

Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM041323\  
 Data File : BM039412.D  
 Acq On : 13 Apr 2023 15:37  
 Operator : CG/JU  
 Sample : PB152103BL  
 Misc :  
 ALS Vial : 3 Sample Multiplier: 1

Instrument :  
 BNA\_M  
 ClientSampleId :  
 PB152103BL

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-BM032923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM039412.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         | 4.952       | 294           | 300         | 315          | rBV      | 2404383        | 3323619       | 32.45%          | 5.217%        |
| 2         | 5.440       | 377           | 383         | 412          | rBV      | 5295796        | 8005964       | 78.16%          | 12.568%       |
| 3         | 7.069       | 652           | 660         | 683          | rBV      | 4693018        | 7847237       | 76.61%          | 12.319%       |
| 4         | 7.863       | 788           | 795         | 810          | rBV      | 894491         | 1489637       | 14.54%          | 2.338%        |
| 5         | 9.034       | 986           | 994         | 1019         | rBV      | 2672935        | 4918717       | 48.02%          | 7.721%        |
| 6         | 10.675      | 1265          | 1273        | 1297         | rBV      | 1061922        | 1990971       | 19.44%          | 3.125%        |
| 7         | 13.139      | 1685          | 1692        | 1716         | rBV      | 6519239        | 10039533      | 98.01%          | 15.760%       |
| 8         | 14.516      | 1919          | 1926        | 1943         | rBV      | 1465734        | 2313138       | 22.58%          | 3.631%        |
| 9         | 16.016      | 2174          | 2181        | 2206         | rBV      | 4138003        | 6344321       | 61.93%          | 9.959%        |
| 10        | 17.268      | 2388          | 2394        | 2411         | rBV      | 1523069        | 2362662       | 23.06%          | 3.709%        |
| 11        | 18.168      | 2542          | 2547        | 2563         | rBV      | 180284         | 459521        | 4.49%           | 0.721%        |
| 12        | 19.451      | 2761          | 2765        | 2778         | rBV3     | 145655         | 356407        | 3.48%           | 0.559%        |
| 13        | 19.586      | 2785          | 2788        | 2793         | rVB      | 102879         | 118327        | 1.16%           | 0.186%        |
| 14        | 19.898      | 2835          | 2841        | 2855         | rBV      | 7852034        | 10243532      | 100.00%         | 16.080%       |
| 15        | 21.456      | 3102          | 3106        | 3116         | rBV      | 1443231        | 1972964       | 19.26%          | 3.097%        |
| 16        | 23.844      | 3507          | 3512        | 3523         | rVB2     | 926399         | 1916281       | 18.71%          | 3.008%        |

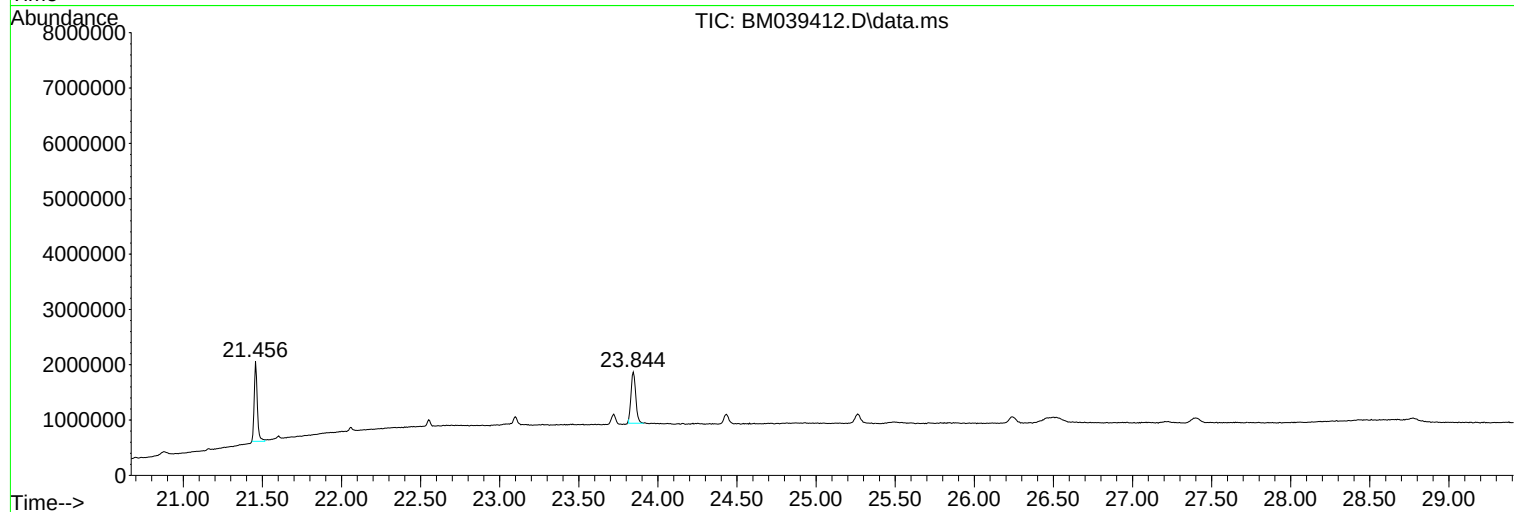
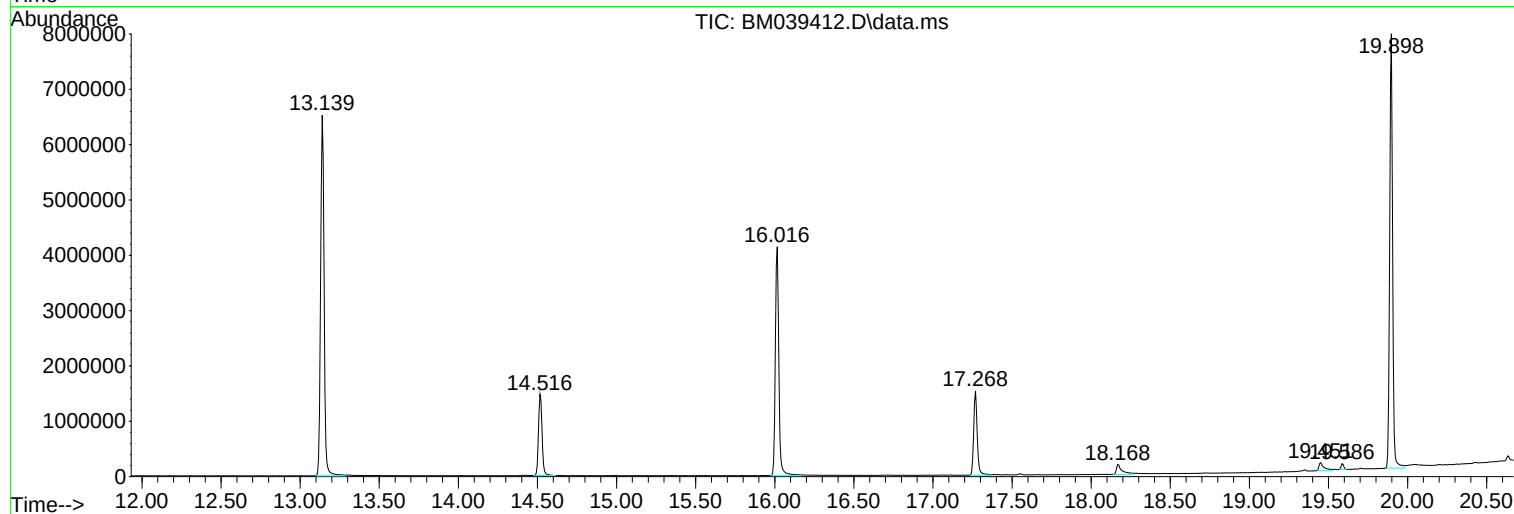
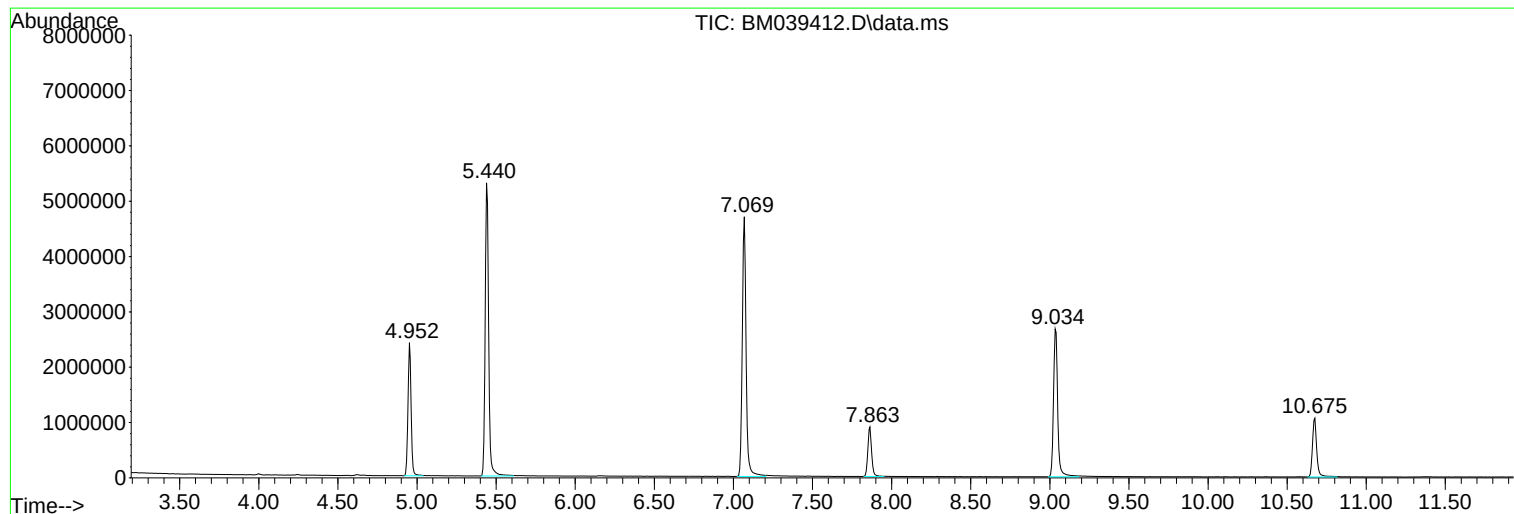
Sum of corrected areas: 63702831

Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM041323\  
Data File : BM039412.D  
Acq On : 13 Apr 2023 15:37  
Operator : CG/JU  
Sample : PB152103BL  
Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
PB152103BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM032923.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM041323\  
Data File : BM039412.D  
Acq On : 13 Apr 2023 15:37  
Operator : CG/JU  
Sample : PB152103BL  
Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
PB152103BL

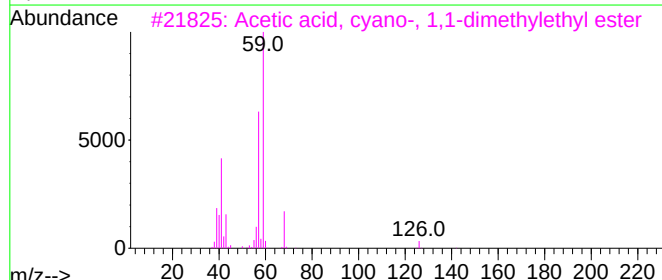
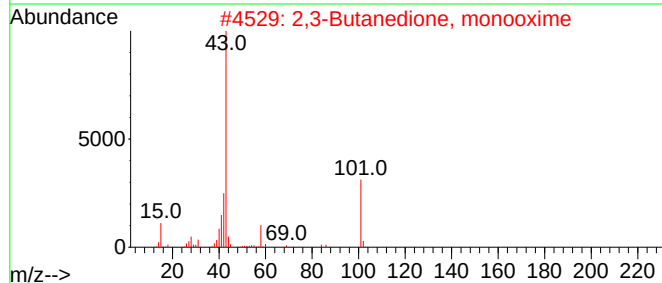
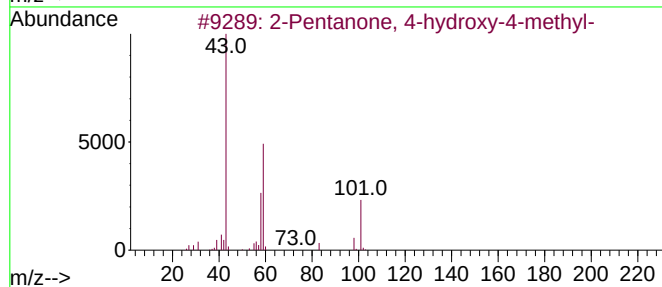
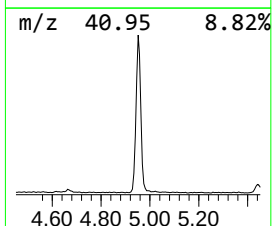
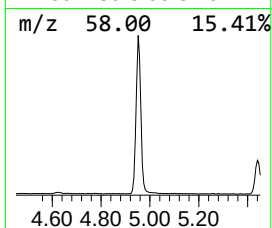
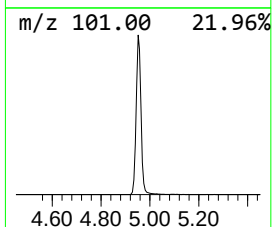
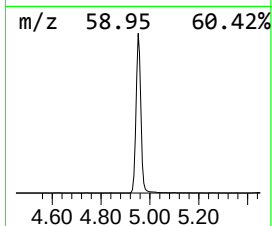
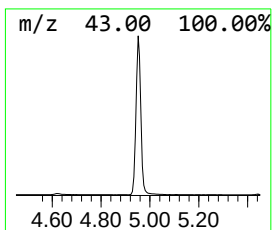
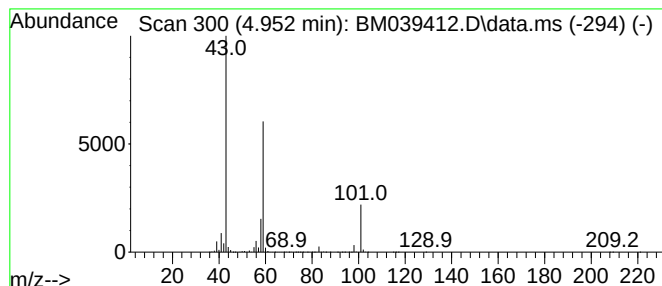
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM032923.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*

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

| R.T.      | EstConc                             | Area    | Relative to ISTD       |          |             | R.T.  |
|-----------|-------------------------------------|---------|------------------------|----------|-------------|-------|
| 4.952     | 44.62 ng                            | 3323620 | 1,4-Dichlorobenzene-d4 |          |             | 7.863 |
| Hit# of 5 | Tentative ID                        |         | MW                     | MolForm  | CAS#        | Qual  |
| 1         | 2-Pentanone, 4-hydroxy-4-methyl-    |         | 116                    | C6H12O2  | 000123-42-2 | 64    |
| 2         | 2,3-Butanedione, monooxime          |         | 101                    | C4H7NO2  | 000057-71-6 | 17    |
| 3         | Acetic acid, cyano-, 1,1-dimethy... |         | 141                    | C7H11NO2 | 001116-98-9 | 17    |
| 4         | Butane, 1-ethoxy-                   |         | 102                    | C6H14O   | 000628-81-9 | 9     |
| 5         | Morpholine, 4-methyl-               |         | 101                    | C5H11NO  | 000109-02-4 | 9     |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM041323\  
Data File : BM039412.D  
Acq On : 13 Apr 2023 15:37  
Operator : CG/JU  
Sample : PB152103BL  
Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
PB152103BL

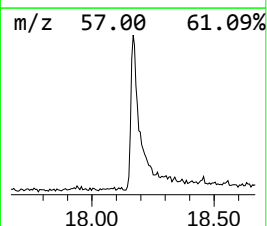
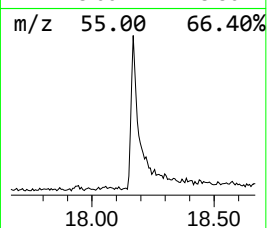
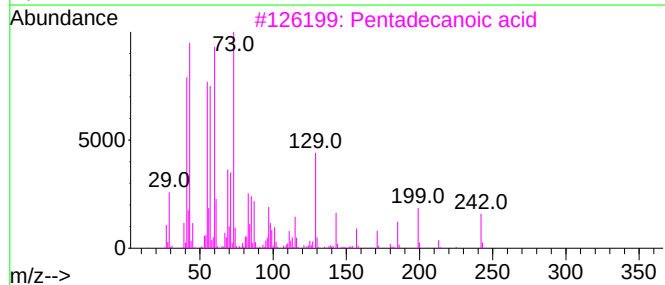
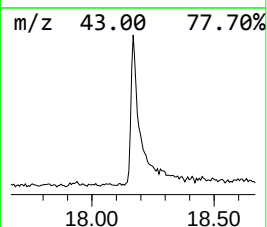
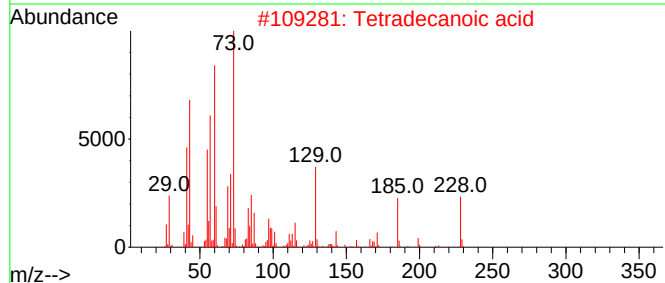
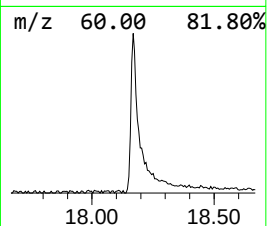
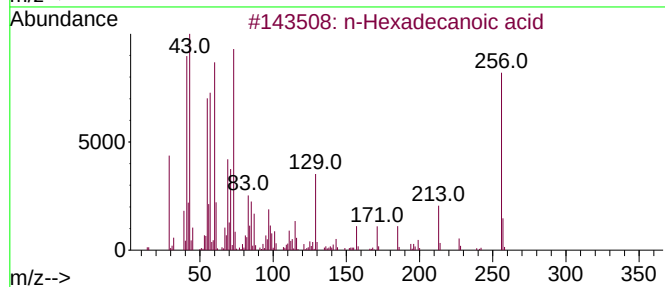
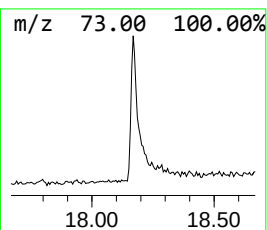
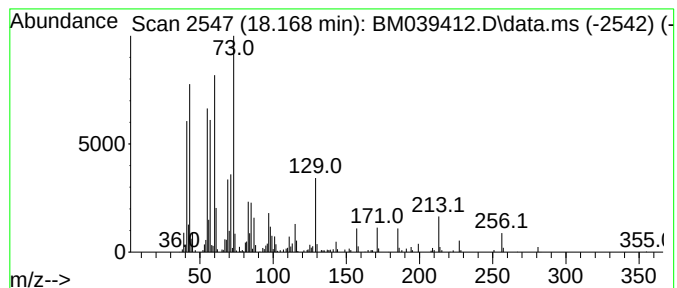
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM032923.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 18.168 | 3.89 ng | 459521 | Phenanthrene-d10 | 17.268 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 99   |
| 2    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 93   |
| 3    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 90   |
| 4    |    |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 87   |
| 5    |    |   | n-Decanoic acid     | 172 | C10H20O2 | 000334-48-5 | 50   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM041323\  
Data File : BM039412.D  
Acq On : 13 Apr 2023 15:37  
Operator : CG/JU  
Sample : PB152103BL  
Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
PB152103BL

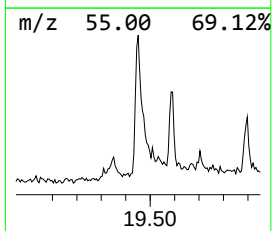
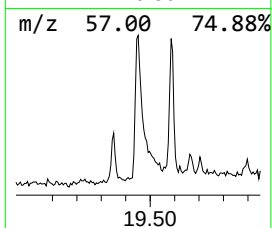
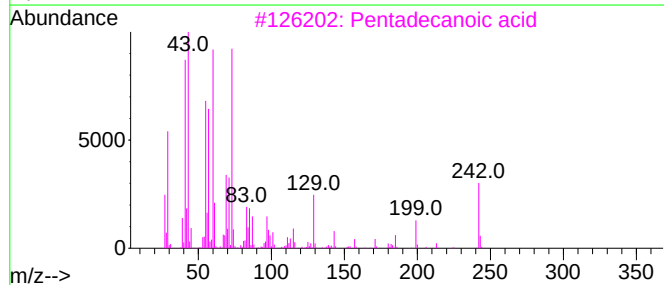
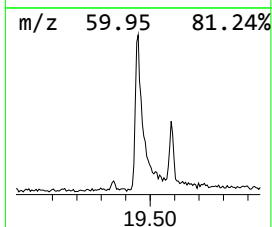
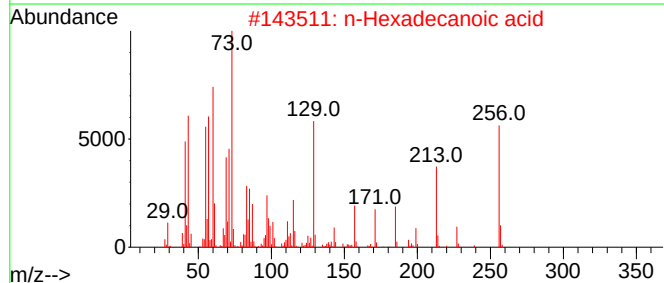
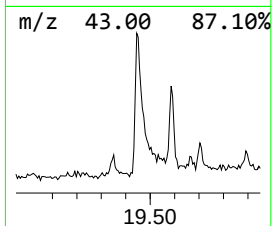
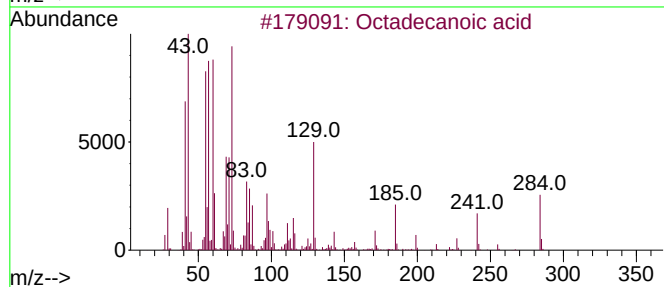
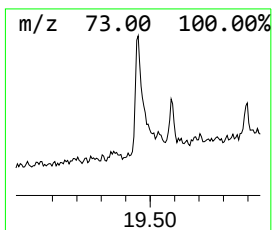
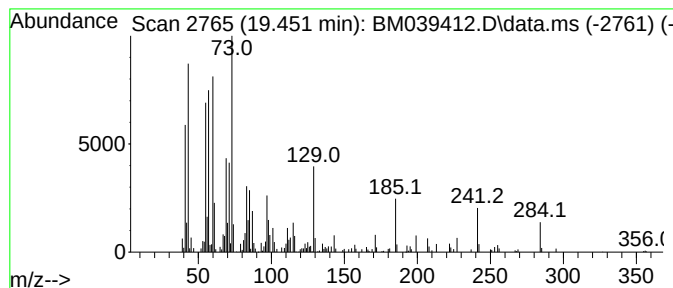
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM032923.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 3 Octadecanoic acid Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 19.451 | 3.61 ng | 356407 | Chrysene-d12     | 21.456 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | Octadecanoic acid                   | 284 | C18H36O2 | 000057-11-4 | 99   |
| 2    |    |   | n-Hexadecanoic acid                 | 256 | C16H32O2 | 000057-10-3 | 90   |
| 3    |    |   | Pentadecanoic acid                  | 242 | C15H30O2 | 001002-84-2 | 90   |
| 4    |    |   | Octadecanoic acid, 2-(2-hydroxye... | 372 | C22H44O4 | 000106-11-6 | 87   |
| 5    |    |   | Tetradecanoic acid                  | 228 | C14H28O2 | 000544-63-8 | 83   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM041323\  
Data File : BM039412.D  
Acq On : 13 Apr 2023 15:37  
Operator : CG/JU  
Sample : PB152103BL  
Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
PB152103BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM032923.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |         |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|---------|------|
|                    |        |         |       |          | #                     | RT     | Resp    | Conc |
| 2-Pentanone, 4-... | 4.952  | 44.6    | ng    | 3323620  | 1                     | 7.863  | 1489640 | 20.0 |
| n-Hexadecanoic ... | 18.168 | 3.9     | ng    | 459521   | 4                     | 17.268 | 2362660 | 20.0 |
| Octadecanoic acid  | 19.451 | 3.6     | ng    | 356407   | 5                     | 21.456 | 1972960 | 20.0 |