

Data Path : Z:\HPCHEM1\BNA G\DATA\BG011217\  
 Data File : BG025497.D  
 Acq On : 13 Jan 2017 00:54  
 Operator : UM/SJ  
 Sample : I1125-04  
 Misc :  
 ALS Vial : 17 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 W-23

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\_G\METHODS\8270-BG122116.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         | 5.265       | 405           | 413         | 423          | rVB      | 178409         | 299564        | 3.75%           | 0.954%        |
| 2         | 5.740       | 486           | 494         | 506          | rBV      | 580263         | 1071588       | 13.42%          | 3.412%        |
| 3         | 7.362       | 762           | 770         | 779          | rBV      | 391302         | 786585        | 9.85%           | 2.504%        |
| 4         | 7.732       | 826           | 833         | 841          | rBV      | 1139295        | 2051121       | 25.69%          | 6.530%        |
| 5         | 8.202       | 906           | 913         | 921          | rBV      | 252344         | 446506        | 5.59%           | 1.422%        |
| 6         | 8.525       | 961           | 968         | 978          | rVB      | 1017935        | 1844616       | 23.10%          | 5.873%        |
| 7         | 9.383       | 1106          | 1114        | 1129         | rBV      | 900735         | 1760026       | 22.04%          | 5.604%        |
| 8         | 11.028      | 1386          | 1394        | 1405         | rBV      | 314814         | 626360        | 7.85%           | 1.994%        |
| 9         | 13.449      | 1797          | 1806        | 1813         | rBV      | 2571933        | 4102651       | 51.39%          | 13.062%       |
| 10        | 14.830      | 2031          | 2041        | 2047         | rBV      | 576761         | 961272        | 12.04%          | 3.061%        |
| 11        | 16.316      | 2286          | 2294        | 2305         | rBV      | 2716648        | 4291169       | 53.75%          | 13.662%       |
| 12        | 17.574      | 2502          | 2508        | 2514         | rVB      | 782745         | 1192022       | 14.93%          | 3.795%        |
| 13        | 17.914      | 2561          | 2566        | 2570         | rBV5     | 56122          | 118133        | 1.48%           | 0.376%        |
| 14        | 18.408      | 2646          | 2650        | 2655         | rBV4     | 128419         | 187976        | 2.35%           | 0.598%        |
| 15        | 19.671      | 2861          | 2865        | 2871         | rBV5     | 86732          | 133787        | 1.68%           | 0.426%        |
| 16        | 20.153      | 2941          | 2947        | 2955         | rBV      | 6160760        | 7983820       | 100.00%         | 25.419%       |
| 17        | 21.863      | 3231          | 3238        | 3247         | rVB      | 1008518        | 1747978       | 21.89%          | 5.565%        |
| 18        | 25.259      | 3806          | 3816        | 3827         | rVB2     | 571102         | 1803594       | 22.59%          | 5.742%        |

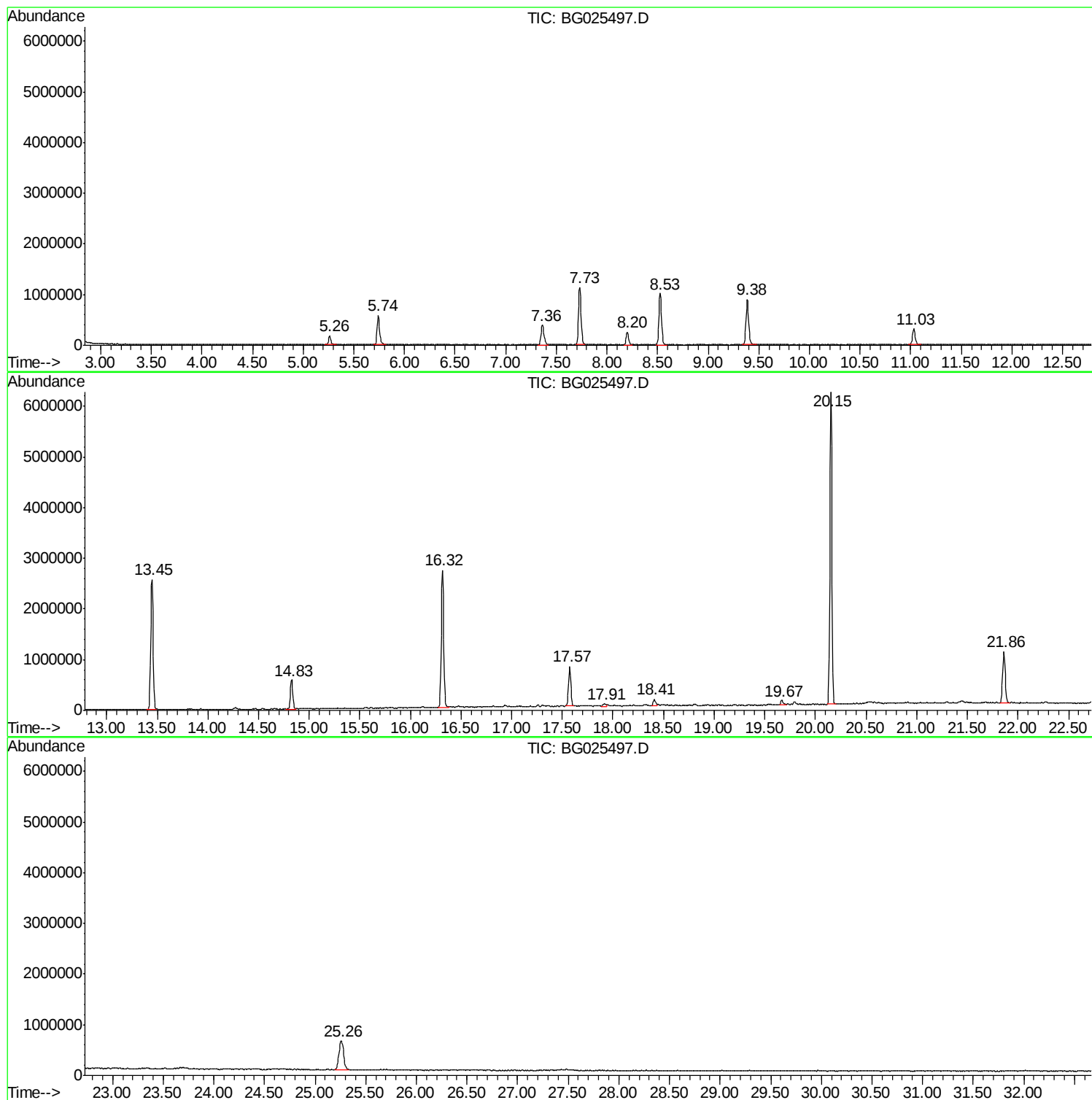
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG122116.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Misc :  
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Instrument :  
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG122116.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

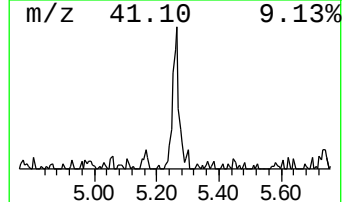
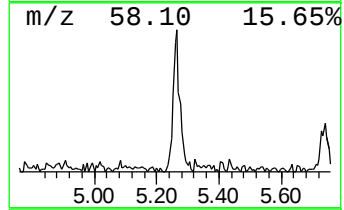
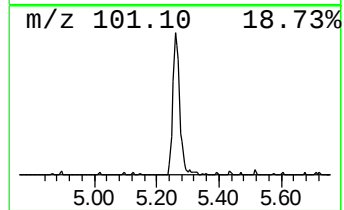
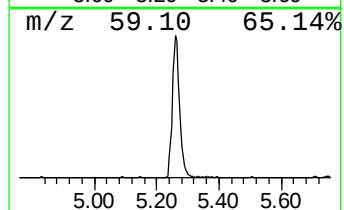
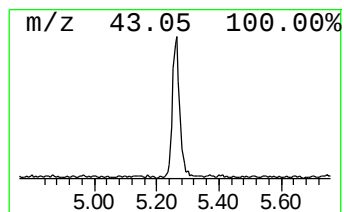
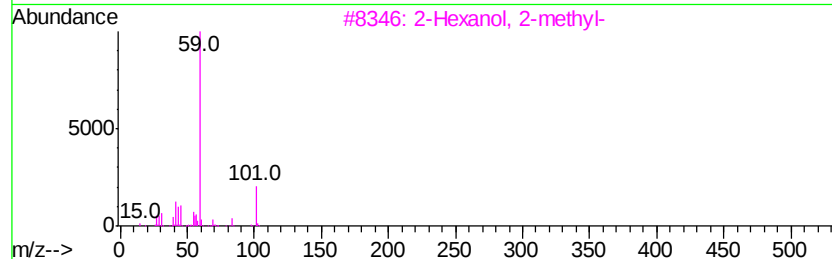
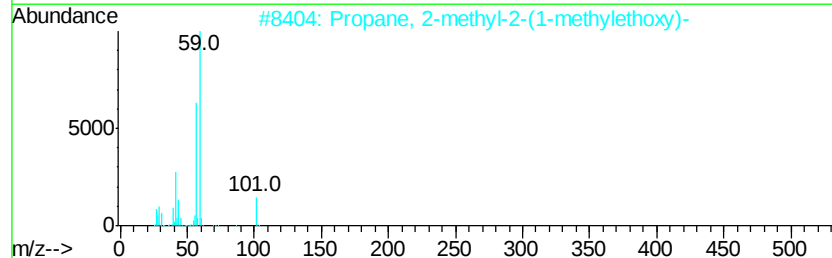
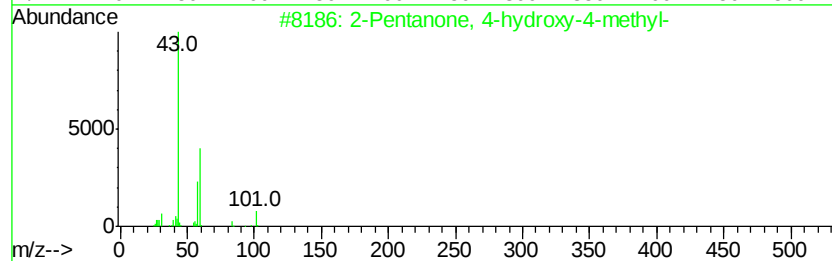
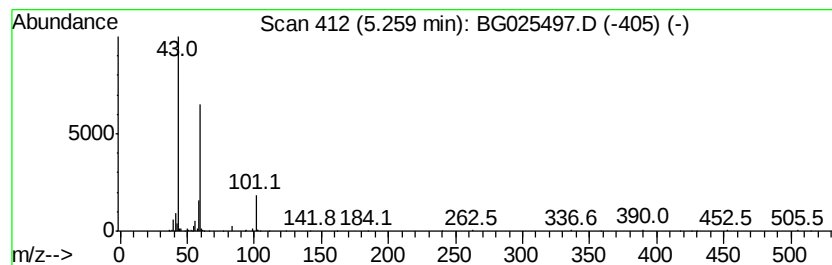
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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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. |
|------|----------|--------|------------------------|------|
| 5.26 | 13.42 ng | 299564 | 1,4-Dichlorobenzene-d4 | 8.20 |

| Hit# | of | 5 | Tentative ID                          | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------------------------|-----|----------|-------------|------|
| 1    |    |   | 2-Pentanone, 4-hydroxy-4-methyl-      | 116 | C6H12O2  | 000123-42-2 | 42   |
| 2    |    |   | Propane, 2-methyl-2-(1-methylethoxy)- | 116 | C7H16O   | 017348-59-3 | 28   |
| 3    |    |   | 2-Hexanol, 2-methyl-                  | 116 | C7H16O   | 000625-23-0 | 25   |
| 4    |    |   | 3-Hexanol, 4-methyl-                  | 116 | C7H16O   | 000615-29-2 | 23   |
| 5    |    |   | Acetic acid, cyano-, 1,1-dimethyl-    | 141 | C7H11NO2 | 001116-98-9 | 17   |



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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG122116.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

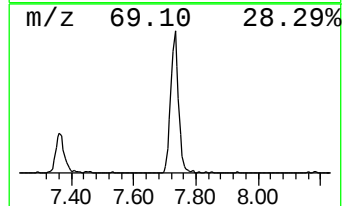
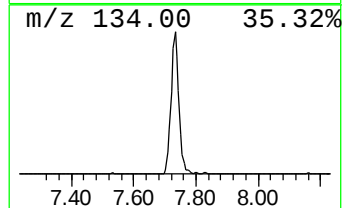
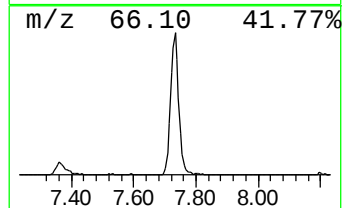
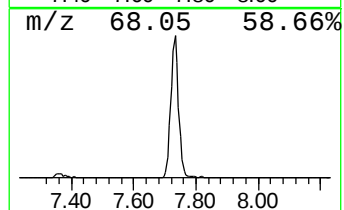
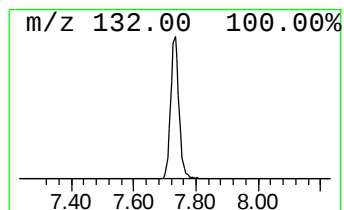
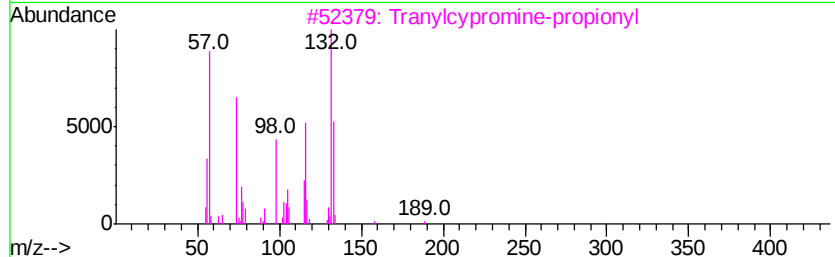
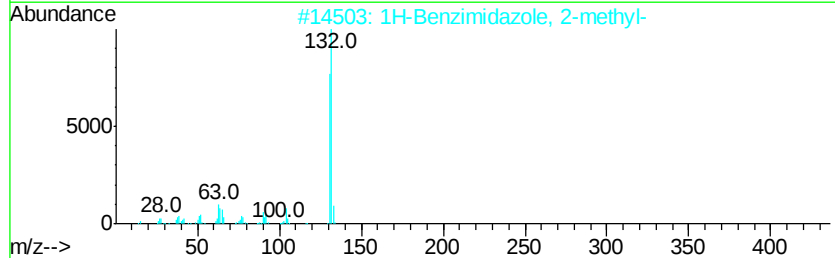
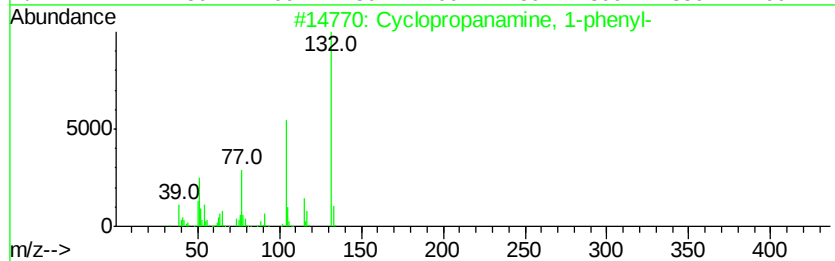
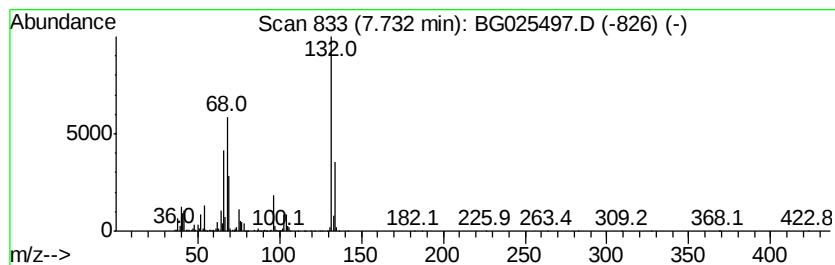
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Peak Number 2 unknown7.73 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 7.73 | 91.87 ng | 2051120 | 1,4-Dichlorobenzene-d4 | 8.20 |

| Hit# | of | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|------|----|-------------------------------------|-----|----------|--------------|------|
| 1    | 5  | Cyclopropanamine, 1-phenyl-         | 133 | C9H11N   | 1000351-26-2 | 10   |
| 2    |    | 1H-Benzimidazole, 2-methyl-         | 132 | C8H8N2   | 000615-15-6  | 10   |
| 3    |    | Tranvlcyproamine-propionyl          | 189 | C12H15NO | 1000123-86-3 | 10   |
| 4    |    | Imidazole, 4,5-dicyano-1-methyl-    | 132 | C6H4N4   | 019485-35-9  | 9    |
| 5    |    | Benzene, 1-methyl-4-(1-methyleth... | 132 | C10H12   | 001195-32-0  | 9    |



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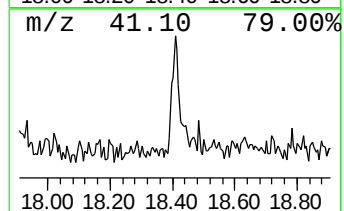
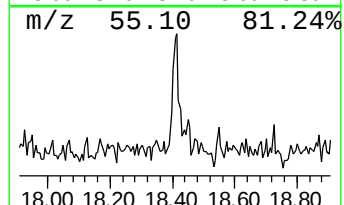
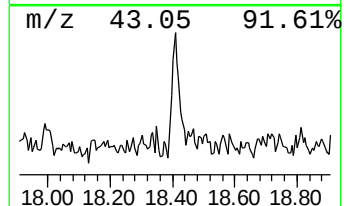
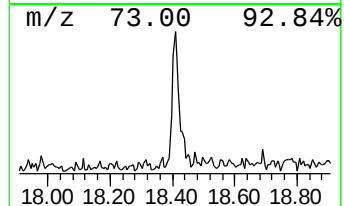
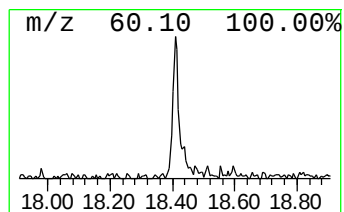
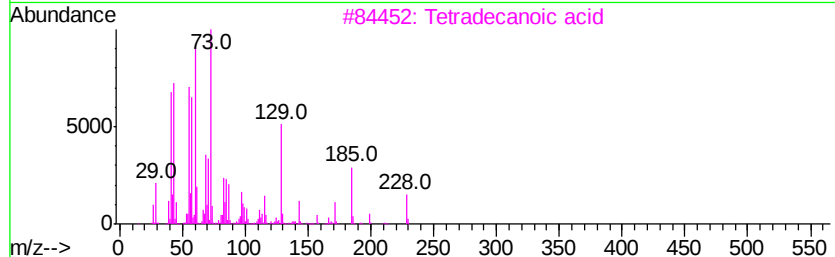
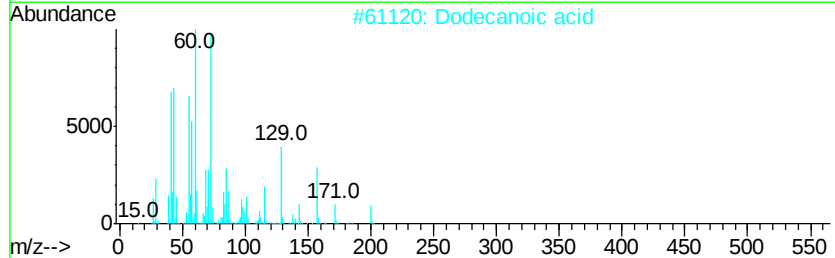
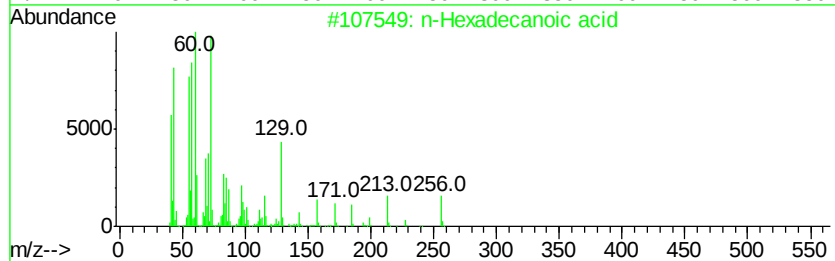
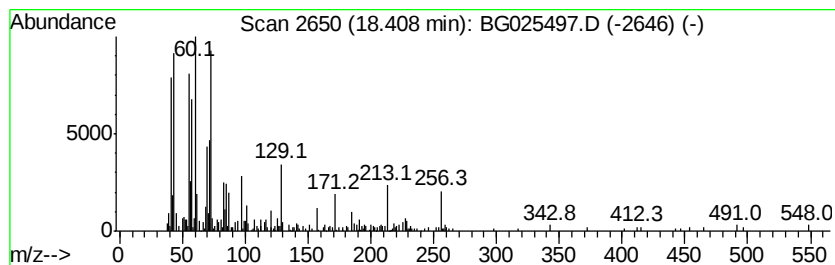
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 18.41 | 3.15 ng | 187976 | Phenanthrene-d10 | 17.57 |

| Hit# of 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|-----------|---------------------|-----|----------|-------------|------|
| 1         | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 93   |
| 2         | Dodecanoic acid     | 200 | C12H24O2 | 000143-07-7 | 70   |
| 3         | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 70   |
| 4         | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 62   |
| 5         | Undecanoic acid     | 186 | C11H22O2 | 000112-37-8 | 50   |



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

| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |         |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|---------|------|
|                      |       |         |       |          | #                     | RT    | Resp    | Conc |
| 2-Pentanone, 4-hy... | 5.26  | 13.4    | ng    | 299564   | 1                     | 8.20  | 446506  | 20.0 |
| unknown7.73          | 7.73  | 91.9    | ng    | 2051120  | 1                     | 8.20  | 446506  | 20.0 |
| n-Hexadecanoic acid  | 18.41 | 3.1     | ng    | 187976   | 4                     | 17.57 | 1192020 | 20.0 |