

Data Path : Z:\svoasrv\HPCHEM1\BNA\_P\Data\BP102320\  
 Data File : BP003723.D  
 Acq On : 23 Oct 2020 16:36  
 Operator : CG/JU  
 Sample : L4491-01  
 Misc :  
 ALS Vial : 8 Sample Multiplier: 1

Instrument :  
 BNA\_P  
 ClientSampleId :  
 COMP-1

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\_P\METHODS\8270-BP101920.M  
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP003723.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         | 3.105       | 32            | 37          | 55           | rVB      | 3125009        | 3815995       | 56.80%          | 10.780%       |
| 2         | 3.270       | 57            | 65          | 75           | rVB      | 62358          | 134717        | 2.01%           | 0.381%        |
| 3         | 3.358       | 75            | 80          | 87           | rBV      | 179352         | 228606        | 3.40%           | 0.646%        |
| 4         | 6.022       | 525           | 533         | 545          | rBV      | 1955796        | 2938990       | 43.75%          | 8.302%        |
| 5         | 7.675       | 805           | 814         | 826          | rBV      | 1795184        | 2956613       | 44.01%          | 8.352%        |
| 6         | 8.528       | 951           | 959         | 966          | rBV      | 412623         | 682781        | 10.16%          | 1.929%        |
| 7         | 9.693       | 1148          | 1157        | 1167         | rBV      | 1248652        | 2083869       | 31.02%          | 5.887%        |
| 8         | 11.369      | 1435          | 1442        | 1450         | rBV      | 503233         | 858221        | 12.77%          | 2.424%        |
| 9         | 13.751      | 1839          | 1847        | 1858         | rBV      | 3245848        | 4558973       | 67.86%          | 12.879%       |
| 10        | 14.540      | 1973          | 1981        | 1987         | rBV      | 188718         | 256053        | 3.81%           | 0.723%        |
| 11        | 15.122      | 2073          | 2080        | 2090         | rBV      | 788643         | 1130058       | 16.82%          | 3.192%        |
| 12        | 16.592      | 2323          | 2330        | 2346         | rBV      | 2365786        | 3377797       | 50.28%          | 9.542%        |
| 13        | 17.839      | 2535          | 2542        | 2552         | rBV      | 971901         | 1368532       | 20.37%          | 3.866%        |
| 14        | 18.645      | 2675          | 2679        | 2688         | rBV      | 96334          | 148913        | 2.22%           | 0.421%        |
| 15        | 20.310      | 2956          | 2962        | 2972         | rBV      | 5644187        | 6718186       | 100.00%         | 18.978%       |
| 16        | 21.480      | 3157          | 3161        | 3166         | rBV      | 421921         | 483187        | 7.19%           | 1.365%        |
| 17        | 21.857      | 3219          | 3225        | 3230         | rVB      | 1142177        | 1569975       | 23.37%          | 4.435%        |
| 18        | 21.939      | 3236          | 3239        | 3245         | rVB2     | 78569          | 92398         | 1.38%           | 0.261%        |
| 19        | 22.421      | 3318          | 3321        | 3329         | rVB4     | 64891          | 97619         | 1.45%           | 0.276%        |
| 20        | 22.945      | 3406          | 3410        | 3415         | rBV2     | 57808          | 82842         | 1.23%           | 0.234%        |
| 21        | 23.527      | 3505          | 3509        | 3515         | rVB3     | 48980          | 78270         | 1.17%           | 0.221%        |
| 22        | 24.433      | 3655          | 3663        | 3672         | rBV      | 795527         | 1626378       | 24.21%          | 4.594%        |
| 23        | 25.045      | 3762          | 3767        | 3778         | rVB4     | 47054          | 110788        | 1.65%           | 0.313%        |

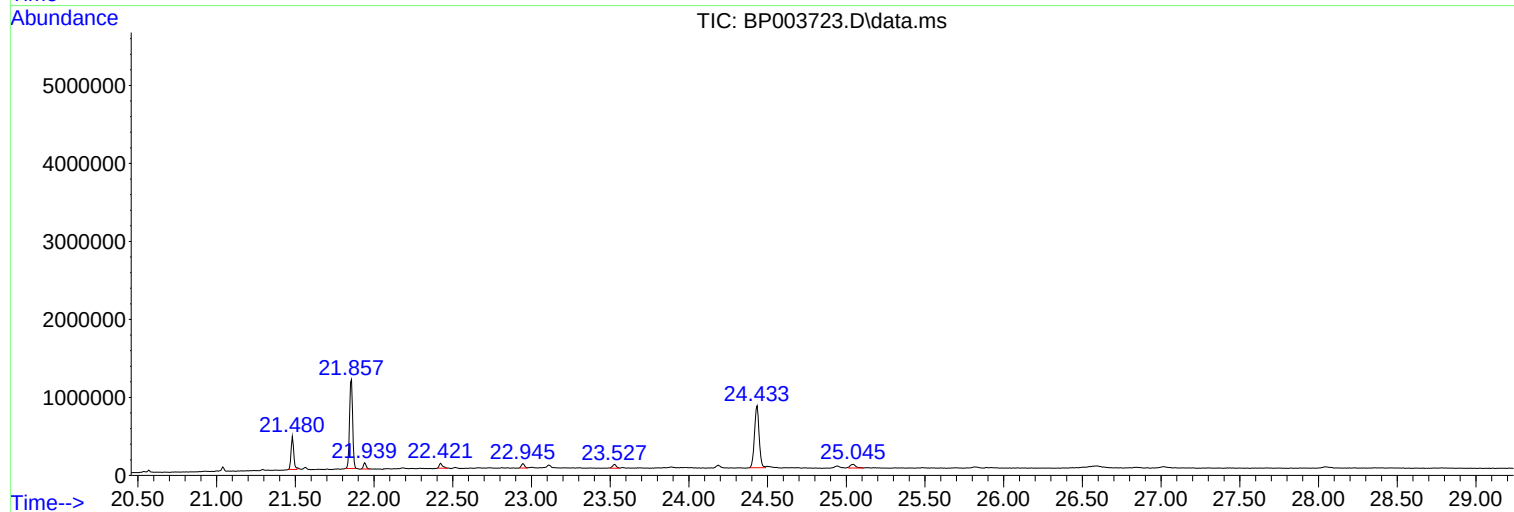
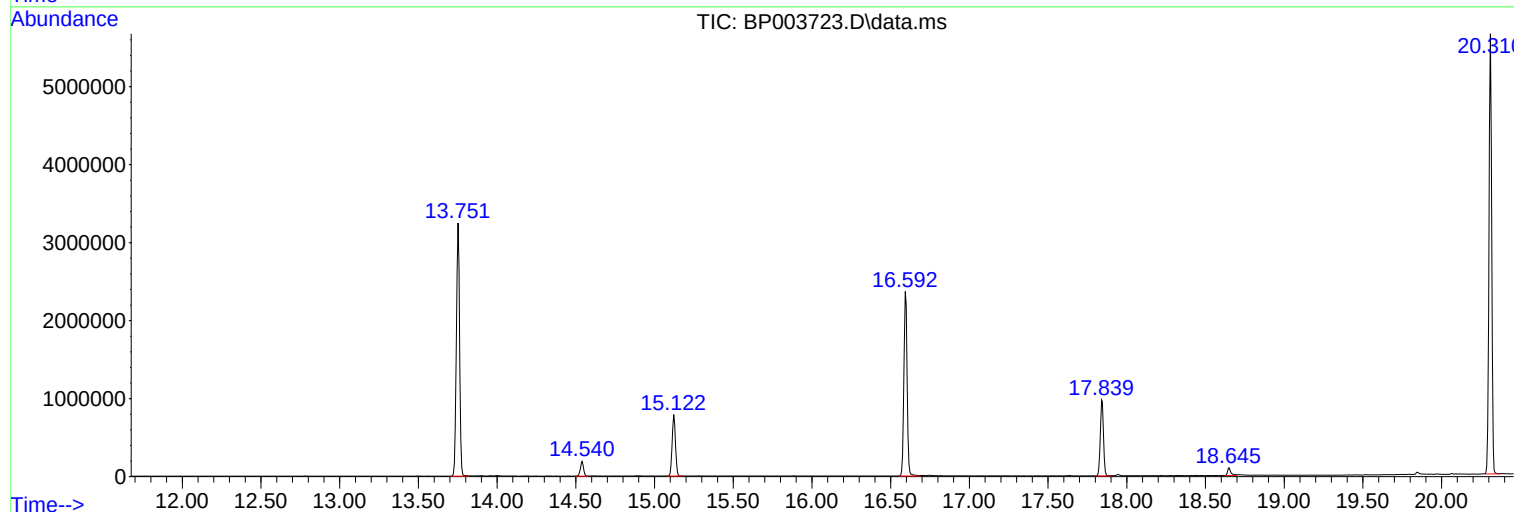
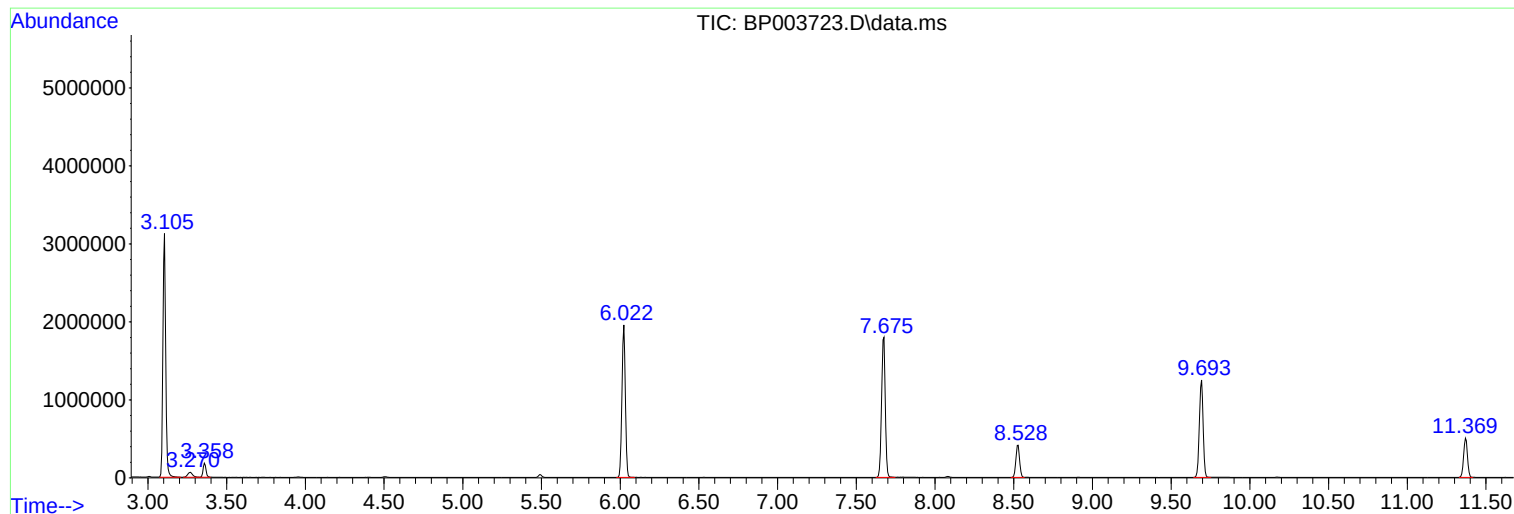
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BNA\_P  
ClientSampleId :  
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_P\METHODS\8270-BP101920.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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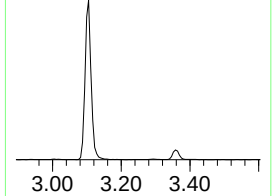
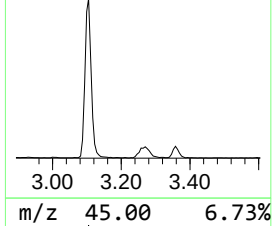
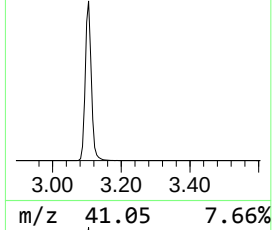
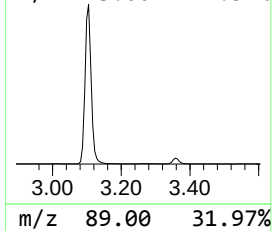
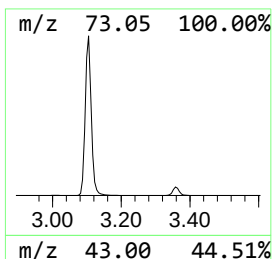
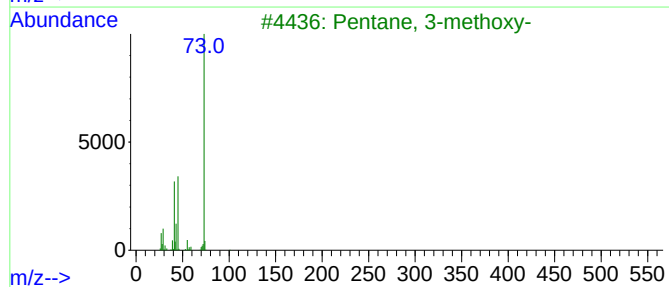
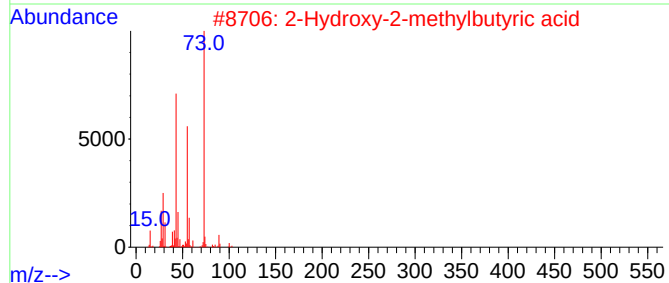
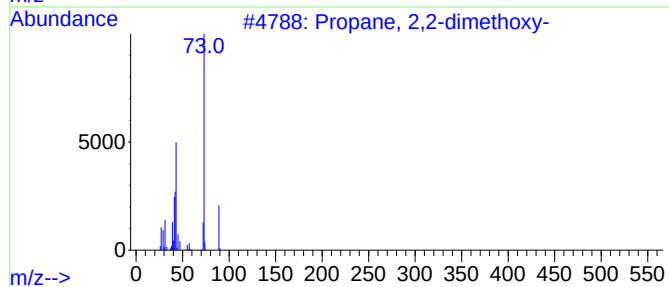
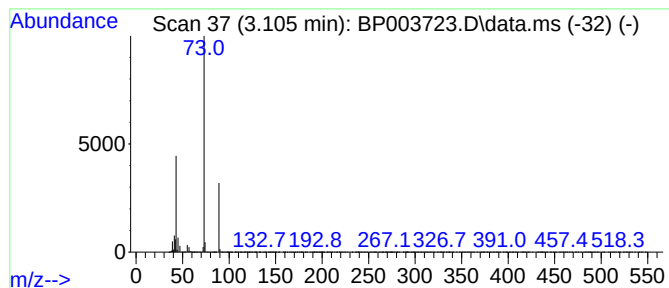
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 unknown3.10 Concentration Rank 1

| R.T.  | EstConc   | Area    | Relative to ISTD       | R.T.  |
|-------|-----------|---------|------------------------|-------|
| 3.105 | 111.78 ng | 3816000 | 1,4-Dichlorobenzene-d4 | 8.528 |

| Hit# | of | 5 | Tentative ID                   | MW  | MolForm | CAS#        | Qual |
|------|----|---|--------------------------------|-----|---------|-------------|------|
| 1    |    |   | Propane, 2,2-dimethoxy-        | 104 | C5H12O2 | 000077-76-9 | 45   |
| 2    |    |   | 2-Hydroxy-2-methylbutyric acid | 118 | C5H10O3 | 003739-30-8 | 9    |
| 3    |    |   | Pentane, 3-methoxy-            | 102 | C6H14O  | 036839-67-5 | 9    |
| 4    |    |   | Propane, 2-methoxy-2-methyl-   | 88  | C5H12O  | 001634-04-4 | 9    |
| 5    |    |   | Methane, isothiocyanato-       | 73  | C2H3NS  | 000556-61-6 | 7    |



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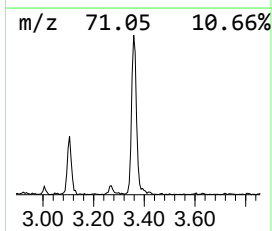
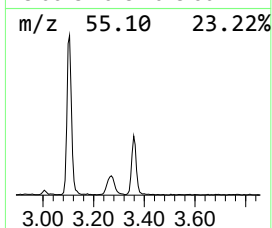
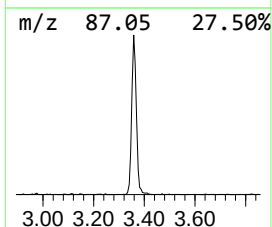
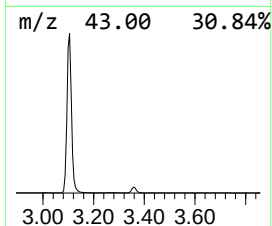
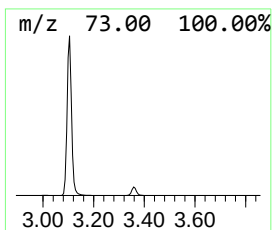
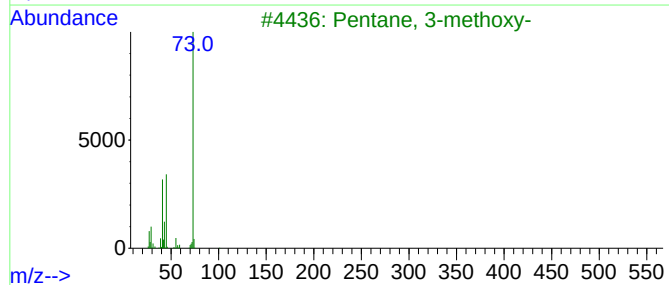
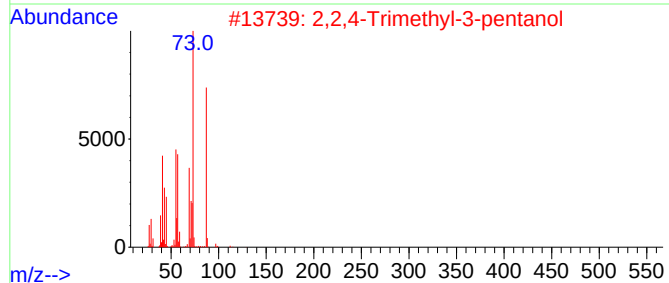
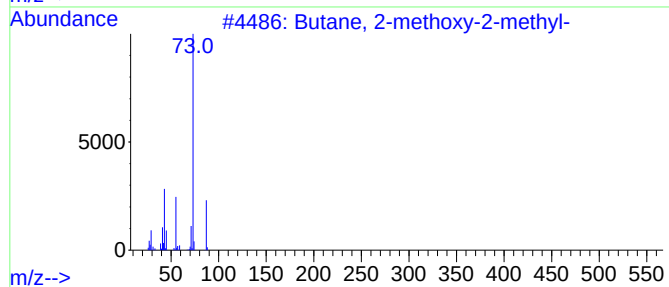
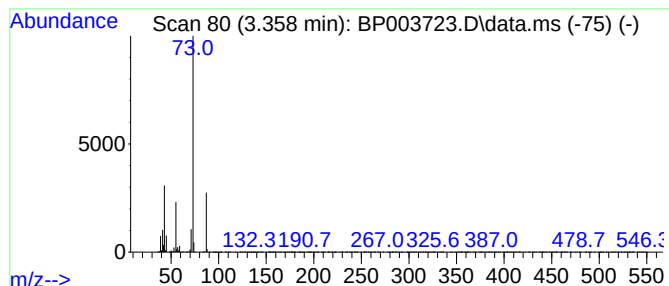
Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_P\METHODS\8270-BP101920.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 2

| R.T.  | EstConc | Area   | Relative to ISTD       | R.T.  |
|-------|---------|--------|------------------------|-------|
| 3.358 | 6.70 ng | 228606 | 1,4-Dichlorobenzene-d4 | 8.528 |

| Hit# | of | 5 | Tentative ID                | MW  | MolForm | CAS#        | Qual |
|------|----|---|-----------------------------|-----|---------|-------------|------|
| 1    |    |   | Butane, 2-methoxy-2-methyl- | 102 | C6H14O  | 000994-05-8 | 90   |
| 2    |    |   | 2,2,4-Trimethyl-3-pentanol  | 130 | C8H18O  | 005162-48-1 | 43   |
| 3    |    |   | Pentane, 3-methoxy-         | 102 | C6H14O  | 036839-67-5 | 23   |
| 4    |    |   | Silane, tetramethyl-        | 88  | C4H12Si | 000075-76-3 | 9    |
| 5    |    |   | N-Ethylformamide            | 73  | C3H7NO  | 000627-45-2 | 9    |



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BNA\_P  
ClientSampleId :  
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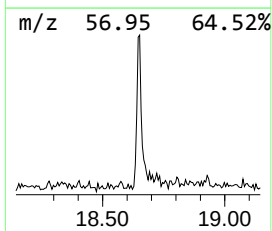
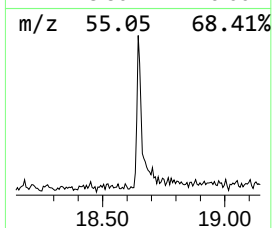
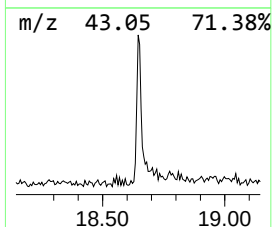
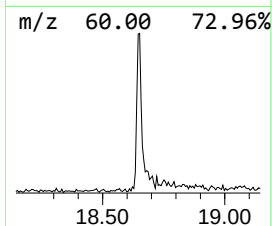
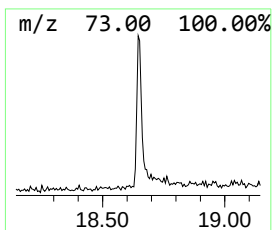
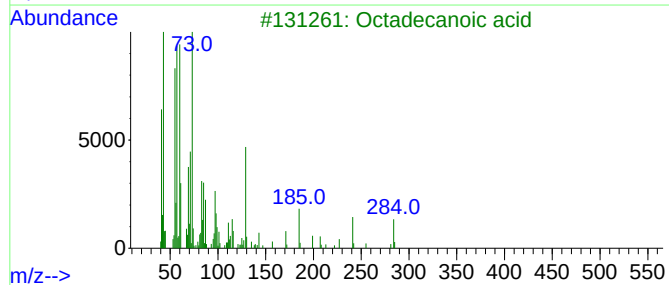
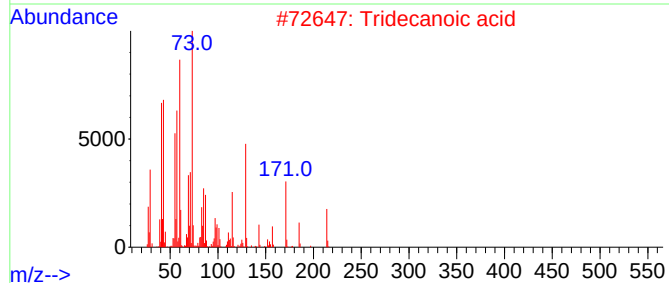
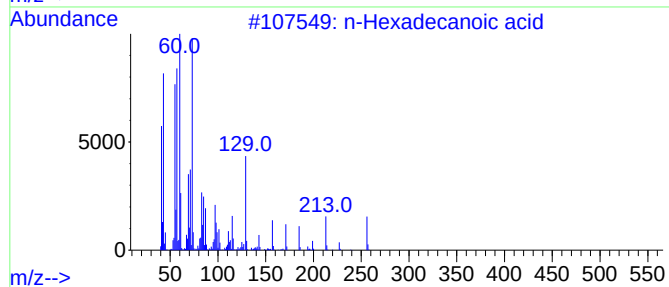
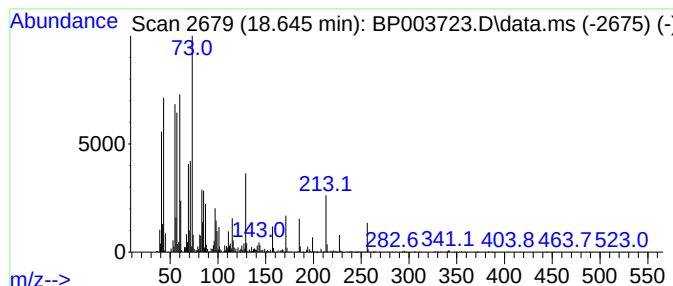
Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_P\METHODS\8270-BP101920.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 18.645 | 2.18 ng | 148913 | Phenanthrene-d10 | 17.839 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 98   |
| 2    |    |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 89   |
| 3    |    |   | Octadecanoic acid   | 284 | C18H36O2 | 000057-11-4 | 87   |
| 4    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 83   |
| 5    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 76   |



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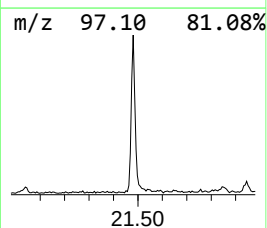
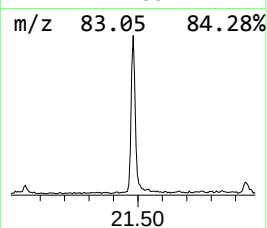
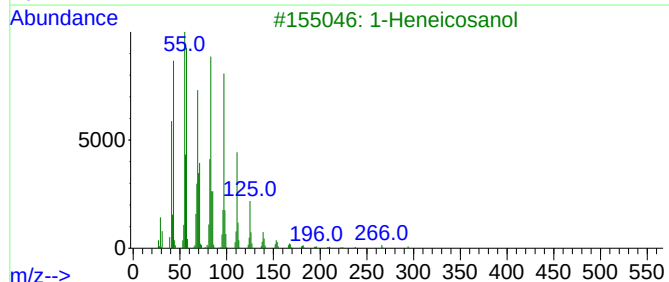
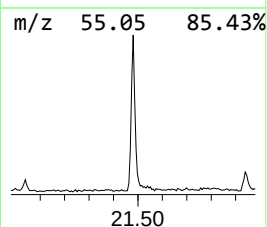
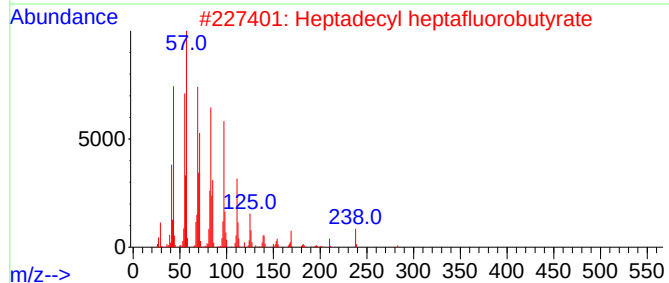
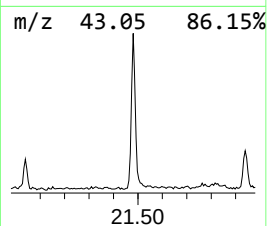
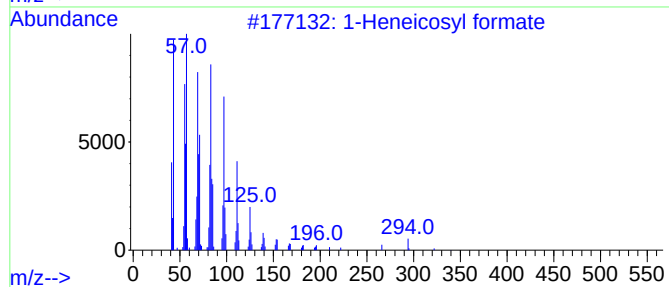
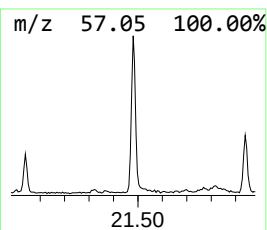
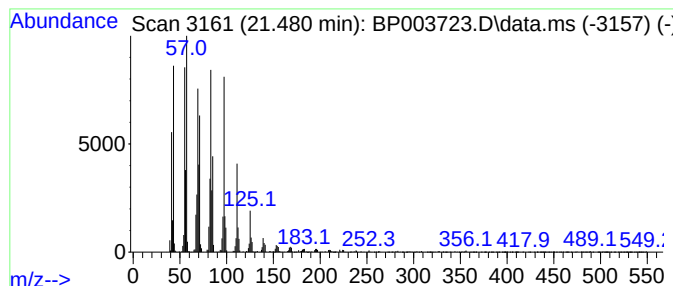
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TIC Library : C:\DATABASE\NIST11.L  
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Peak Number 5 1-Heneicosyl formate Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 21.480 | 6.16 ng | 483187 | Chrysene-d12     | 21.857 |

| Hit# | of | 5 | Tentative ID                   | MW  | MolForm    | CAS#        | Qual |
|------|----|---|--------------------------------|-----|------------|-------------|------|
| 1    |    |   | 1-Heneicosyl formate           | 340 | C22H44O2   | 077899-03-7 | 95   |
| 2    |    |   | Heptadecyl heptafluorobutyrate | 452 | C21H35F7O2 | 959085-66-6 | 94   |
| 3    |    |   | 1-Heneicosanol                 | 312 | C21H44O    | 015594-90-8 | 93   |
| 4    |    |   | Cyclopentadecane               | 210 | C15H30     | 000295-48-7 | 93   |
| 5    |    |   | Behenic alcohol                | 326 | C22H46O    | 000661-19-8 | 93   |



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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 |
| unknown3.10        | 3.105  | 111.8   | ng    | 3816000  | 1                     | 8.528  | 682781  | 20.0 |
| Butane, 2-metho... | 3.358  | 6.7     | ng    | 228606   | 1                     | 8.528  | 682781  | 20.0 |
| n-Hexadecanoic ... | 18.645 | 2.2     | ng    | 148913   | 4                     | 17.839 | 1368530 | 20.0 |
| 1-Heneicosyl fo... | 21.480 | 6.2     | ng    | 483187   | 5                     | 21.857 | 1569980 | 20.0 |