

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF020923\  
 Data File : BF132379.D  
 Acq On : 09 Feb 2023 15:26  
 Operator : CG\JU  
 Sample : 01508-09  
 Misc :  
 ALS Vial : 9 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 RS-3

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-BF013123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132379.D\data.ms

| 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         | 3.890       | 174           | 179         | 184          | rBV      | 48986          | 67119         | 1.61%           | 0.246%        |
| 2         | 4.690       | 310           | 315         | 321          | rBV      | 68475          | 75649         | 1.82%           | 0.277%        |
| 3         | 5.290       | 411           | 417         | 425          | rVB      | 825029         | 1071054       | 25.76%          | 3.925%        |
| 4         | 5.672       | 477           | 482         | 485          | rBV      | 3001078        | 3028496       | 72.85%          | 11.099%       |
| 5         | 6.666       | 645           | 651         | 654          | rBV      | 2796728        | 2957452       | 71.14%          | 10.839%       |
| 6         | 7.048       | 712           | 716         | 719          | rBV      | 956748         | 807576        | 19.43%          | 2.960%        |
| 7         | 7.607       | 806           | 811         | 814          | rBV      | 2061246        | 2029236       | 48.81%          | 7.437%        |
| 8         | 8.331       | 931           | 934         | 937          | rBV      | 1415954        | 1064939       | 25.62%          | 3.903%        |
| 9         | 9.407       | 1113          | 1117        | 1120         | rBV      | 4749646        | 4157403       | 100.00%         | 15.237%       |
| 10        | 10.095      | 1230          | 1234        | 1237         | rBV      | 1557838        | 1242990       | 29.90%          | 4.556%        |
| 11        | 10.807      | 1352          | 1355        | 1359         | rBV      | 633623         | 502650        | 12.09%          | 1.842%        |
| 12        | 10.889      | 1364          | 1369        | 1372         | rBV      | 3371612        | 2917768       | 70.18%          | 10.694%       |
| 13        | 11.589      | 1484          | 1488        | 1492         | rBV      | 1508994        | 1282993       | 30.86%          | 4.702%        |
| 14        | 12.107      | 1567          | 1576        | 1590         | rBV4     | 84321          | 274034        | 6.59%           | 1.004%        |
| 15        | 13.183      | 1755          | 1759        | 1762         | rBV      | 4441410        | 4040287       | 97.18%          | 14.808%       |
| 16        | 14.213      | 1930          | 1934        | 1936         | rBV      | 92076          | 83301         | 2.00%           | 0.305%        |
| 17        | 14.248      | 1936          | 1940        | 1944         | rBV      | 955007         | 822019        | 19.77%          | 3.013%        |
| 18        | 15.818      | 2201          | 2207        | 2218         | rBV      | 621968         | 860196        | 20.69%          | 3.153%        |

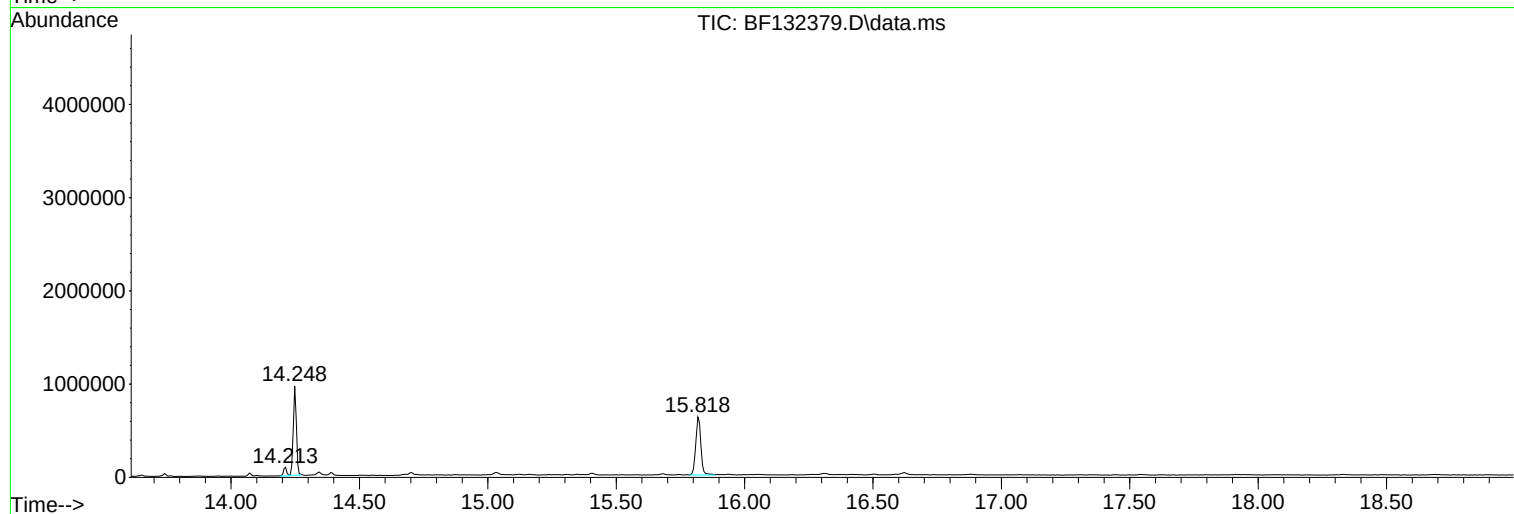
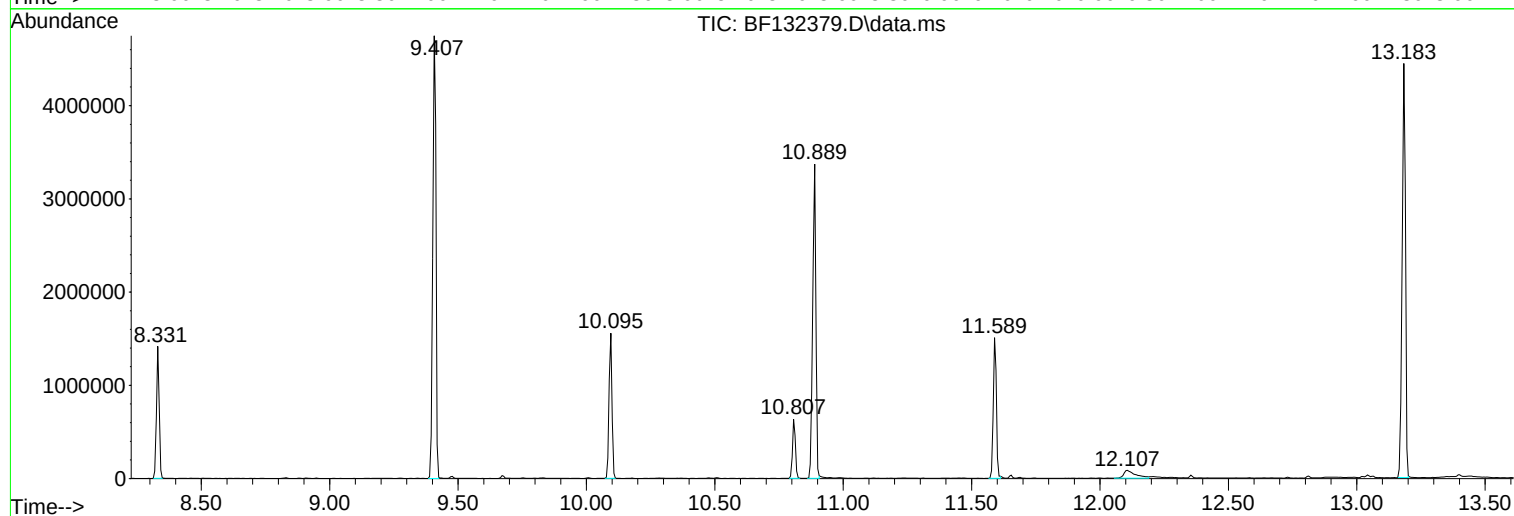
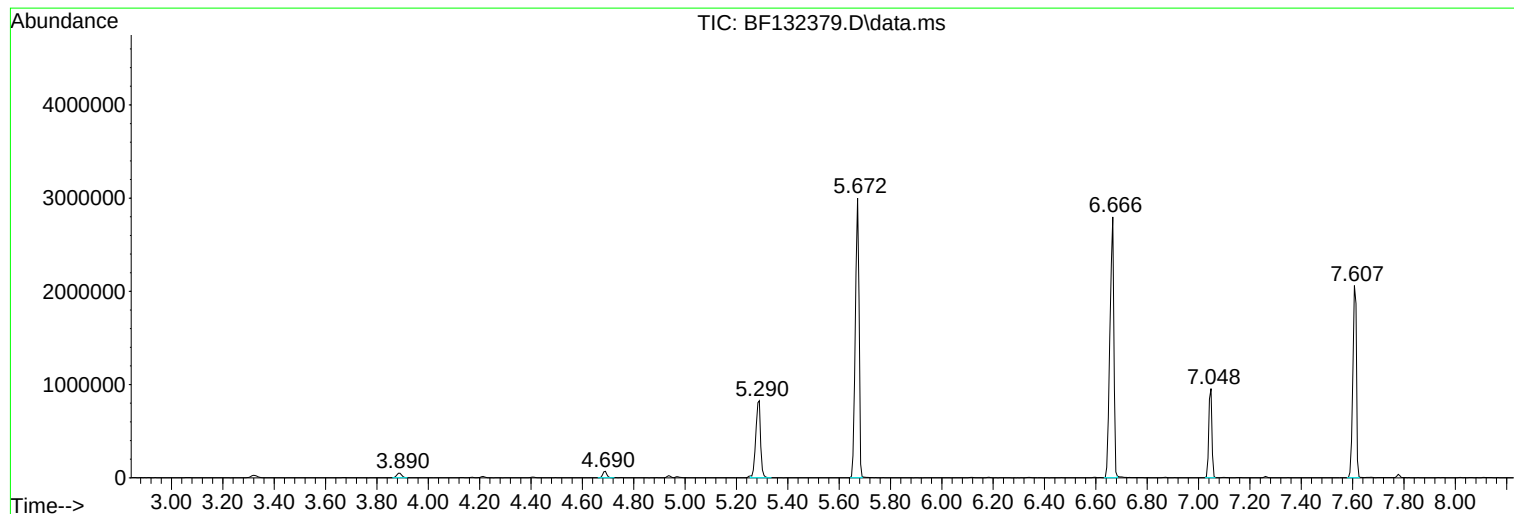
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Instrument :  
BNA\_F  
ClientSampleId :  
RS-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF013123.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P



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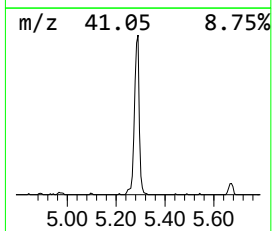
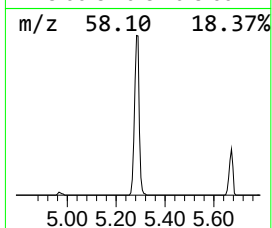
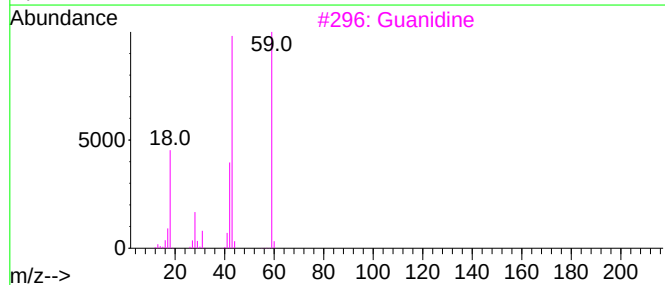
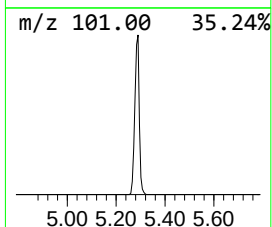
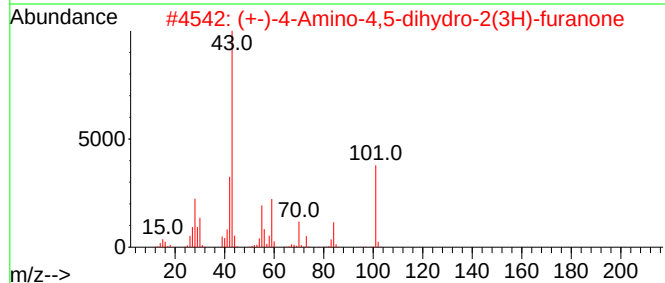
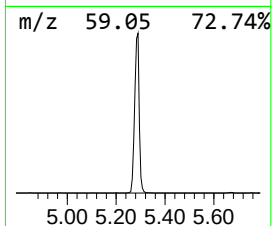
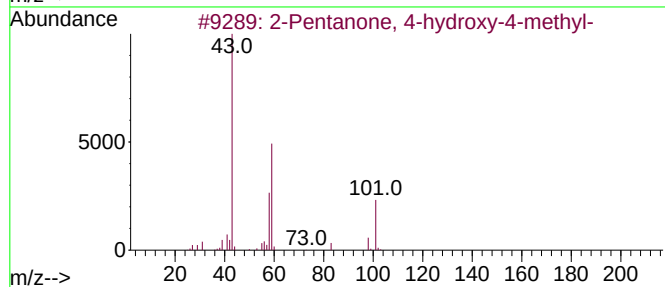
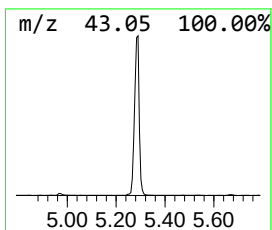
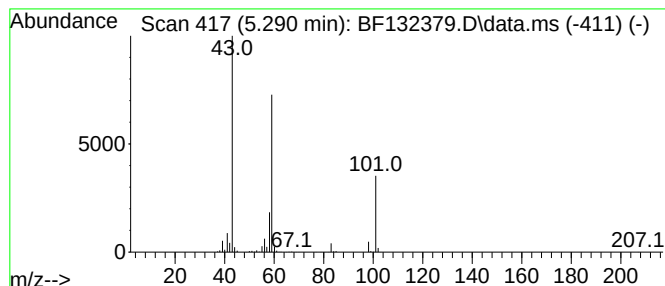
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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

| R.T.  | EstConc  | Area    | Relative to ISTD       | R.T.  |
|-------|----------|---------|------------------------|-------|
| 5.290 | 26.53 ng | 1071050 | 1,4-Dichlorobenzene-d4 | 7.048 |

| Hit# | of | 5 | Tentative ID                       | MW  | MolForm | CAS#        | Qual |
|------|----|---|------------------------------------|-----|---------|-------------|------|
| 1    |    |   | 2-Pentanone, 4-hydroxy-4-methyl-   | 116 | C6H12O2 | 000123-42-2 | 64   |
| 2    |    |   | (+)-4-Amino-4,5-dihydro-2(3H)-f... | 101 | C4H7NO2 | 016504-58-8 | 47   |
| 3    |    |   | Guanidine                          | 59  | CH5N3   | 000113-00-8 | 43   |
| 4    |    |   | 1-Propen-2-ol, acetate             | 100 | C5H8O2  | 000108-22-5 | 10   |
| 5    |    |   | 5-Hexen-2-one                      | 98  | C6H10O  | 000109-49-9 | 9    |



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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

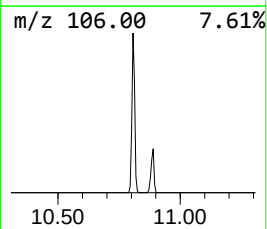
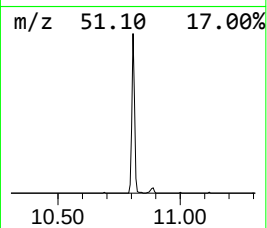
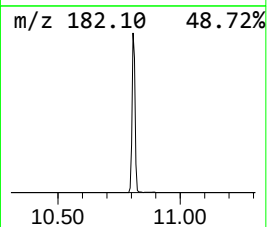
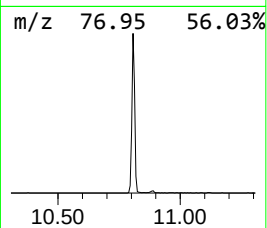
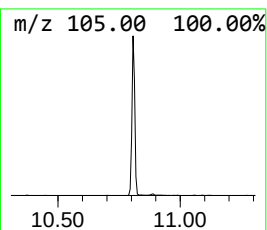
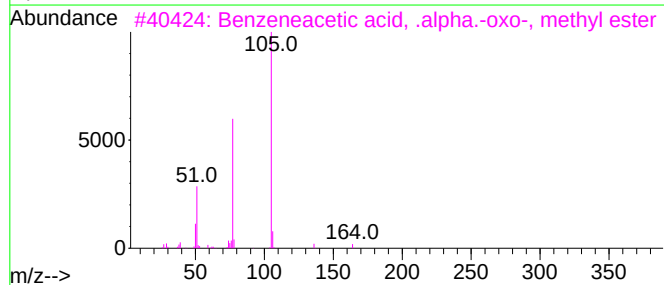
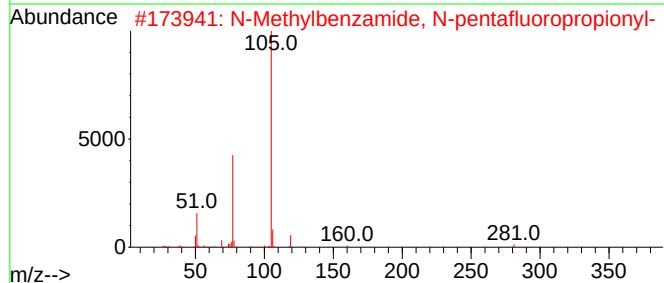
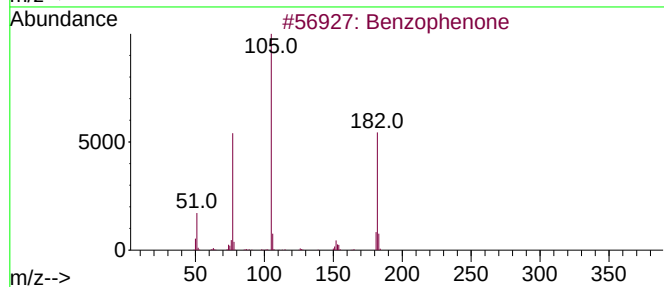
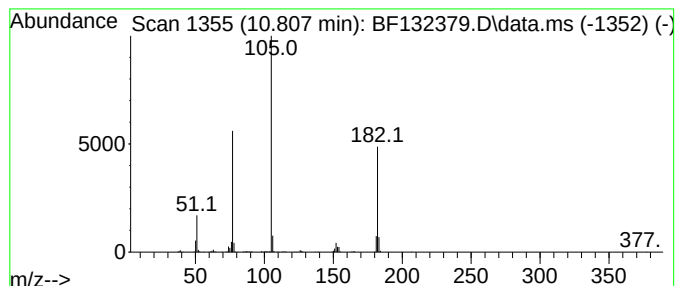
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Peak Number 2 Benzophenone Concentration Rank 2

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 10.807 | 8.09 ng | 502650 | Acenaphthene-d10 | 10.095 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|------------|--------------|------|
| 1    |    |   | Benzophenone                        | 182 | C13H10O    | 000119-61-9  | 96   |
| 2    |    |   | N-Methylbenzamide, N-pentafluoro... | 281 | C11H8F5NO2 | 1000446-98-1 | 43   |
| 3    |    |   | Benzeneacetic acid, .alpha.-oxo-... | 164 | C9H8O3     | 015206-55-0  | 43   |
| 4    |    |   | Benzofurazan-5-carbohydrazide, N... | 282 | C14H10N4O3 | 1000272-94-4 | 43   |
| 5    |    |   | 1-Propanone, 2-bromo-1-phenyl-      | 212 | C9H9BrO    | 002114-00-3  | 43   |



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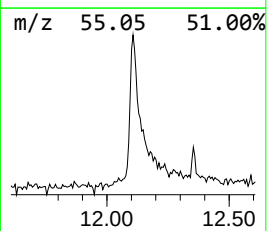
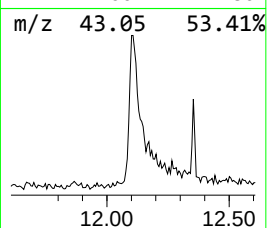
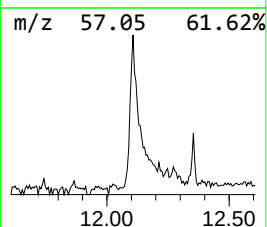
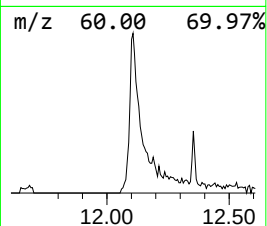
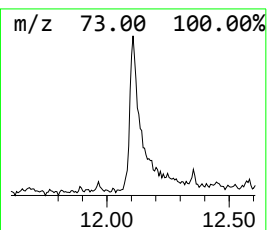
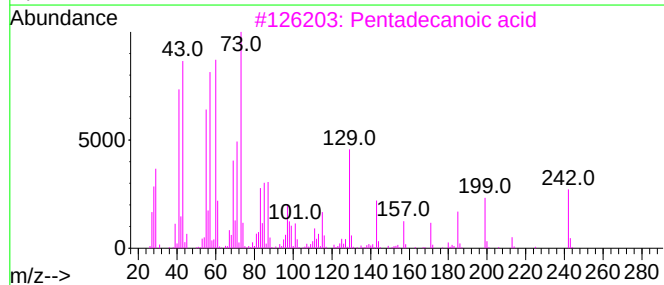
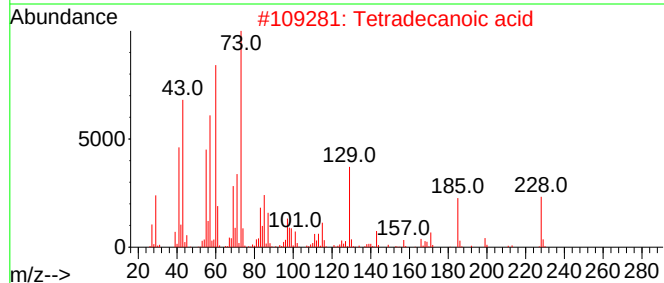
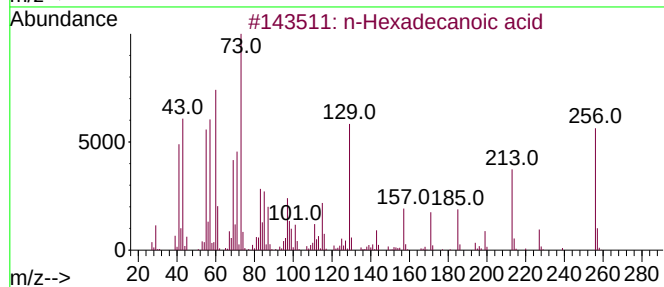
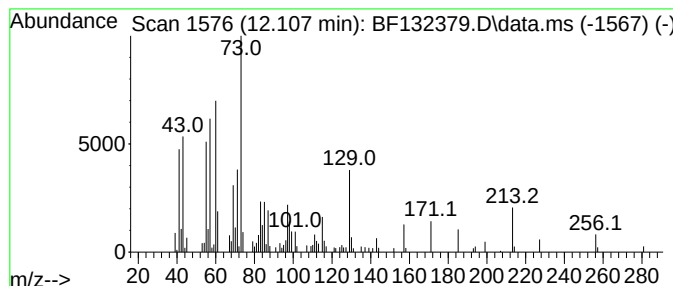
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 12.107 | 4.27 ng | 274034 | Phenanthrene-d10 | 11.589 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|----------|--------------|------|
| 1    |    |   | n-Hexadecanoic acid                 | 256 | C16H32O2 | 000057-10-3  | 99   |
| 2    |    |   | Tetradecanoic acid                  | 228 | C14H28O2 | 000544-63-8  | 72   |
| 3    |    |   | Pentadecanoic acid                  | 242 | C15H30O2 | 001002-84-2  | 72   |
| 4    |    |   | Tridecanoic acid                    | 214 | C13H26O2 | 000638-53-9  | 70   |
| 5    |    |   | Oxalic acid, cyclobutyl octadecy... | 396 | C24H44O4 | 1000309-70-8 | 25   |



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TIC Library : C:\Database\NIST20.L  
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| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |         |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|---------|------|
|                    |        |         |       |          | #                     | RT     | Resp    | Conc |
| 2-Pentanone, 4-... | 5.290  | 26.5    | ng    | 1071050  | 1                     | 7.048  | 807576  | 20.0 |
| Benzophenone       | 10.807 | 8.1     | ng    | 502650   | 3                     | 10.095 | 1242990 | 20.0 |
| n-Hexadecanoic ... | 12.107 | 4.3     | ng    | 274034   | 4                     | 11.589 | 1282990 | 20.0 |