

Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM041625\  
 Data File : BM049945.D  
 Acq On : 16 Apr 2025 10:07  
 Operator : RC/JU  
 Sample : PB167561BL  
 Misc :  
 ALS Vial : 3 Sample Multiplier: 1

Instrument :  
 BNA\_M  
 ClientSampleId :  
 PB167561BL

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\_M\Methods\8270-BM040825.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM049945.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         | 4.887       | 318           | 323         | 334          | rBV      | 1600948        | 2138101       | 12.36%          | 2.818%        |
| 2         | 5.357       | 397           | 403         | 416          | rBV      | 5107231        | 7335027       | 42.40%          | 9.667%        |
| 3         | 5.963       | 501           | 506         | 516          | rVB      | 282112         | 399453        | 2.31%           | 0.526%        |
| 4         | 6.951       | 666           | 674         | 699          | rBV      | 4414678        | 7244649       | 41.87%          | 9.547%        |
| 5         | 7.769       | 806           | 813         | 828          | rVB      | 1087488        | 1680162       | 9.71%           | 2.214%        |
| 6         | 8.928       | 1002          | 1010        | 1024         | rBV      | 2767687        | 4641890       | 26.83%          | 6.117%        |
| 7         | 10.563      | 1280          | 1288        | 1304         | rBV      | 1183151        | 2066661       | 11.94%          | 2.724%        |
| 8         | 13.033      | 1701          | 1708        | 1721         | rBV      | 7807782        | 11349841      | 65.60%          | 14.958%       |
| 9         | 14.416      | 1935          | 1943        | 1962         | rBV      | 1771682        | 2741706       | 15.85%          | 3.613%        |
| 10        | 15.910      | 2189          | 2197        | 2220         | rBV      | 5510838        | 8833164       | 51.05%          | 11.641%       |
| 11        | 17.162      | 2403          | 2410        | 2423         | rBV2     | 2059620        | 3097409       | 17.90%          | 4.082%        |
| 12        | 18.062      | 2558          | 2563        | 2578         | rBV3     | 117316         | 366215        | 2.12%           | 0.483%        |
| 13        | 19.786      | 2851          | 2856        | 2868         | rBV      | 14868757       | 17301606      | 100.00%         | 22.801%       |
| 14        | 21.403      | 3125          | 3131        | 3141         | rBV      | 2095667        | 3277744       | 18.94%          | 4.320%        |
| 15        | 24.409      | 3634          | 3642        | 3654         | rVB      | 1344838        | 3406678       | 19.69%          | 4.490%        |

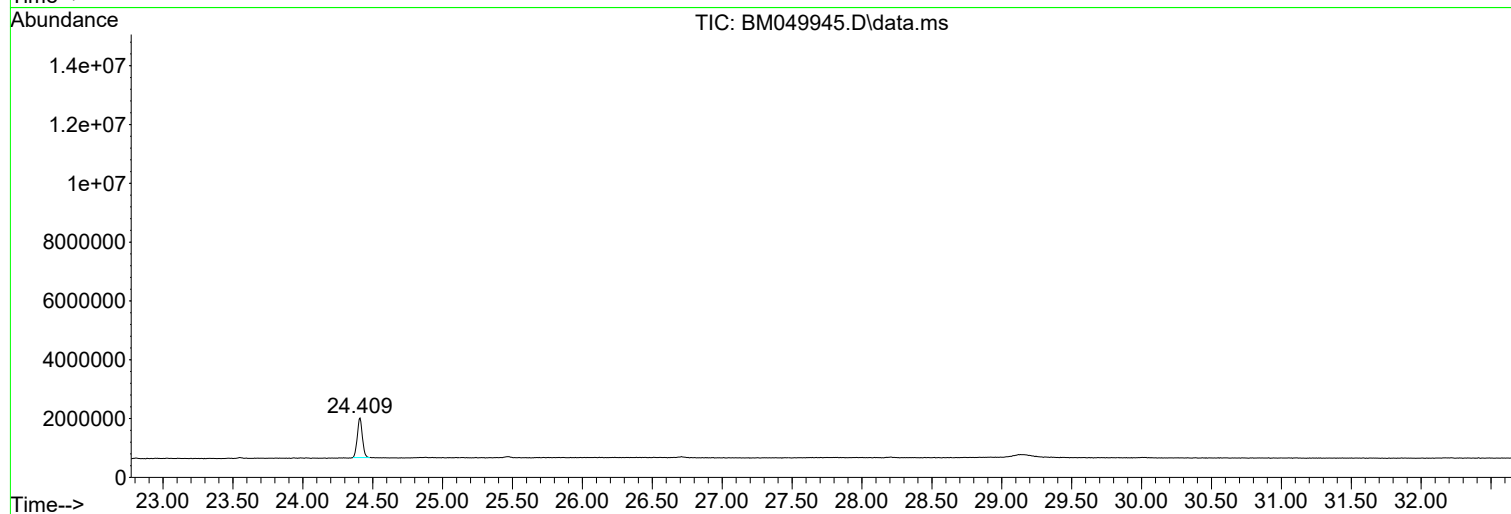
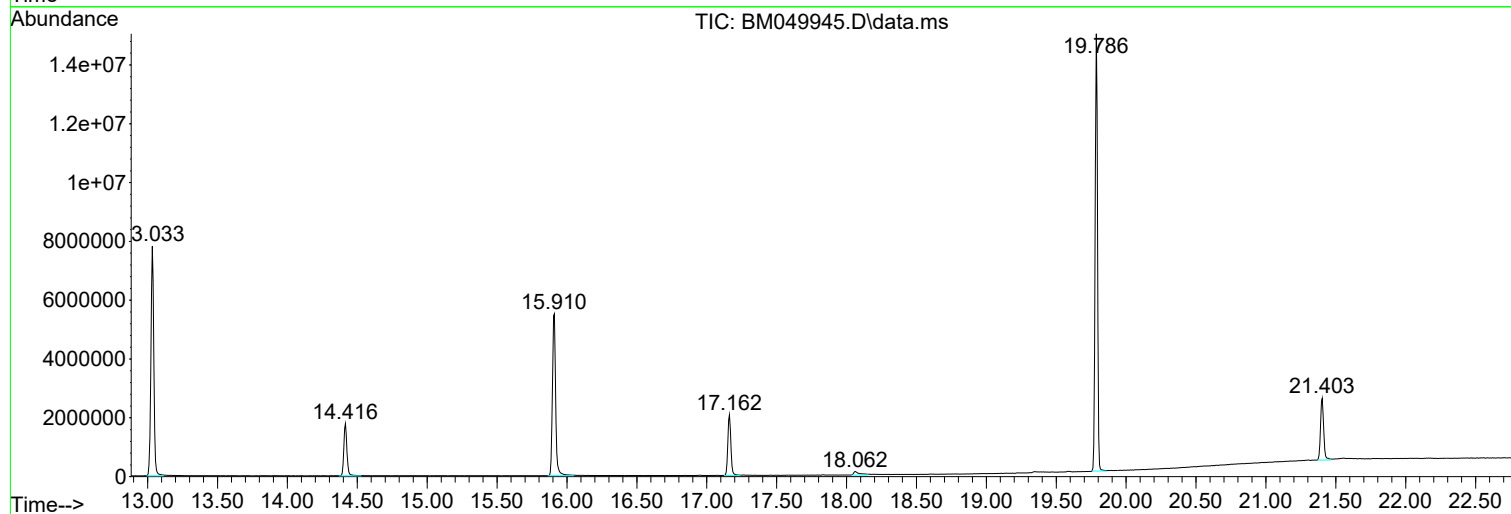
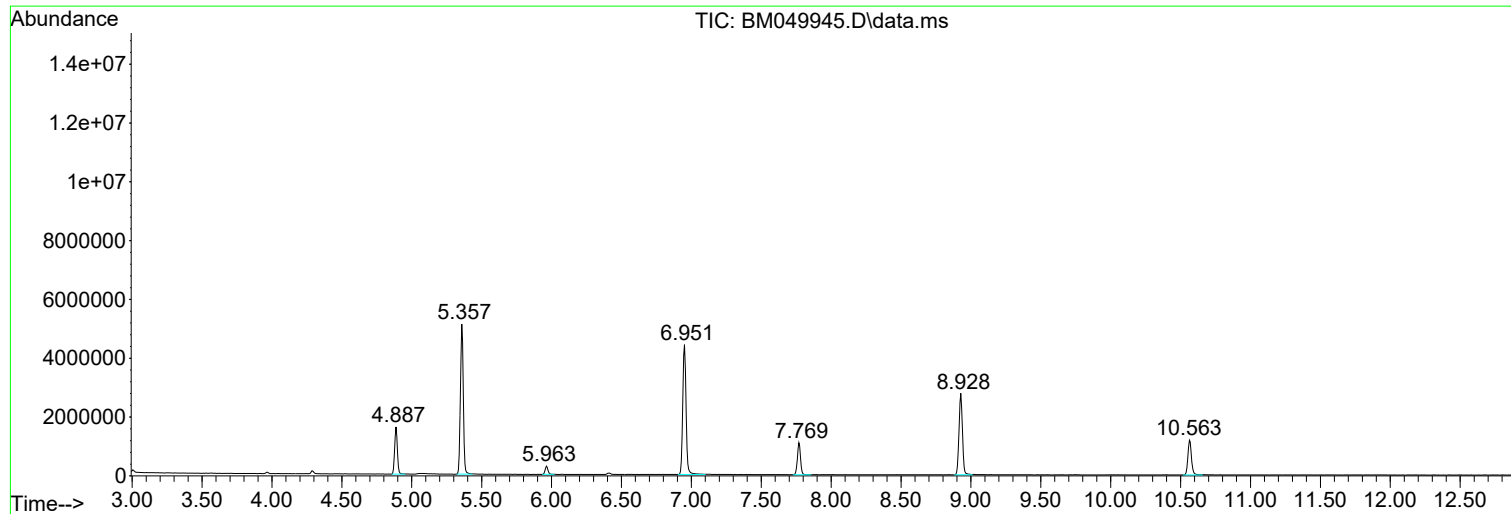
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Instrument :  
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ClientSampleId :  
PB167561BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM040825.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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Sample : PB167561BL  
Misc :  
ALS Vial : 3 Sample Multiplier: 1

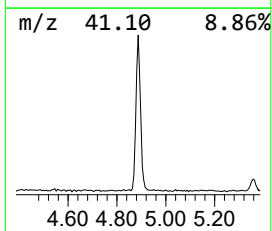
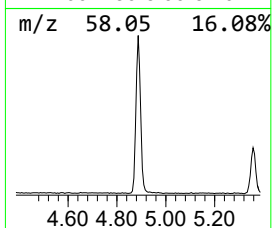
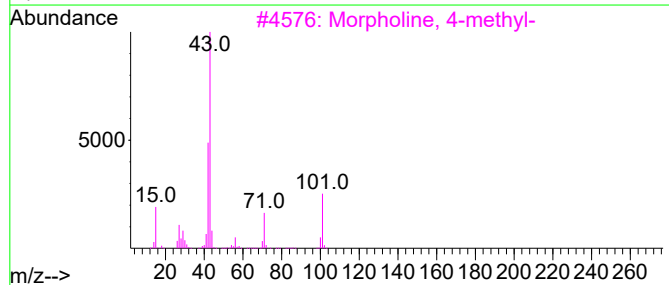
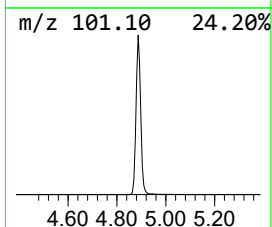
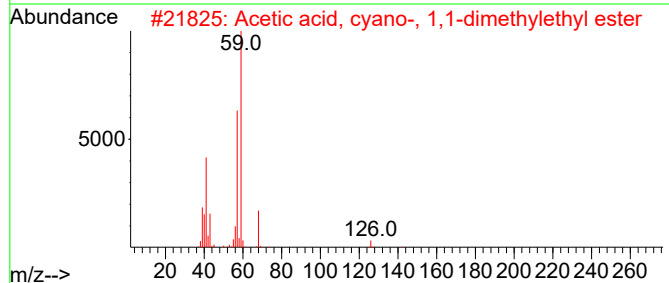
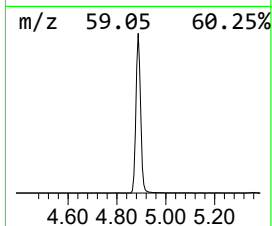
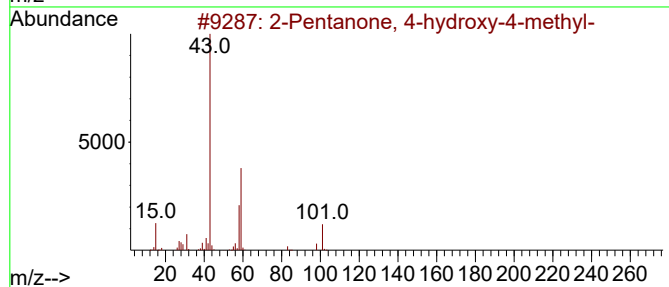
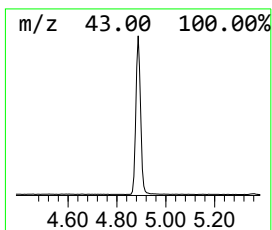
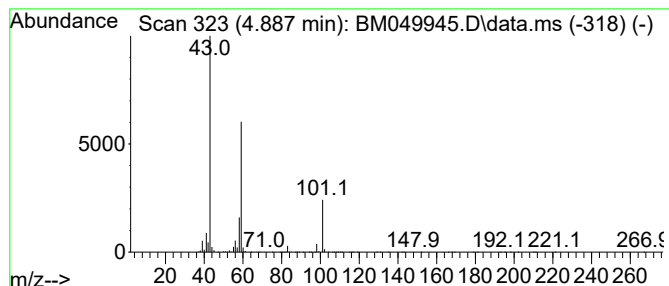
Instrument :  
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ClientSampleId :  
PB167561BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM040825.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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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

| R.T.    | EstConc                             | Area         | Relative to ISTD       |         |             | R.T.  |
|---------|-------------------------------------|--------------|------------------------|---------|-------------|-------|
| 4.887   | 25.45 ng                            | 2138100      | 1,4-Dichlorobenzene-d4 |         |             | 7.769 |
| Hit# of | 5                                   | Tentative ID | MW                     | MolForm | CAS#        | Qual  |
| 1       | 2-Pentanone, 4-hydroxy-4-methyl-    | 116          | C6H12O2                |         | 000123-42-2 | 50    |
| 2       | Acetic acid, cyano-, 1,1-dimethy... | 141          | C7H11NO2               |         | 001116-98-9 | 17    |
| 3       | Morpholine, 4-methyl-               | 101          | C5H11NO                |         | 000109-02-4 | 9     |
| 4       | 5-Hexen-2-one                       | 98           | C6H10O                 |         | 000109-49-9 | 9     |
| 5       | Butane, 1-ethoxy-                   | 102          | C6H14O                 |         | 000628-81-9 | 9     |



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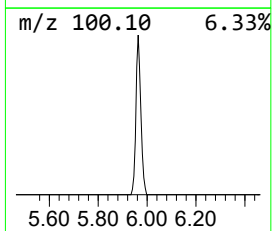
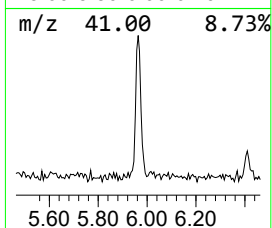
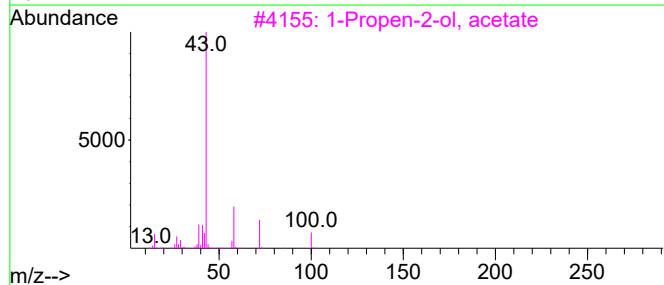
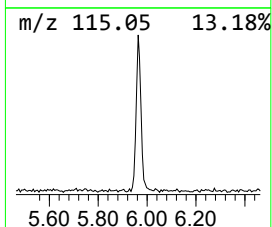
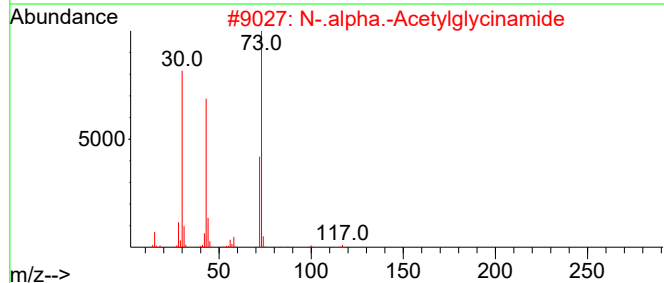
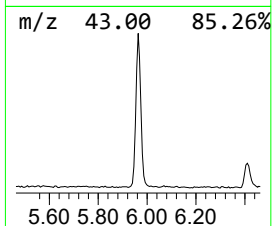
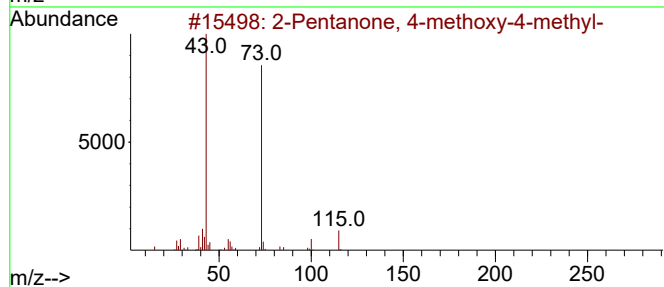
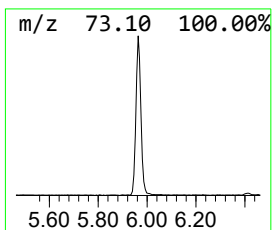
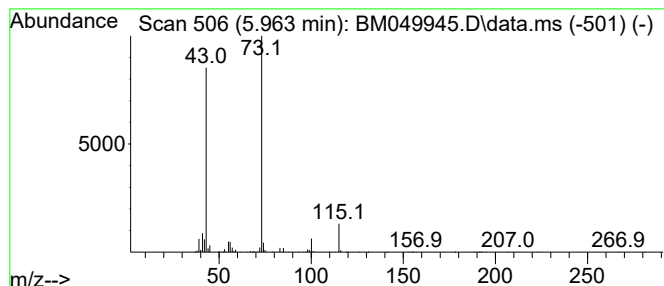
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Peak Number 2 2-Pentanone, 4-methoxy-4-me... Concentration Rank 2

| R.T.      | EstConc                           | Area   | Relative to ISTD       |          |             | R.T.  |
|-----------|-----------------------------------|--------|------------------------|----------|-------------|-------|
| 5.963     | 4.75 ng                           | 399453 | 1,4-Dichlorobenzene-d4 |          |             | 7.769 |
| Hit# of 5 | Tentative ID                      |        | MW                     | MolForm  | CAS#        | Qual  |
| 1         | 2-Pentanone, 4-methoxy-4-methyl-  |        | 130                    | C7H14O2  | 000107-70-0 | 83    |
| 2         | N-.alpha.-Acetylglycinamide       |        | 116                    | C4H8N2O2 | 002620-63-5 | 28    |
| 3         | 1-Propen-2-ol, acetate            |        | 100                    | C5H8O2   | 000108-22-5 | 12    |
| 4         | 1,3-Dioxolane, 2-(1-methylethyl)- |        | 116                    | C6H12O2  | 000822-83-3 | 10    |
| 5         | Borane, dimethoxy-                |        | 74                     | C2H7BO2  | 004542-61-4 | 9     |



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BNA\_M  
ClientSampleId :  
PB167561BL

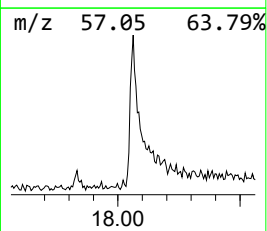
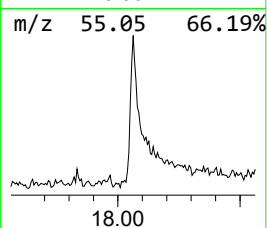
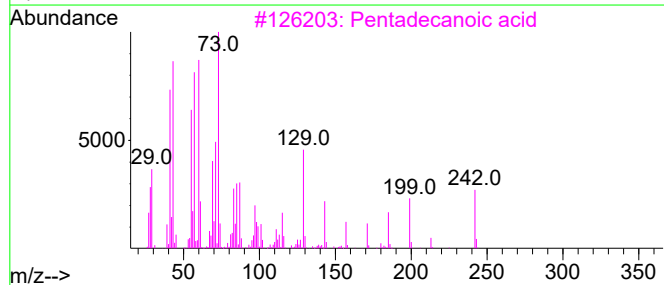
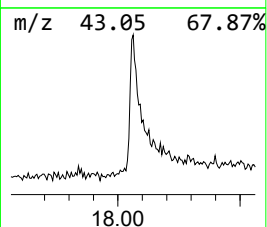
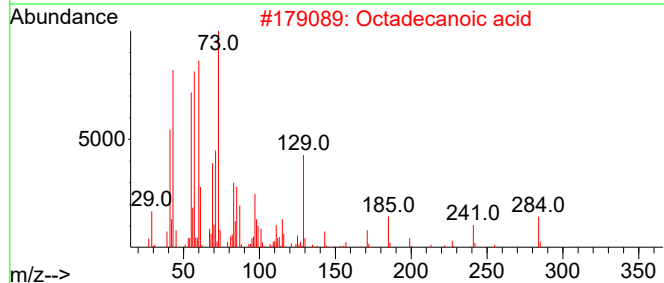
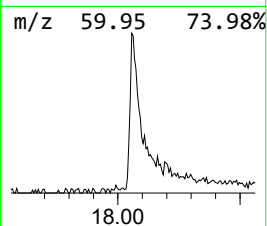
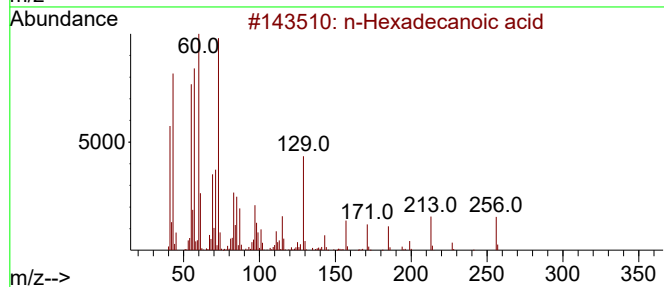
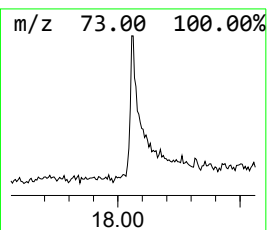
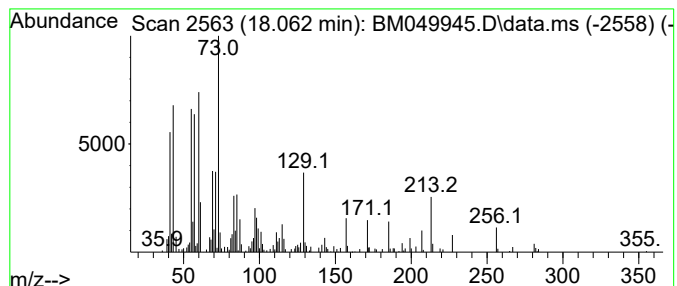
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.   |
|--------|---------|--------|------------------|--------|
| 18.062 | 2.36 ng | 366215 | Phenanthrene-d10 | 17.162 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 99   |
| 2    |    |   | Octadecanoic acid   | 284 | C18H36O2 | 000057-11-4 | 81   |
| 3    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 81   |
| 4    |    |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 76   |
| 5    |    |   | n-Decanoic acid     | 172 | C10H20O2 | 000334-48-5 | 55   |



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Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
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| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |         |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|---------|------|
|                    |        |         |       |          | #                     | RT     | Resp    | Conc |
| 2-Pentanone, 4-... | 4.887  | 25.4    | ng    | 2138100  | 1                     | 7.769  | 1680160 | 20.0 |
| 2-Pentanone, 4-... | 5.963  | 4.8     | ng    | 399453   | 1                     | 7.769  | 1680160 | 20.0 |
| n-Hexadecanoic ... | 18.062 | 2.4     | ng    | 366215   | 4                     | 17.162 | 3097410 | 20.0 |