          | 7.531%        |
| 7         | 7.385       | 443           | 446         | 448          | rBV      | 3208514        | 3339749       | 53.99%          | 7.864%        |
| 8         | 8.105       | 506           | 509         | 511          | rBV      | 2474922        | 2223691       | 35.95%          | 5.236%        |
| 9         | 9.179       | 600           | 603         | 606          | rBV      | 5011061        | 4962591       | 80.22%          | 11.685%       |
| 10        | 9.853       | 659           | 662         | 664          | rBV      | 2665986        | 2336297       | 37.77%          | 5.501%        |
| 11        | 10.642      | 728           | 731         | 734          | rBV      | 3572360        | 3773214       | 60.99%          | 8.884%        |
| 12        | 11.339      | 789           | 792         | 794          | rBV      | 2257709        | 2430436       | 39.29%          | 5.723%        |
| 13        | 11.865      | 836           | 838         | 841          | rBV2     | 193757         | 283037        | 4.58%           | 0.666%        |
| 14        | 12.574      | 897           | 900         | 902          | rBV3     | 25730          | 63388         | 1.02%           | 0.149%        |
| 15        | 12.654      | 905           | 907         | 914          | rBV      | 451793         | 553162        | 8.94%           | 1.302%        |
| 16        | 12.928      | 928           | 931         | 933          | rBV      | 5440533        | 6186244       | 100.00%         | 14.566%       |
| 17        | 13.968      | 1019          | 1022        | 1024         | rBV      | 2261797        | 2295730       | 37.11%          | 5.405%        |
| 18        | 15.385      | 1142          | 1146        | 1148         | rBV      | 1225751        | 1594123       | 25.77%          | 3.753%        |

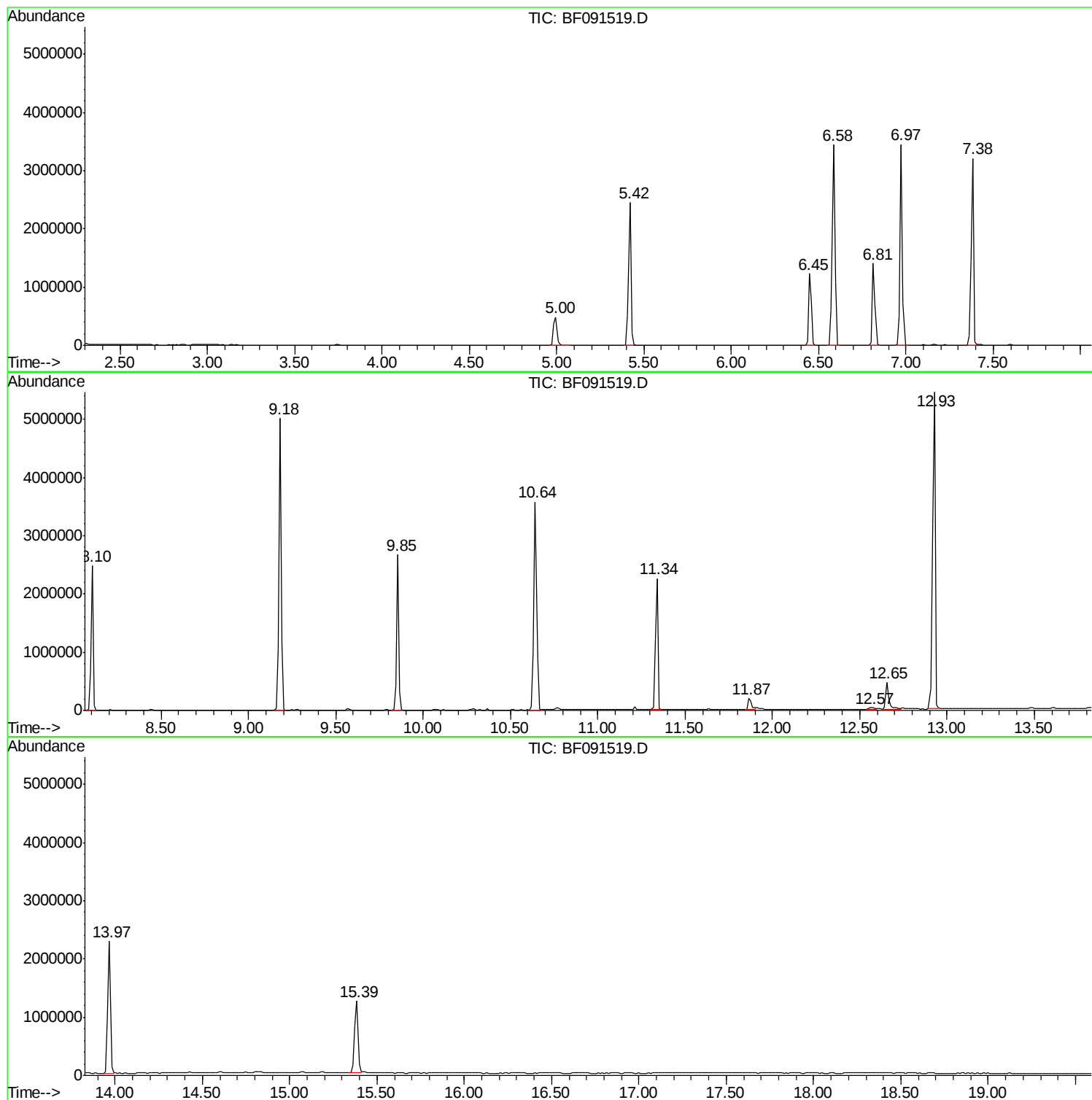
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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF112916.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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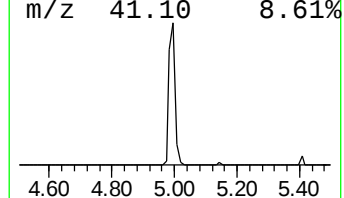
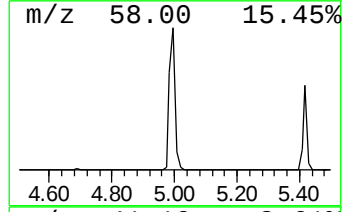
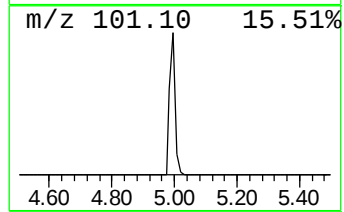
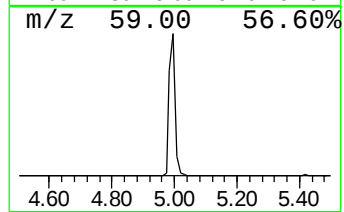
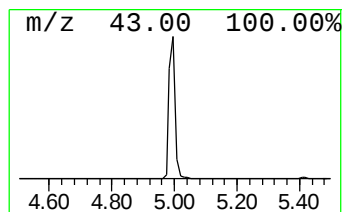
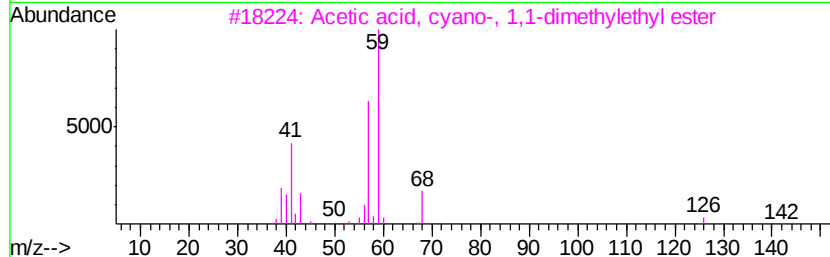
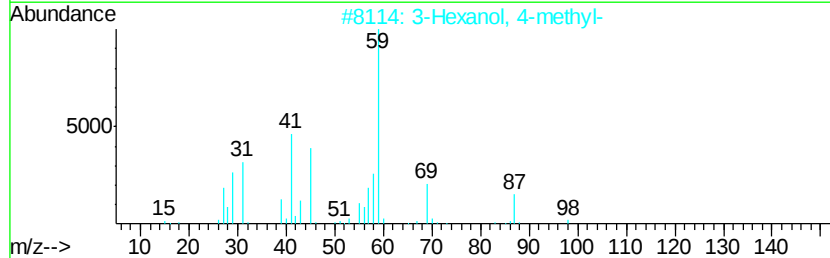
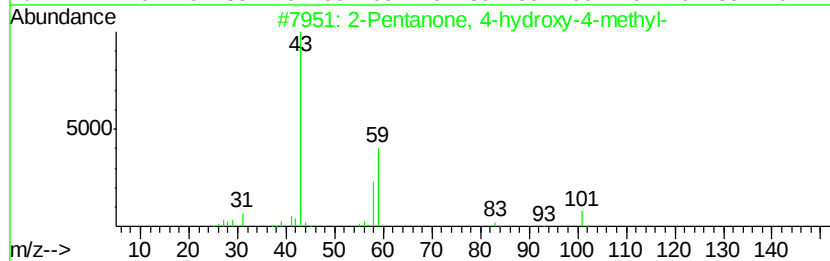
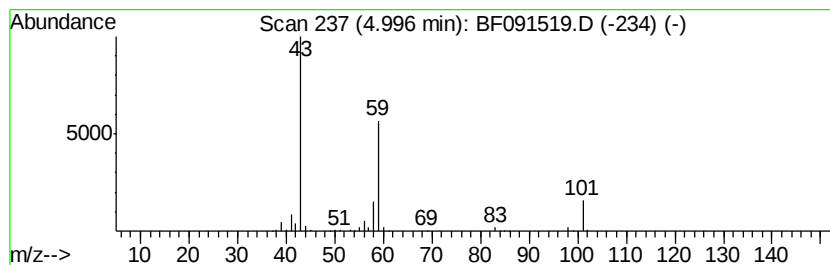
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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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. |
|------|---------|--------|------------------------|------|
| 5.00 | 8.61 ng | 635286 | 1,4-Dichlorobenzene-d4 | 6.81 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2  | 000123-42-2 | 50   |
| 2    |    |   | 3-Hexanol, 4-methyl-                | 116 | C7H16O   | 000615-29-2 | 33   |
| 3    |    |   | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 25   |
| 4    |    |   | Guanidine                           | 59  | CH5N3    | 000113-00-8 | 9    |
| 5    |    |   | 2,3-Butanedione, monooxime          | 101 | C4H7NO2  | 000057-71-6 | 9    |



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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

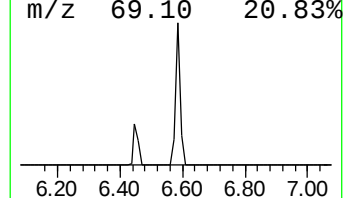
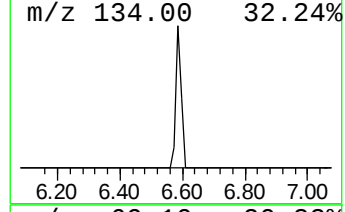
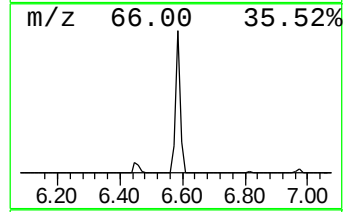
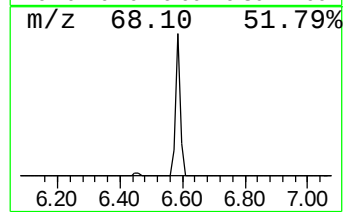
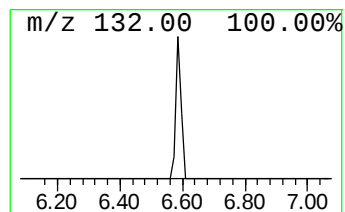
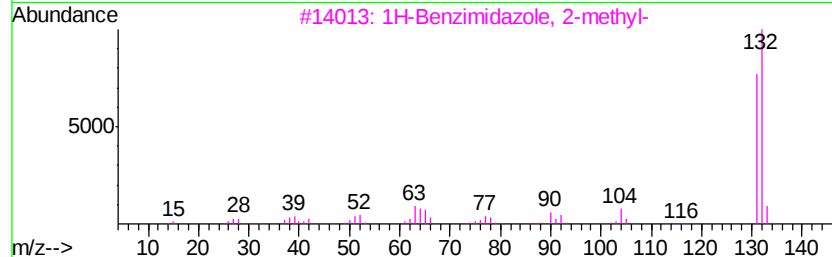
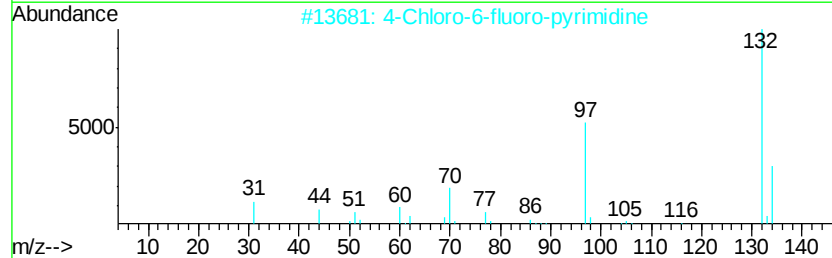
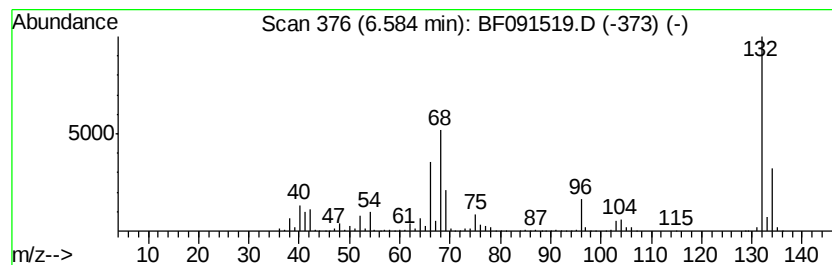
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Peak Number 2 unknown6.58 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.58 | 47.77 ng | 3524180 | 1,4-Dichlorobenzene-d4 | 6.81 |

| Hit# | of | Tentative ID                 | MW  | MolForm   | CAS#         | Qual |
|------|----|------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 3-Chloro-6-fluoro-pyrazine   | 132 | C4H2ClFN2 | 1000146-10-7 | 27   |
| 2    |    | 4-Chloro-6-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-01-6  | 27   |
| 3    |    | 1H-Benzimidazole, 2-methyl-  | 132 | C8H8N2    | 000615-15-6  | 22   |
| 4    |    | 5-Fluoro-2-chloropyrimidine  | 132 | C4H2ClFN2 | 062802-42-0  | 12   |
| 5    |    | Tranylcypromine-propionyl    | 189 | C12H15NO  | 1000123-86-3 | 10   |



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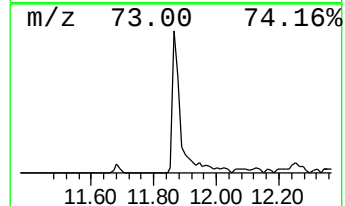
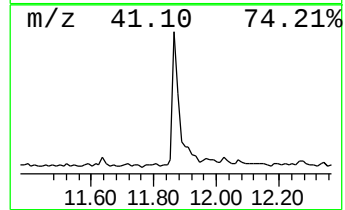
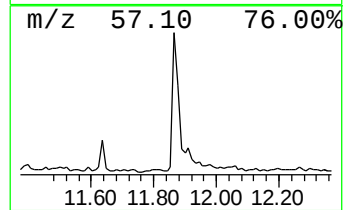
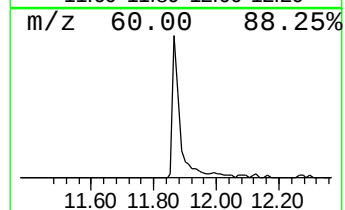
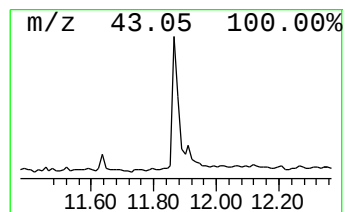
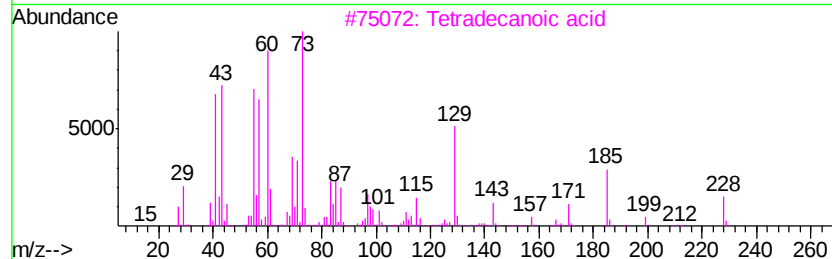
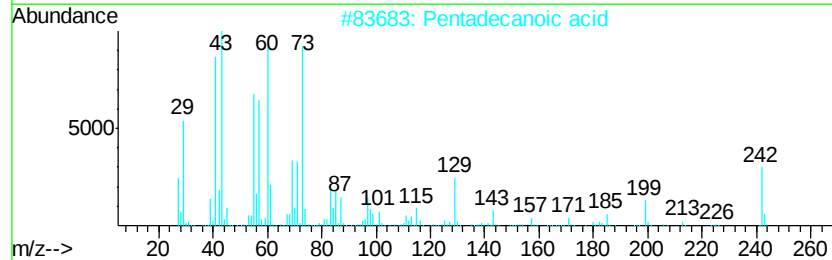
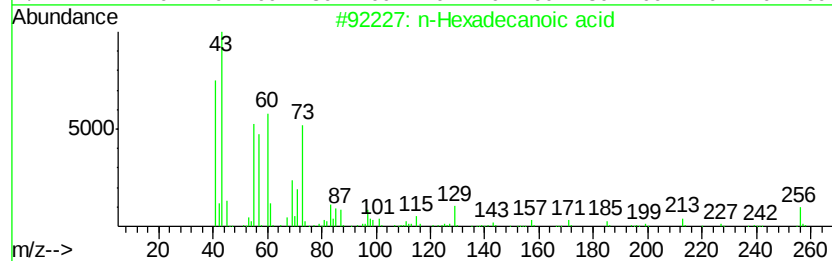
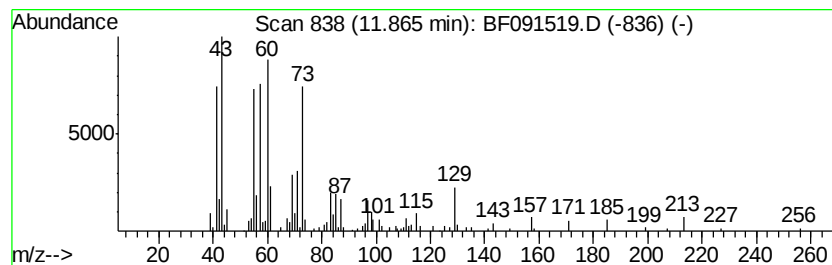
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 11.87 | 2.33 ng | 283037 | Phenanthrene-d10 | 11.34 |

| Hit# of 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|-----------|---------------------|-----|----------|-------------|------|
| 1         | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 95   |
| 2         | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 91   |
| 3         | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 83   |
| 4         | Undecanoic acid     | 186 | C11H22O2 | 000112-37-8 | 80   |
| 5         | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 64   |



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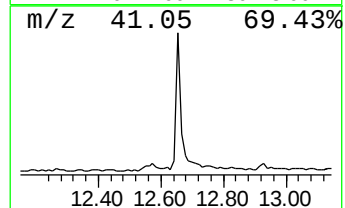
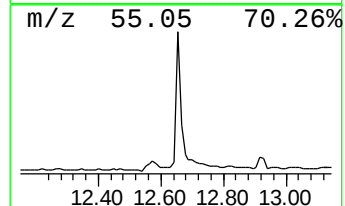
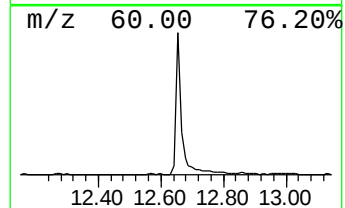
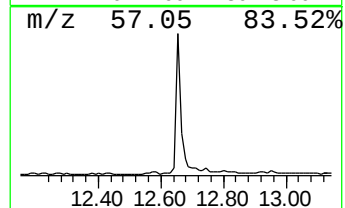
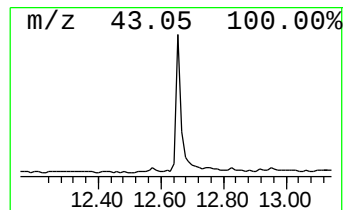
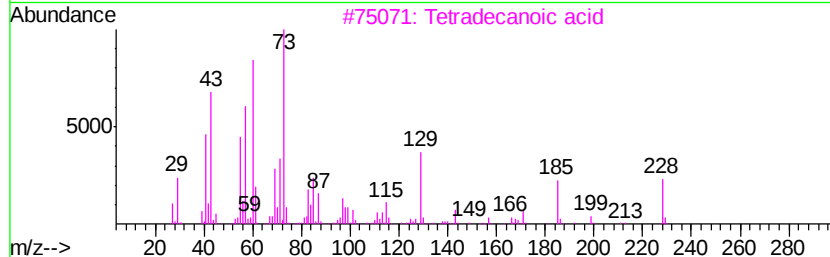
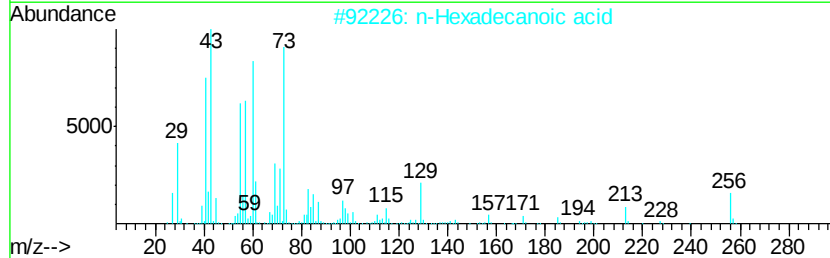
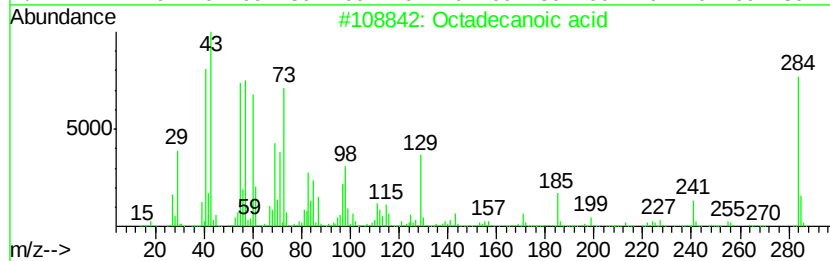
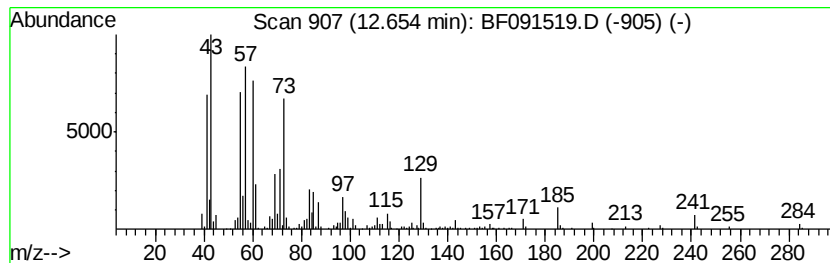
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TIC Integration Parameters: LSCINT.P

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Peak Number 5 Octadecanoic acid Concentration Rank 4

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 12.65 | 4.82 ng | 553162 | Chrysene-d12     | 13.97 |

| Hit# of | 5 | Tentative ID            | MW  | MolForm    | CAS#        | Qual |
|---------|---|-------------------------|-----|------------|-------------|------|
| 1       |   | Octadecanoic acid       | 284 | C18H36O2   | 000057-11-4 | 94   |
| 2       |   | n-Hexadecanoic acid     | 256 | C16H32O2   | 000057-10-3 | 72   |
| 3       |   | Tetradecanoic acid      | 228 | C14H28O2   | 000544-63-8 | 60   |
| 4       |   | 12-Bromododecanoic acid | 278 | C12H23BrO2 | 073367-80-3 | 53   |
| 5       |   | Dodecanoic acid         | 200 | C12H24O2   | 000143-07-7 | 53   |



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| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |         |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|---------|------|
|                      |       |         |       |          | #                     | RT    | Resp    | Conc |
| 2-Pentanone, 4-hy... | 5.00  | 8.6     | ng    | 635286   | 1                     | 6.81  | 1475570 | 20.0 |
| unknown6.58          | 6.58  | 47.8    | ng    | 3524180  | 1                     | 6.81  | 1475570 | 20.0 |
| n-Hexadecanoic acid  | 11.87 | 2.3     | ng    | 283037   | 4                     | 11.34 | 2430440 | 20.0 |
| Octadecanoic acid    | 12.65 | 4.8     | ng    | 553162   | 5                     | 13.97 | 2295730 | 20.0 |