

Data Path : Z:\HPCHEM1\BNA M\DATA\BM051617\  
 Data File : BM010064.D  
 Acq On : 16 May 2017 21:39  
 Operator : SJ/MA  
 Sample : I3180-01  
 Misc :  
 ALS Vial : 11 Sample Multiplier: 1

Instrument :  
 BNA\_M  
 ClientSampleId :  
 EFF-170515-05

Integration Parameters: rteint.p  
 Integrator: RTE  
 Smoothing : ON  
 Sampling : 1  
 Start Thrs: 0.2  
 Stop Thrs : 0  
 Filtering: 5  
 Min Area: 3 % of largest Peak  
 Max Peaks: 100  
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >  
 Peak separation: 5

Method : Z:\HPCHEM1\BNA\_M\METHODS\8270-BM051117.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         | 4.287       | 199           | 204         | 218          | rBV      | 1337337        | 1786823       | 34.90%          | 7.050%        |
| 2         | 4.893       | 301           | 307         | 323          | rVB      | 2086910        | 2769406       | 54.09%          | 10.928%       |
| 3         | 5.346       | 377           | 384         | 402          | rBV2     | 512831         | 825443        | 16.12%          | 3.257%        |
| 4         | 5.946       | 480           | 486         | 495          | rBV      | 321896         | 483508        | 9.44%           | 1.908%        |
| 5         | 6.934       | 649           | 654         | 668          | rBV      | 374773         | 664202        | 12.97%          | 2.621%        |
| 6         | 7.287       | 708           | 714         | 728          | rBV      | 872659         | 1415562       | 27.65%          | 5.586%        |
| 7         | 7.751       | 788           | 793         | 804          | rBV      | 222835         | 364259        | 7.11%           | 1.437%        |
| 8         | 8.069       | 840           | 847         | 857          | rBV      | 1152949        | 1823844       | 35.62%          | 7.197%        |
| 9         | 8.928       | 986           | 993         | 1006         | rBV      | 1023487        | 1744769       | 34.08%          | 6.885%        |
| 10        | 10.551      | 1262          | 1269        | 1282         | rBV      | 252430         | 451429        | 8.82%           | 1.781%        |
| 11        | 13.016      | 1681          | 1688        | 1699         | rBV      | 2205938        | 3248258       | 63.44%          | 12.817%       |
| 12        | 13.874      | 1829          | 1834        | 1841         | rBV2     | 38469          | 64328         | 1.26%           | 0.254%        |
| 13        | 14.410      | 1919          | 1925        | 1937         | rBV2     | 344255         | 564219        | 11.02%          | 2.226%        |
| 14        | 15.910      | 2173          | 2180        | 2197         | rBV2     | 1161248        | 1778488       | 34.74%          | 7.018%        |
| 15        | 17.162      | 2387          | 2393        | 2403         | rBV      | 432653         | 687430        | 13.43%          | 2.712%        |
| 16        | 18.039      | 2538          | 2542        | 2552         | rBV3     | 52467          | 75913         | 1.48%           | 0.300%        |
| 17        | 19.315      | 2756          | 2759        | 2764         | rBV4     | 41865          | 56479         | 1.10%           | 0.223%        |
| 18        | 19.786      | 2833          | 2839        | 2847         | rBV      | 4469219        | 5119908       | 100.00%         | 20.202%       |
| 19        | 21.356      | 3101          | 3106        | 3112         | rBV      | 549462         | 757903        | 14.80%          | 2.991%        |
| 20        | 23.644      | 3489          | 3495        | 3504         | rBV2     | 314968         | 661074        | 12.91%          | 2.608%        |

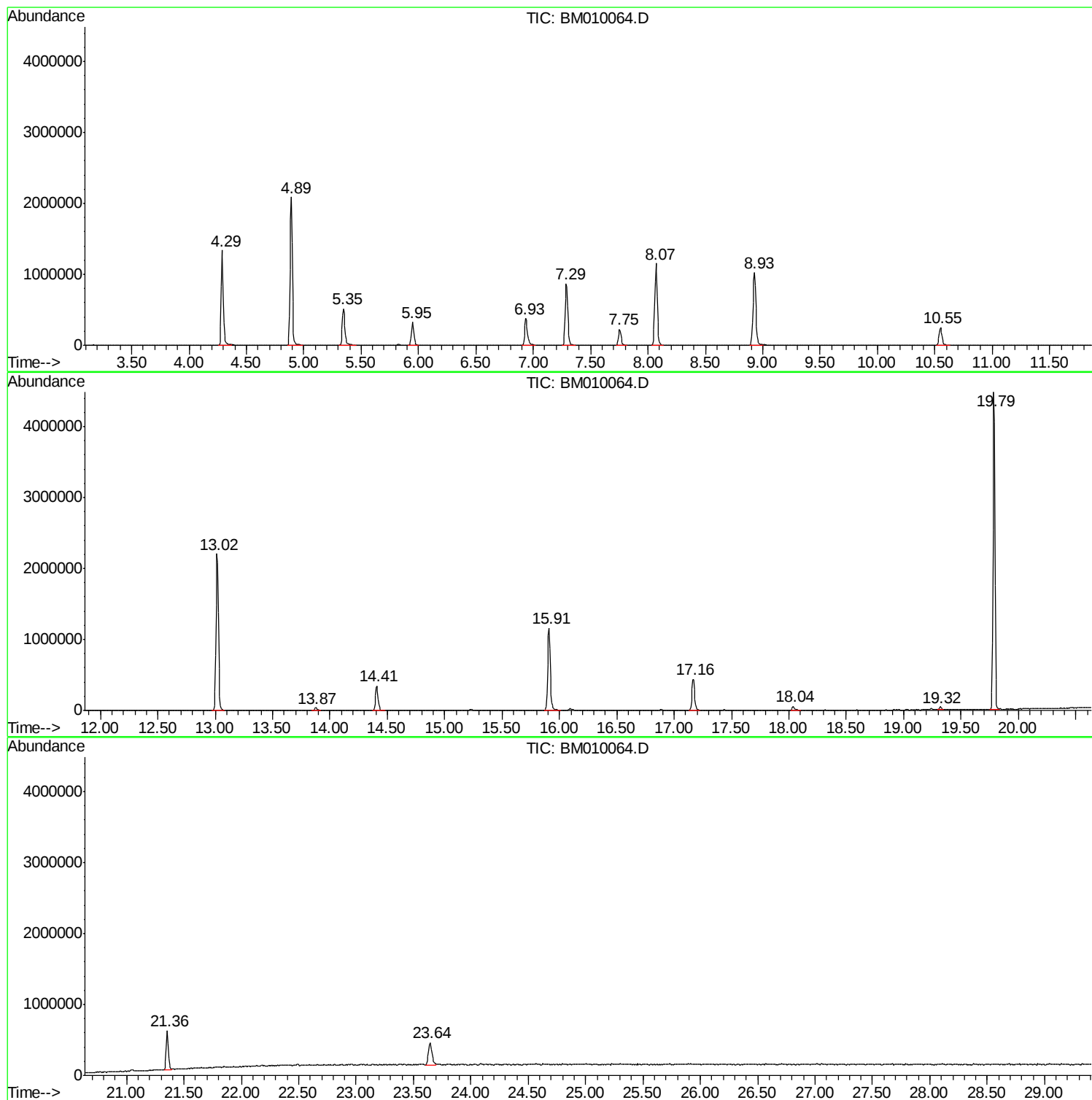
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ALS Vial : 11 Sample Multiplier: 1

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BNA\_M  
ClientSampleId :  
EFF-170515-05

Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM051117.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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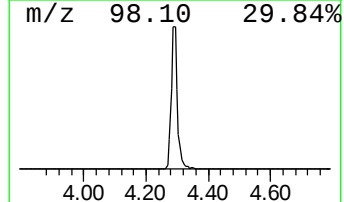
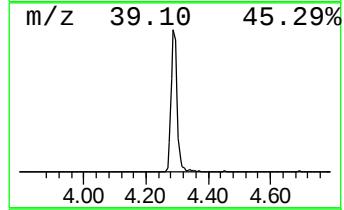
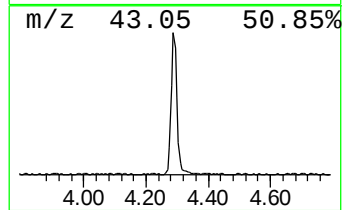
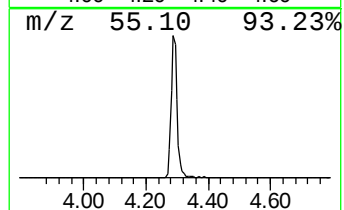
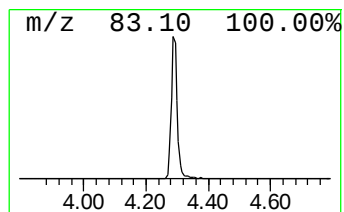
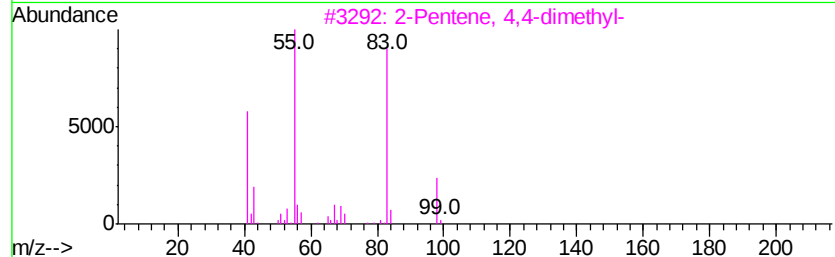
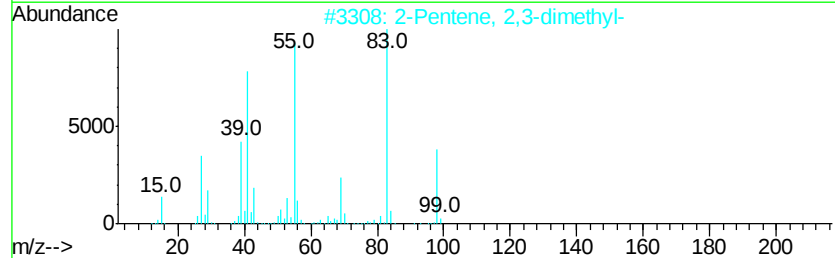
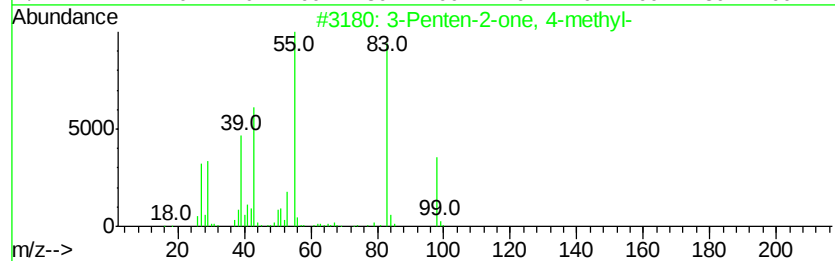
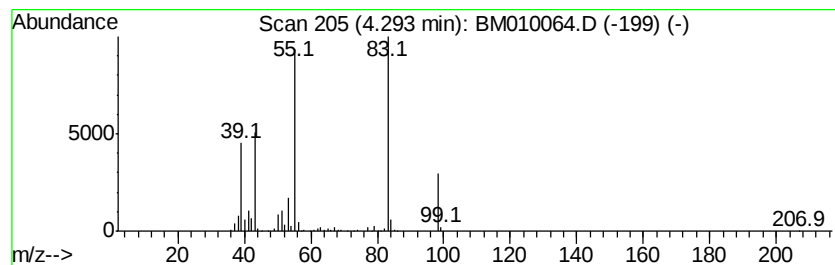
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 3

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 4.29 | 98.11 ng | 1786820 | 1,4-Dichlorobenzene-d4 | 7.75 |

| Hit# | of | 5 | Tentative ID                   | MW | MolForm | CAS#        | Qual |
|------|----|---|--------------------------------|----|---------|-------------|------|
| 1    |    |   | 3-Penten-2-one, 4-methyl-      | 98 | C6H10O  | 000141-79-7 | 91   |
| 2    |    |   | 2-Pentene, 2,3-dimethyl-       | 98 | C7H14   | 010574-37-5 | 72   |
| 3    |    |   | 2-Pentene, 4,4-dimethyl-       | 98 | C7H14   | 026232-98-4 | 64   |
| 4    |    |   | 2-Pentene, 3,4-dimethyl-, (Z)- | 98 | C7H14   | 004914-91-4 | 53   |
| 5    |    |   | 3-Hexen-2-one                  | 98 | C6H10O  | 000763-93-9 | 52   |



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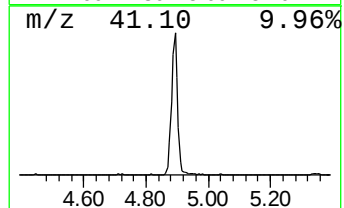
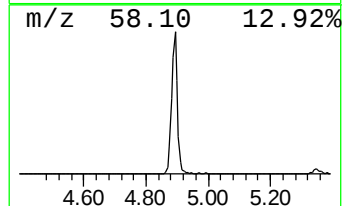
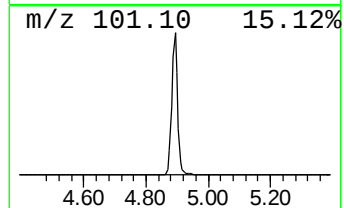
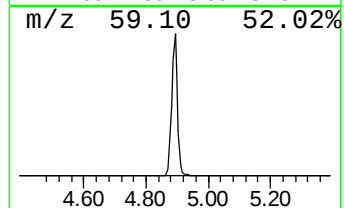
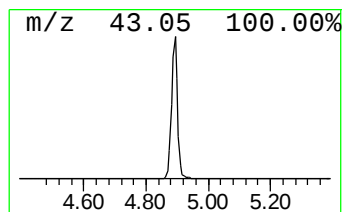
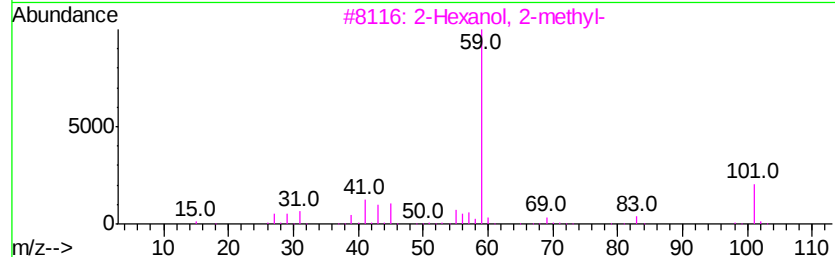
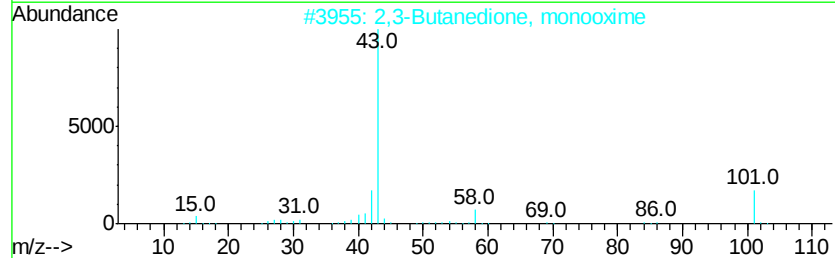
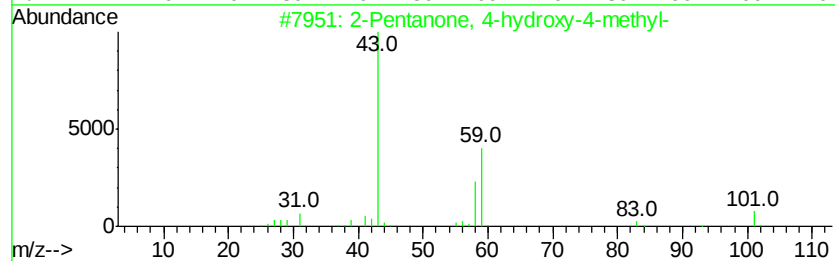
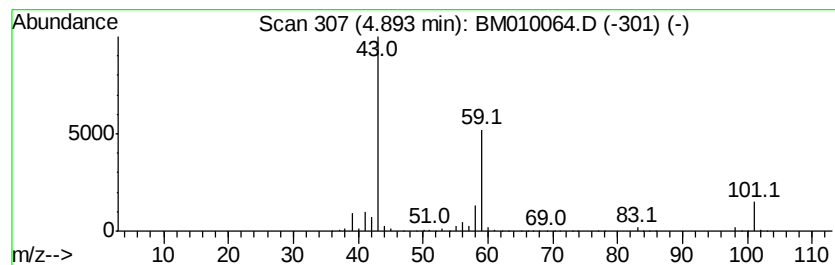
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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

| R.T. | EstConc   | Area    | Relative to ISTD       | R.T. |
|------|-----------|---------|------------------------|------|
| 4.89 | 152.06 ng | 2769410 | 1,4-Dichlorobenzene-d4 | 7.75 |

| Hit# | of | Tentative ID                     | MW  | MolForm | CAS#        | Qual |
|------|----|----------------------------------|-----|---------|-------------|------|
| 1    | 5  | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 64   |
| 2    |    | 2,3-Butanedione, monooxime       | 101 | C4H7NO2 | 000057-71-6 | 27   |
| 3    |    | 2-Hexanol, 2-methyl-             | 116 | C7H16O  | 000625-23-0 | 25   |
| 4    |    | Butyl aldoxime, 3-methyl-, syn-  | 101 | C5H11NO | 005780-40-5 | 23   |
| 5    |    | 1-Butene, 4-ethoxy-              | 100 | C6H12O  | 044611-46-3 | 23   |



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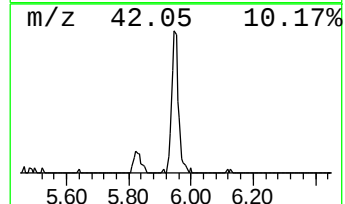
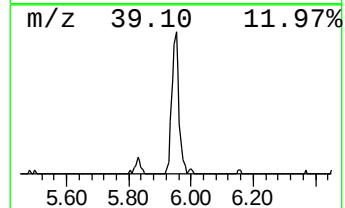
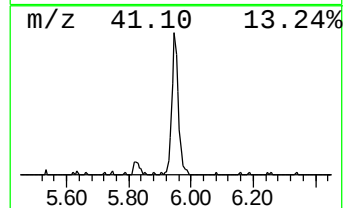
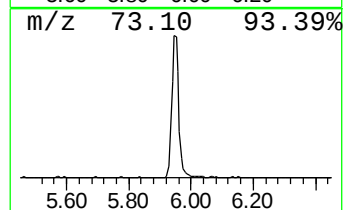
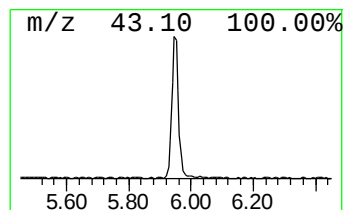
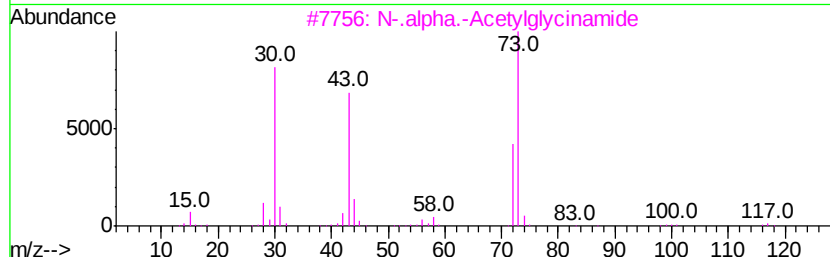
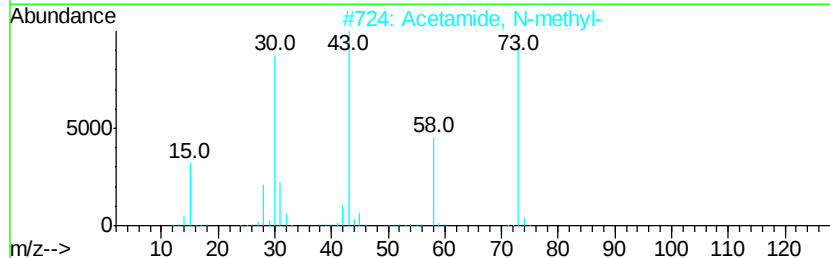
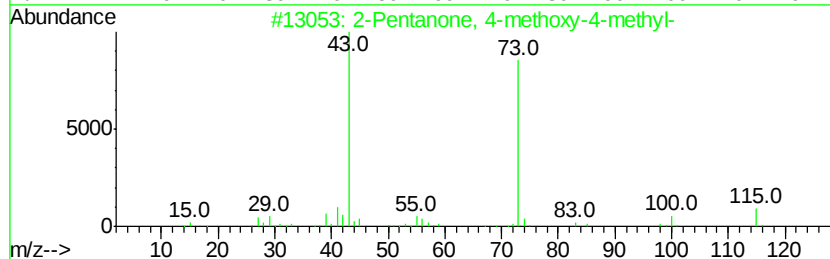
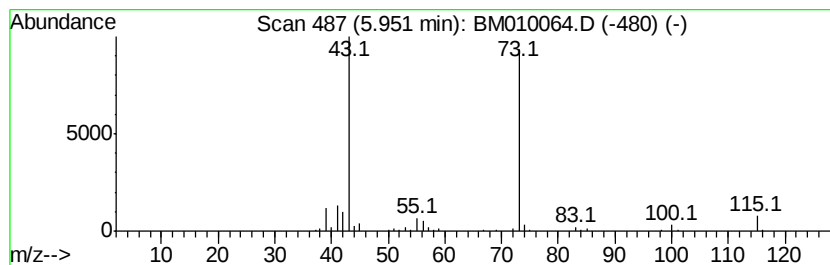
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TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

| R.T. | EstConc  | Area   | Relative to ISTD       | R.T. |
|------|----------|--------|------------------------|------|
| 5.95 | 26.55 ng | 483508 | 1,4-Dichlorobenzene-d4 | 7.75 |

| Hit# | of | Tentative ID                     | MW  | MolForm  | CAS#        | Qual |
|------|----|----------------------------------|-----|----------|-------------|------|
| 1    | 5  | 2-Pentanone, 4-methoxy-4-methyl- | 130 | C7H14O2  | 000107-70-0 | 90   |
| 2    |    | Acetamide, N-methyl-             | 73  | C3H7NO   | 000079-16-3 | 64   |
| 3    |    | N-.alpha.-Acetylglucosinamide    | 116 | C4H8N2O2 | 002620-63-5 | 50   |
| 4    |    | 2-Pentanone, 3-methyl-           | 100 | C6H12O   | 000565-61-7 | 25   |
| 5    |    | 2-Butanone, 3-methoxy-3-methyl-  | 116 | C6H12O2  | 036687-98-6 | 25   |



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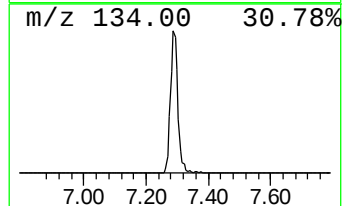
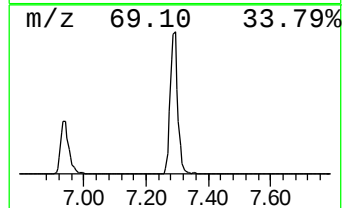
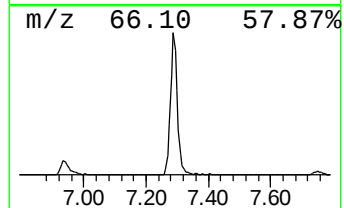
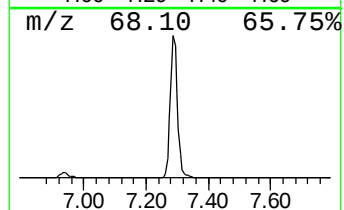
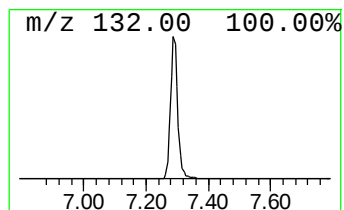
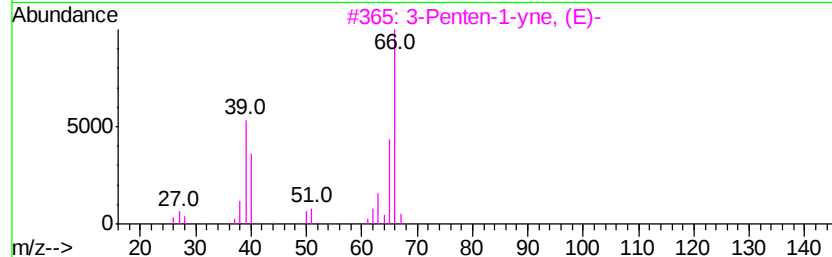
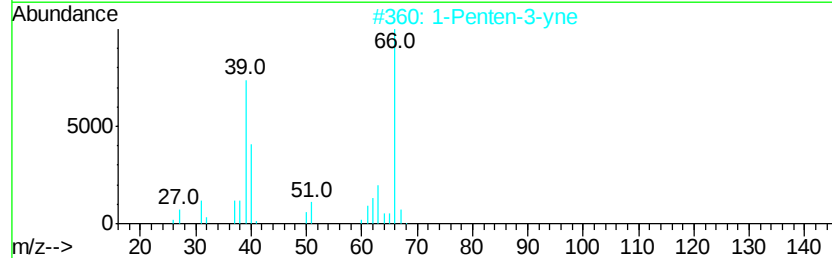
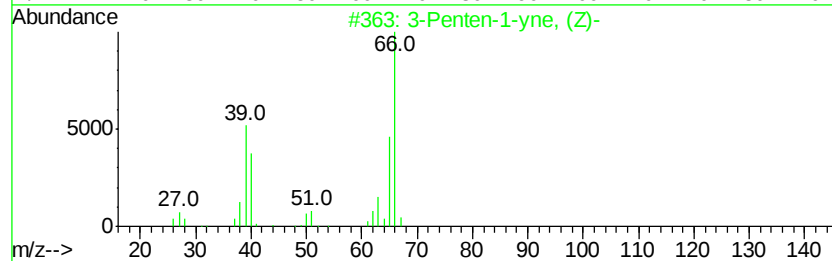
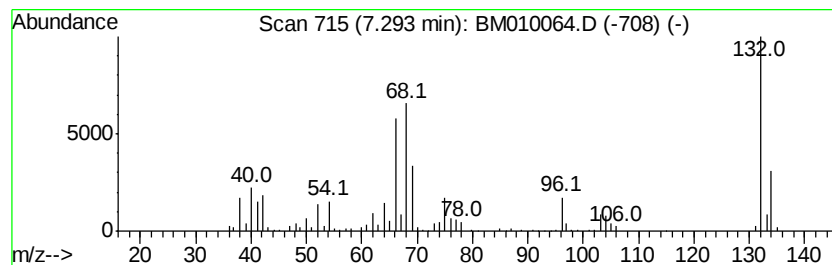
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TIC Library : C:\DATABASE\NIST02.L  
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\*\*\*\*\*  
Peak Number 4 unknown7.29 Concentration Rank 4

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 7.29 | 77.72 ng | 1415560 | 1,4-Dichlorobenzene-d4 | 7.75 |

| Hit# | of | Tentative ID            | MW  | MolForm | CAS#        | Qual |
|------|----|-------------------------|-----|---------|-------------|------|
| 1    | 5  | 3-Penten-1-yne, (Z)-    | 66  | C5H6    | 001574-40-9 | 35   |
| 2    |    | 1-Penten-3-yne          | 66  | C5H6    | 000646-05-9 | 35   |
| 3    |    | 3-Penten-1-yne, (E)-    | 66  | C5H6    | 002004-69-5 | 25   |
| 4    |    | 5-Norbornene-2-methanol | 124 | C8H12O  | 000095-12-5 | 25   |
| 5    |    | Propanedinitrile        | 66  | C3H2N2  | 000109-77-3 | 25   |



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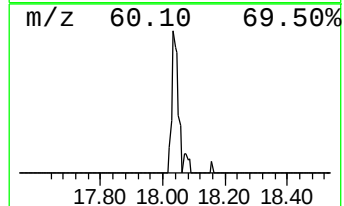
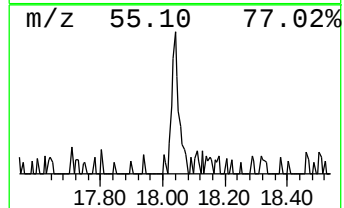
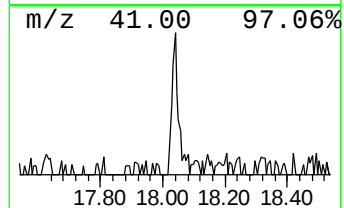
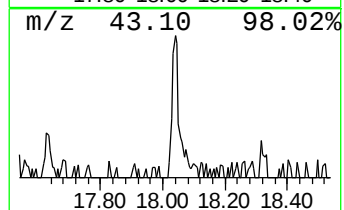
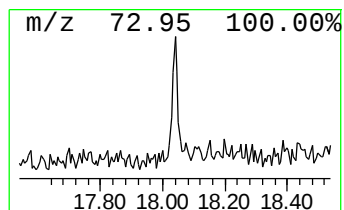
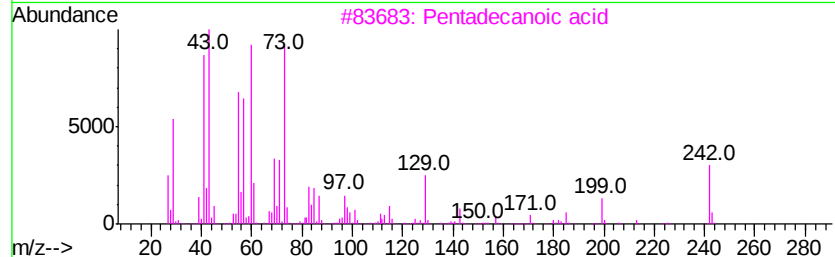
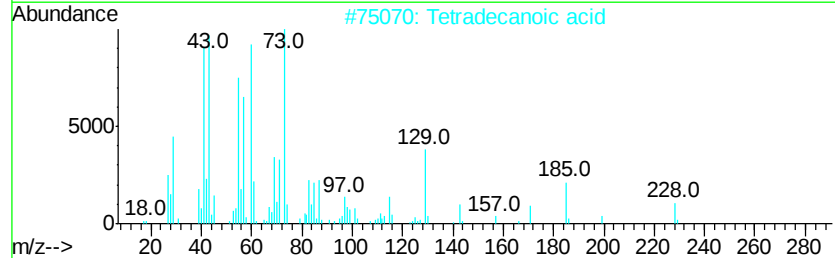
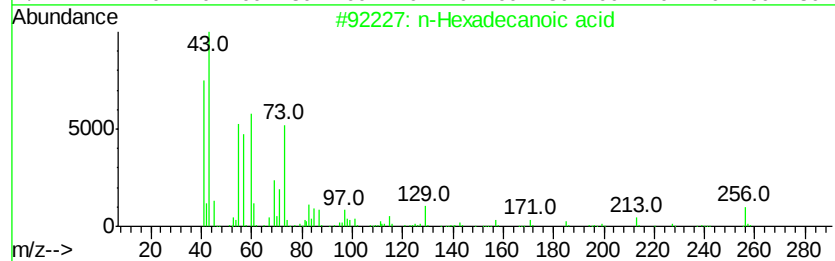
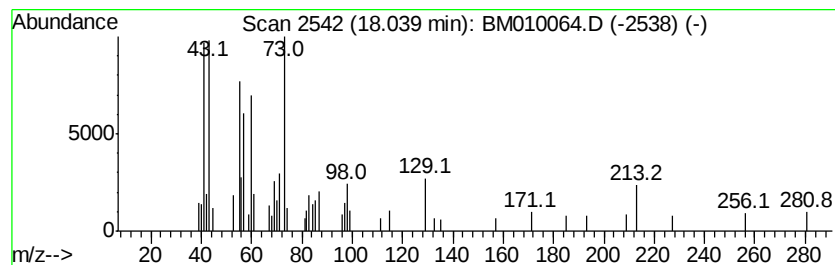
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 6 n-Hexadecanoic acid Concentration Rank 6

| R.T.  | EstConc | Area  | Relative to ISTD | R.T.  |
|-------|---------|-------|------------------|-------|
| 18.04 | 2.21 ng | 75913 | Phenanthrene-d10 | 17.16 |

| Hit# | of | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---------------------|-----|----------|-------------|------|
| 1    | 5  | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 95   |
| 2    |    | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 58   |
| 3    |    | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 53   |
| 4    |    | n-Decanoic acid     | 172 | C10H20O2 | 000334-48-5 | 47   |
| 5    |    | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 43   |



Data Path : Z:\HPCHEM1\BNA\_M\DATA\BM051617\  
Data File : BM010064.D  
Acq On : 16 May 2017 21:39  
Operator : SJ/MA  
Sample : I3180-01  
Misc :  
ALS Vial : 11 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
EFF-170515-05

Quant Method : Z:\HPCHEM1\BNA\_M\METHODS\8270-BM051117.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                      |       |         |       |          | #                     | RT    | Resp   | Conc |
| 3-Penten-2-one, 4... | 4.29  | 98.1    | ng    | 1786820  | 1                     | 7.75  | 364259 | 20.0 |
| 2-Pentanone, 4-hy... | 4.89  | 152.1   | ng    | 2769410  | 1                     | 7.75  | 364259 | 20.0 |
| 2-Pentanone, 4-me... | 5.95  | 26.6    | ng    | 483508   | 1                     | 7.75  | 364259 | 20.0 |
| unknown7.29          | 7.29  | 77.7    | ng    | 1415560  | 1                     | 7.75  | 364259 | 20.0 |
| n-Hexadecanoic acid  | 18.04 | 2.2     | ng    | 75913    | 4                     | 17.16 | 687430 | 20.0 |