

Data Path : Z:\HPCHEM1\BNA M\DATA\BM071717\  
 Data File : BM010856.D  
 Acq On : 18 Jul 2017 04:09  
 Operator : SJ/JU  
 Sample : I4199-04  
 Misc :  
 ALS Vial : 16 Sample Multiplier: 1

Instrument :  
 BNA\_M  
 ClientSampleId :  
 3564-PP4

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\_M\METHODS\8270-BM071217.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         | 4.640       | 291           | 298         | 306          | rVB      | 191163         | 279911        | 1.41%           | 0.278%        |
| 2         | 5.081       | 366           | 373         | 383          | rBV      | 2929706        | 3959696       | 19.95%          | 3.929%        |
| 3         | 6.634       | 629           | 637         | 645          | rBV      | 1751387        | 2641418       | 13.31%          | 2.621%        |
| 4         | 6.981       | 689           | 696         | 704          | rBV      | 5377207        | 8185225       | 41.25%          | 8.121%        |
| 5         | 7.440       | 766           | 774         | 783          | rBV      | 1359279        | 2109881       | 10.63%          | 2.093%        |
| 6         | 7.757       | 821           | 828         | 837          | rVB      | 5308602        | 8162186       | 41.13%          | 8.098%        |
| 7         | 8.592       | 961           | 970         | 978          | rBV      | 4516203        | 7349244       | 37.03%          | 7.292%        |
| 8         | 10.204      | 1237          | 1244        | 1251         | rBV      | 1740472        | 2829834       | 14.26%          | 2.808%        |
| 9         | 12.704      | 1661          | 1669        | 1676         | rBV      | 11011403       | 16308141      | 82.18%          | 16.180%       |
| 10        | 13.563      | 1810          | 1815        | 1824         | rVB      | 343470         | 471990        | 2.38%           | 0.468%        |
| 11        | 14.092      | 1896          | 1905        | 1914         | rBV2     | 2458947        | 3615112       | 18.22%          | 3.587%        |
| 12        | 15.592      | 2153          | 2160        | 2172         | rBV      | 8373039        | 11484084      | 57.87%          | 11.394%       |
| 13        | 16.845      | 2367          | 2373        | 2383         | rVB      | 2786827        | 3907947       | 19.69%          | 3.877%        |
| 14        | 17.768      | 2526          | 2530        | 2538         | rBV2     | 384941         | 506505        | 2.55%           | 0.503%        |
| 15        | 19.068      | 2747          | 2751        | 2757         | rBV      | 351684         | 451095        | 2.27%           | 0.448%        |
| 16        | 19.509      | 2819          | 2826        | 2831         | rBV      | 16395184       | 19844599      | 100.00%         | 19.689%       |
| 17        | 20.803      | 3043          | 3046        | 3051         | rBV5     | 212652         | 271550        | 1.37%           | 0.269%        |
| 18        | 21.062      | 3085          | 3090        | 3097         | rBV      | 3502529        | 4249463       | 21.41%          | 4.216%        |
| 19        | 21.909      | 3232          | 3234        | 3241         | rVB6     | 200081         | 199885        | 1.01%           | 0.198%        |
| 20        | 23.191      | 3446          | 3452        | 3460         | rVB      | 2203527        | 3963735       | 19.97%          | 3.933%        |

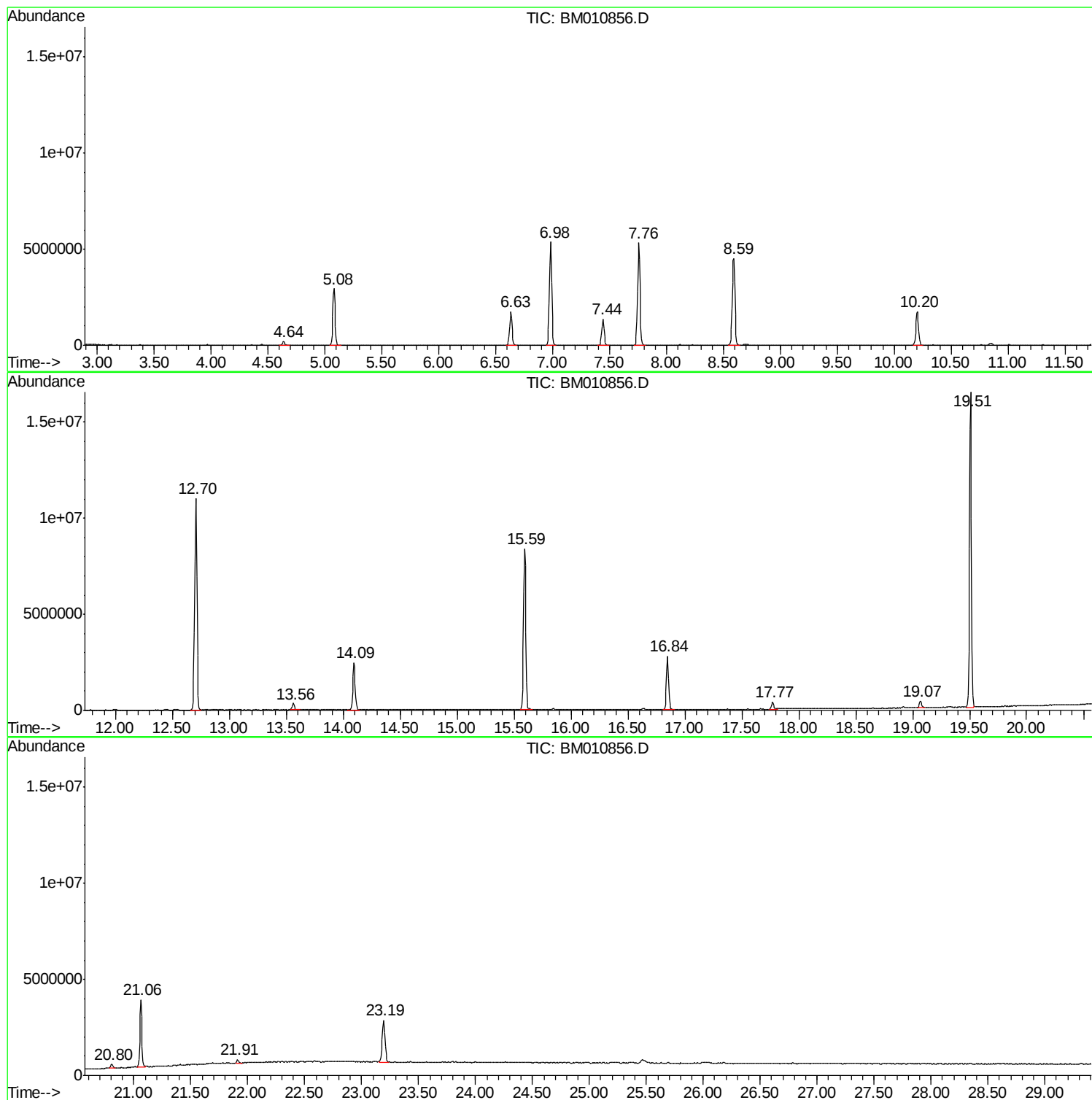
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BNA\_M  
ClientSampleId :  
3564-PP4

Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM071217.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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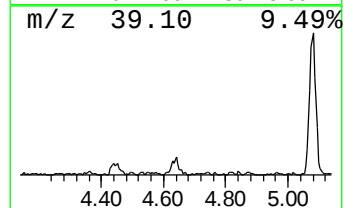
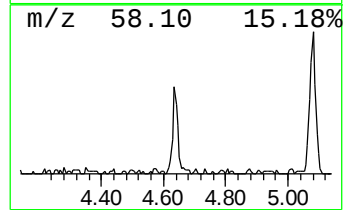
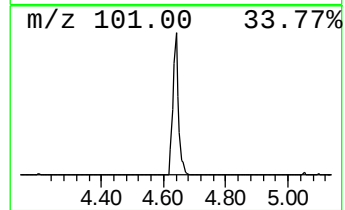
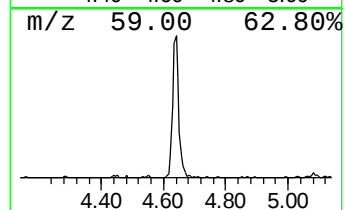
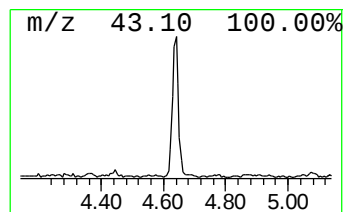
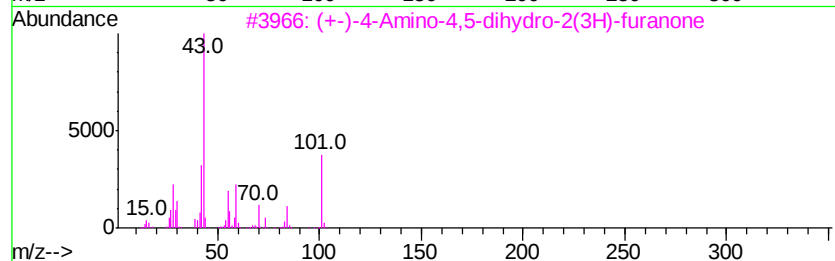
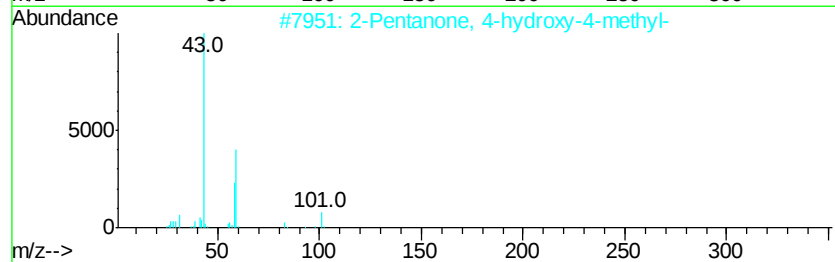
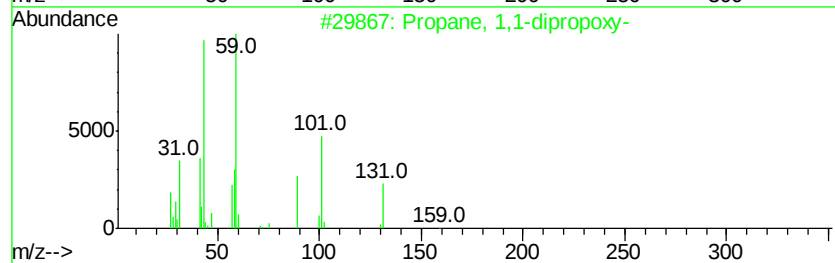
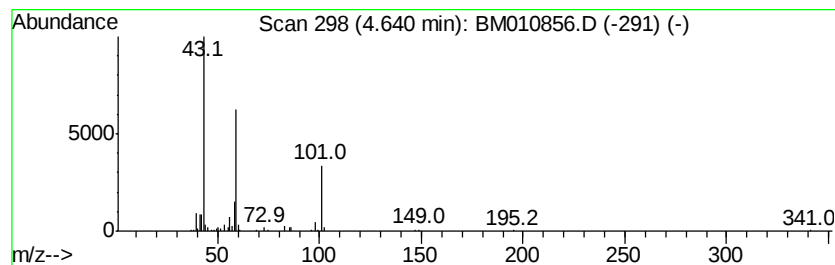
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 Propane, 1,1-dipropoxy- Concentration Rank 3

| R.T. | EstConc | Area   | Relative to ISTD       | R.T. |
|------|---------|--------|------------------------|------|
| 4.64 | 2.65 ng | 279911 | 1,4-Dichlorobenzene-d4 | 7.45 |

| Hit# | of | Tentative ID                           | MW  | MolForm | CAS#        | Qual |
|------|----|----------------------------------------|-----|---------|-------------|------|
| 1    | 5  | Propane, 1,1-dipropoxy-                | 160 | C9H20O2 | 004744-11-0 | 64   |
| 2    |    | 2-Pentanone, 4-hydroxy-4-methyl-       | 116 | C6H12O2 | 000123-42-2 | 45   |
| 3    |    | (+)-4-Amino-4,5-dihydro-2(3H)-furanone | 101 | C4H7NO2 | 016504-58-8 | 42   |
| 4    |    | Hydrazine, 1,1-bis(1-methylethyl)-     | 116 | C6H16N2 | 000921-14-2 | 38   |
| 5    |    | 1,3-Dioxolane, 2,2,4-trimethyl-        | 116 | C6H12O2 | 001193-11-9 | 32   |



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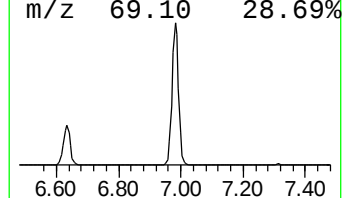
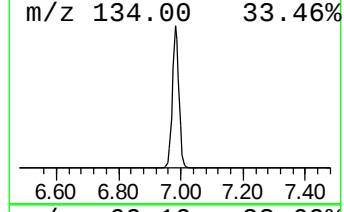
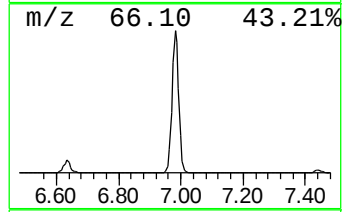
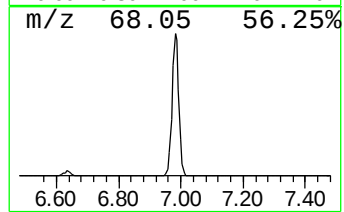
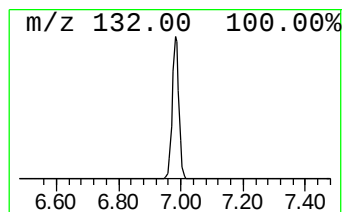
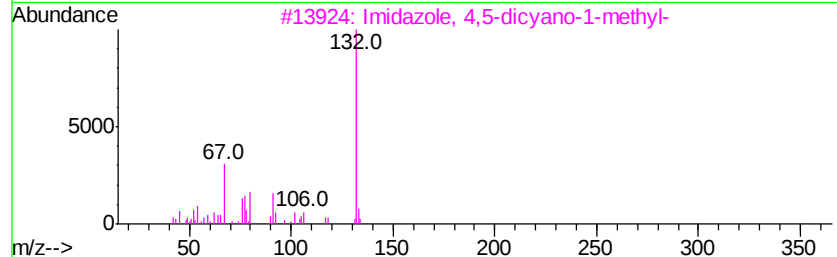
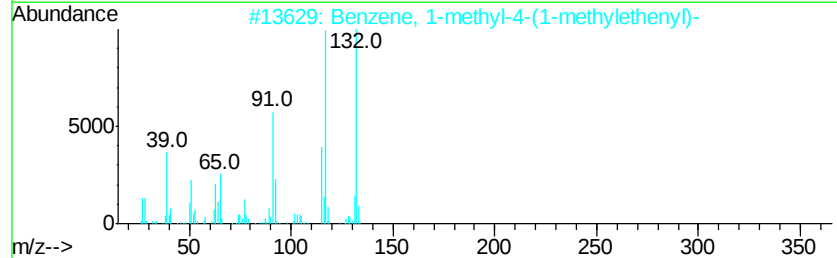
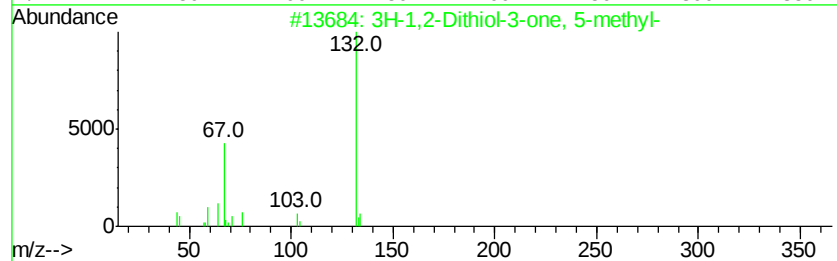
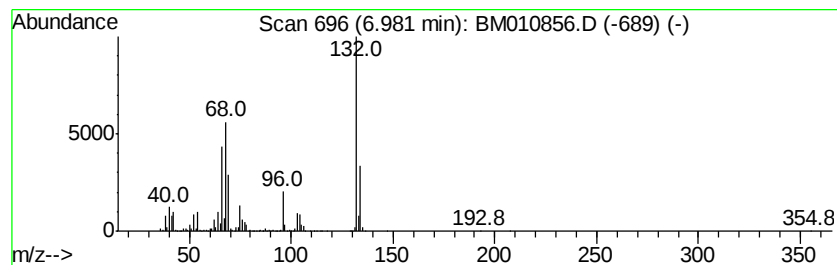
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 unknown6.98 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.98 | 77.59 ng | 8185230 | 1,4-Dichlorobenzene-d4 | 7.45 |

| Hit# | of | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|-------------------------------------|-----|---------|-------------|------|
| 1    | 5  | 3H-1,2-Dithiol-3-one, 5-methyl-     | 132 | C4H4OS2 | 003620-08-4 | 10   |
| 2    |    | Benzene, 1-methyl-4-(1-methyleth... | 132 | C10H12  | 001195-32-0 | 9    |
| 3    |    | Imidazole, 4,5-dicyano-1-methyl-    | 132 | C6H4N4  | 019485-35-9 | 9    |
| 4    |    | (E)-3-Chloro-2-methyl-2-pentenal    | 132 | C6H9ClO | 031357-76-3 | 9    |
| 5    |    | 1,4-Dithiacyclohept-2-ene           | 132 | C5H8S2  | 070063-50-2 | 9    |



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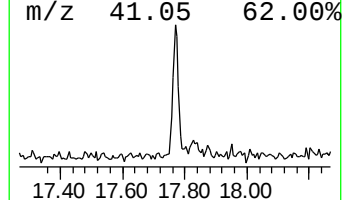
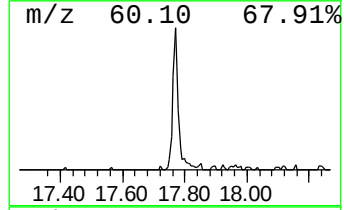
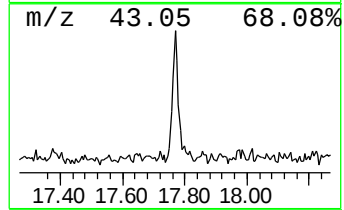
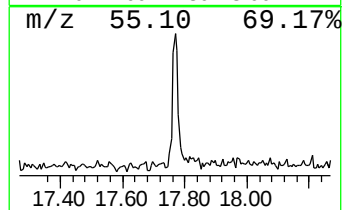
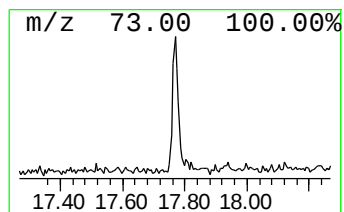
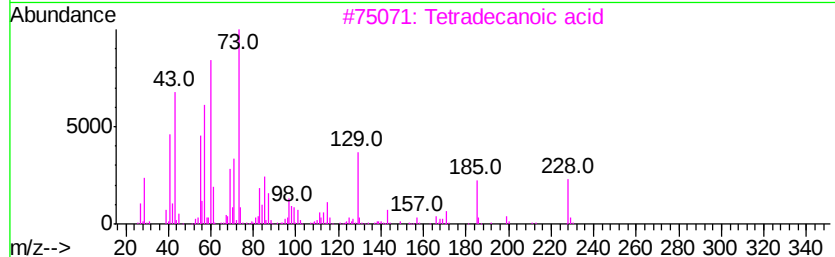
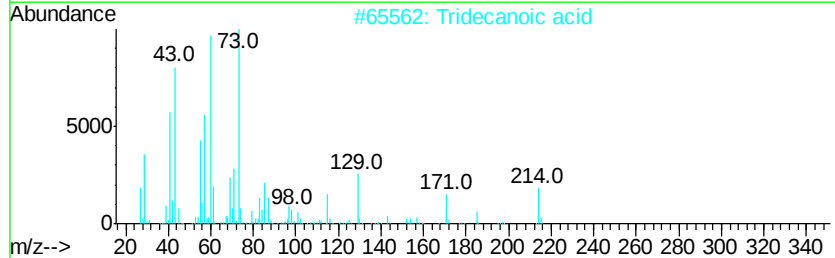
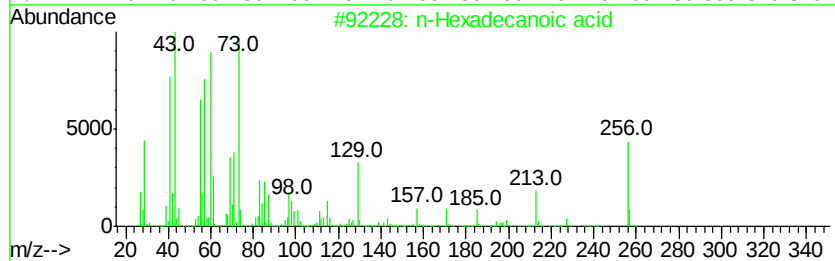
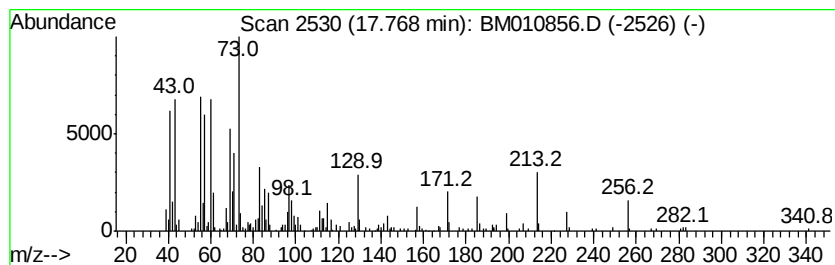
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 17.77 | 2.59 ng | 506505 | Phenanthrene-d10 | 16.84 |

| Hit# of | 5 | Tentative ID             | MW  | MolForm  | CAS#        | Qual |
|---------|---|--------------------------|-----|----------|-------------|------|
| 1       |   | n-Hexadecanoic acid      | 256 | C16H32O2 | 000057-10-3 | 93   |
| 2       |   | Tridecanoic acid         | 214 | C13H26O2 | 000638-53-9 | 58   |
| 3       |   | Tetradecanoic acid       | 228 | C14H28O2 | 000544-63-8 | 52   |
| 4       |   | n-Decanoic acid          | 172 | C10H20O2 | 000334-48-5 | 30   |
| 5       |   | Ether, dodecyl isopropyl | 228 | C15H32O  | 029379-42-8 | 27   |



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Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM071217.M  
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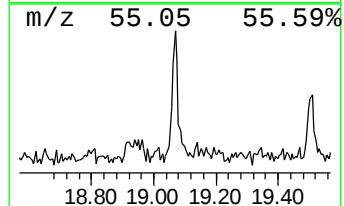
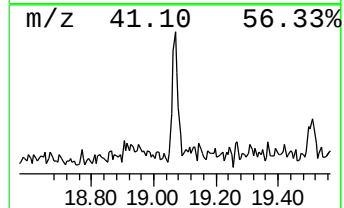
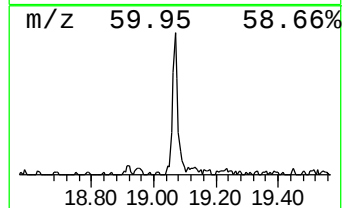
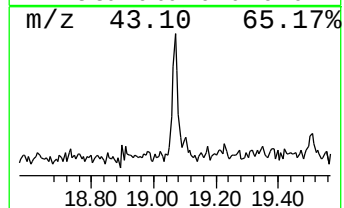
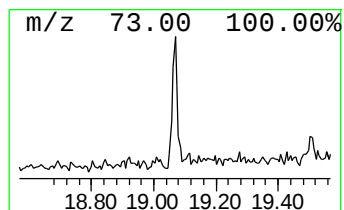
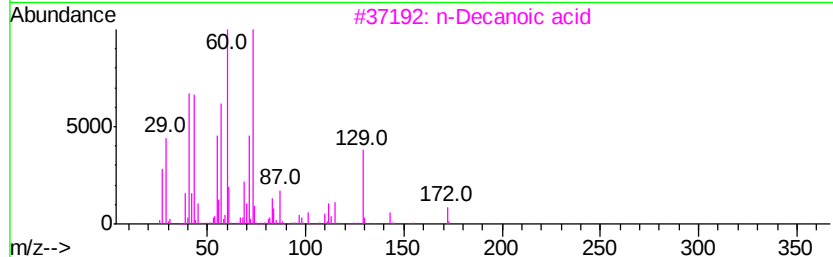
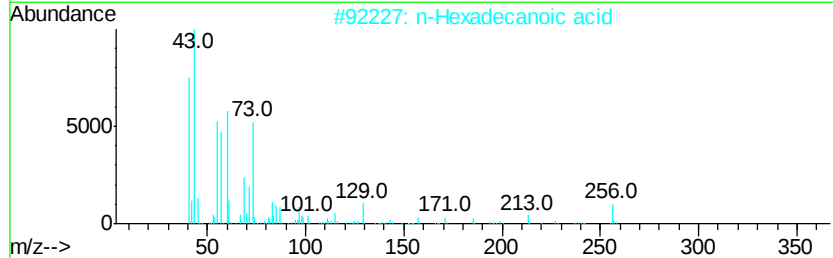
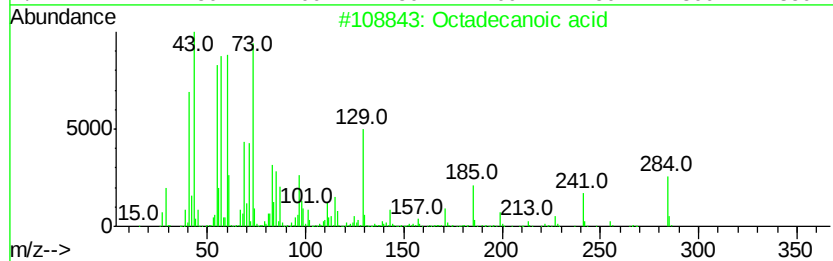
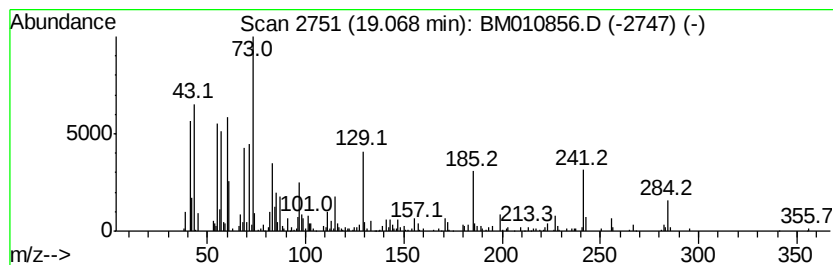
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 Octadecanoic acid Concentration Rank 5

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 19.07 | 2.12 ng | 451095 | Chrysene-d12     | 21.06 |

| Hit# of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|---------|---|---------------------|-----|----------|-------------|------|
| 1       |   | Octadecanoic acid   | 284 | C18H36O2 | 000057-11-4 | 96   |
| 2       |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 55   |
| 3       |   | n-Decanoic acid     | 172 | C10H20O2 | 000334-48-5 | 53   |
| 4       |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 45   |
| 5       |   | Undecanoic acid     | 186 | C11H22O2 | 000112-37-8 | 25   |



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

| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |         |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|---------|------|
|                      |       |         |       |          | #                     | RT    | Resp    | Conc |
| Propane, 1,1-dipr... | 4.64  | 2.6     | ng    | 279911   | 1                     | 7.45  | 2109880 | 20.0 |
| unknown6.98          | 6.98  | 77.6    | ng    | 8185230  | 1                     | 7.45  | 2109880 | 20.0 |
| n-Hexadecanoic acid  | 17.77 | 2.6     | ng    | 506505   | 4                     | 16.84 | 3907950 | 20.0 |
| Octadecanoic acid    | 19.07 | 2.1     | ng    | 451095   | 5                     | 21.06 | 4249460 | 20.0 |