

Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG112522\  
 Data File : BG055784.D  
 Acq On : 25 Nov 2022 17:17  
 Operator : CG/JU  
 Sample : N5741-04  
 Misc :  
 ALS Vial : 5 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 MW-18R

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\_G\Methods\8270-BG111622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055784.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         | 5.286       | 333           | 340         | 351          | rVB      | 65605          | 103582        | 3.40%           | 0.859%        |
| 2         | 5.768       | 415           | 422         | 432          | rVB      | 318285         | 527219        | 17.29%          | 4.370%        |
| 3         | 7.378       | 687           | 696         | 706          | rBV      | 205124         | 359428        | 11.79%          | 2.979%        |
| 4         | 8.235       | 834           | 842         | 849          | rBV      | 140992         | 238195        | 7.81%           | 1.974%        |
| 5         | 9.405       | 1032          | 1041        | 1053         | rBV      | 432833         | 788895        | 25.87%          | 6.539%        |
| 6         | 11.061      | 1316          | 1323        | 1332         | rBV      | 187495         | 343054        | 11.25%          | 2.843%        |
| 7         | 13.482      | 1728          | 1735        | 1744         | rBV      | 1221975        | 1870490       | 61.35%          | 15.503%       |
| 8         | 14.857      | 1963          | 1969        | 1977         | rVB      | 325569         | 514059        | 16.86%          | 4.261%        |
| 9         | 16.203      | 2192          | 2198        | 2203         | rBV      | 31649          | 45947         | 1.51%           | 0.381%        |
| 10        | 16.344      | 2215          | 2222        | 2239         | rBV      | 997207         | 1562892       | 51.26%          | 12.954%       |
| 11        | 17.601      | 2429          | 2436        | 2443         | rBV      | 446830         | 675431        | 22.15%          | 5.598%        |
| 12        | 18.453      | 2577          | 2581        | 2592         | rBV      | 77379          | 137824        | 4.52%           | 1.142%        |
| 13        | 19.716      | 2791          | 2796        | 2807         | rBV3     | 40167          | 78486         | 2.57%           | 0.651%        |
| 14        | 20.186      | 2870          | 2876        | 2884         | rBV      | 2304534        | 3048951       | 100.00%         | 25.270%       |
| 15        | 21.532      | 3099          | 3105        | 3118         | rBV5     | 30530          | 108130        | 3.55%           | 0.896%        |
| 16        | 21.896      | 3160          | 3167        | 3179         | rVB      | 454240         | 801769        | 26.30%          | 6.645%        |
| 17        | 25.292      | 3735          | 3745        | 3759         | rVB3     | 273665         | 860961        | 28.24%          | 7.136%        |

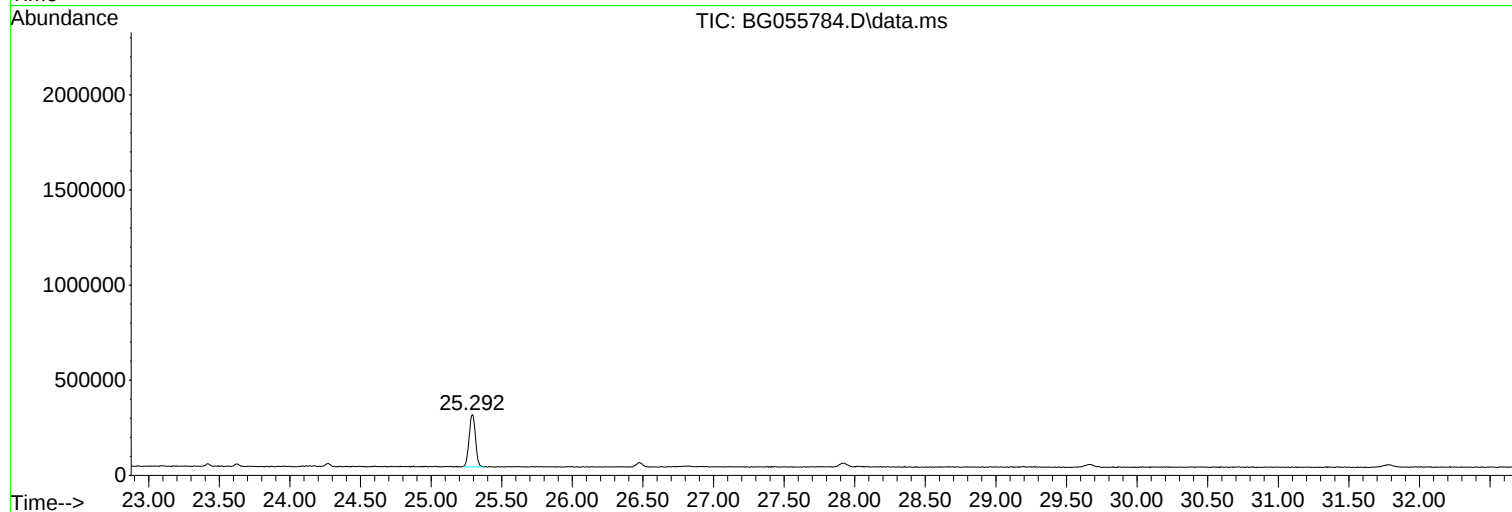
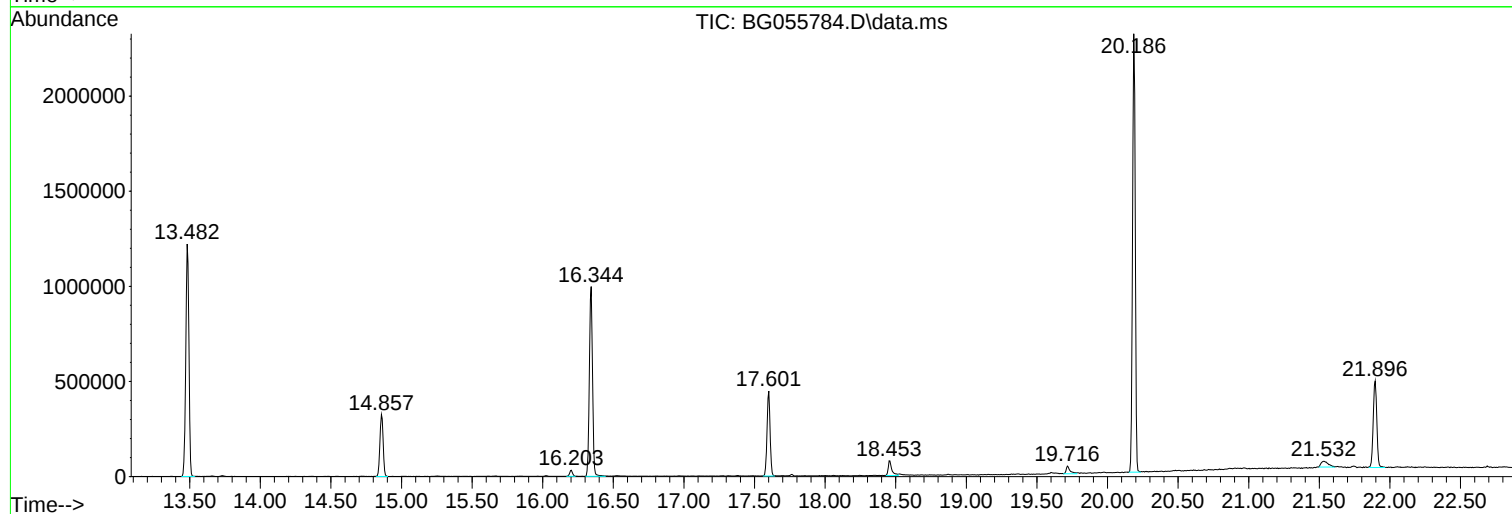
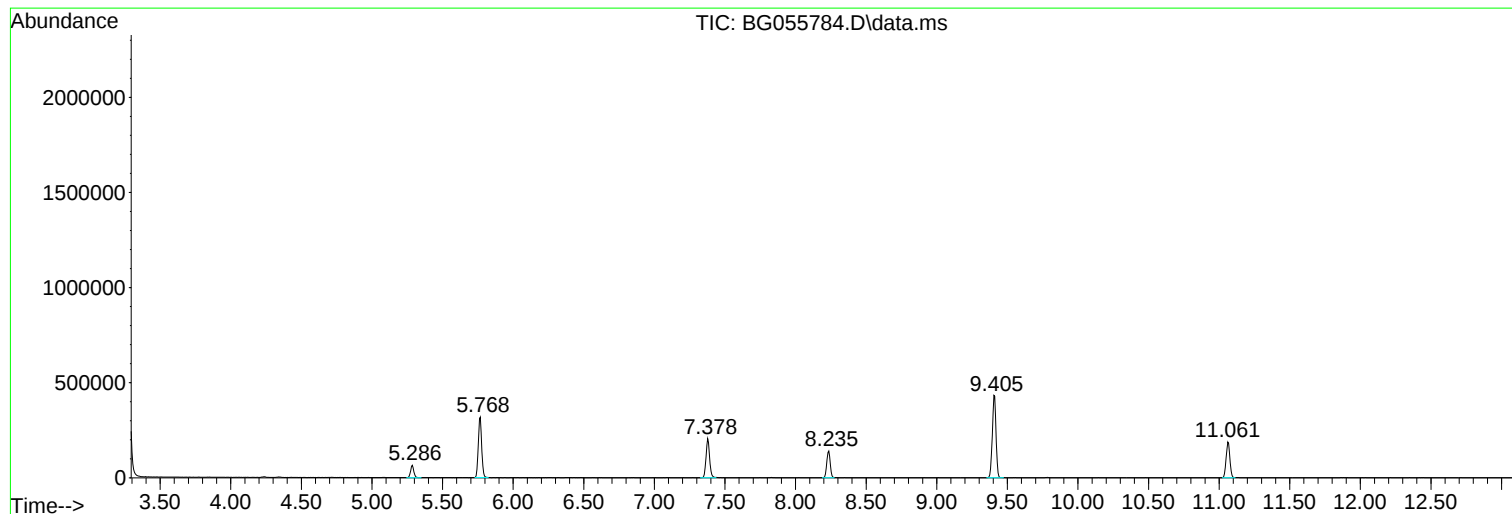
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Instrument :  
BNA\_G  
ClientSampleId :  
MW-18R

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG111622.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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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG11622.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

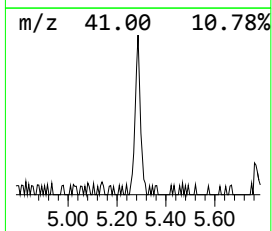
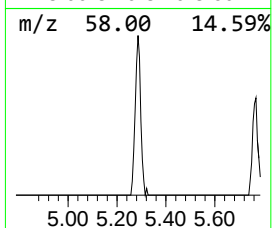
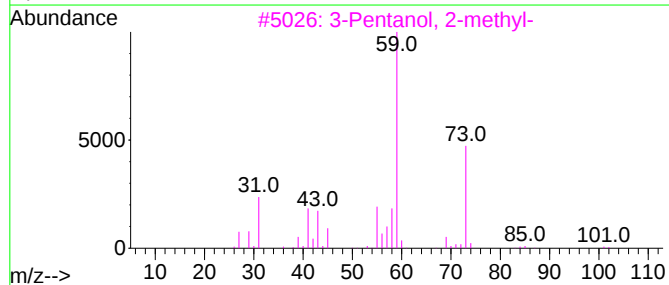
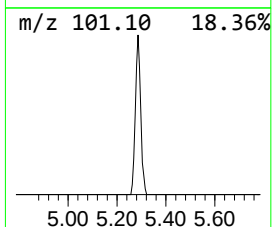
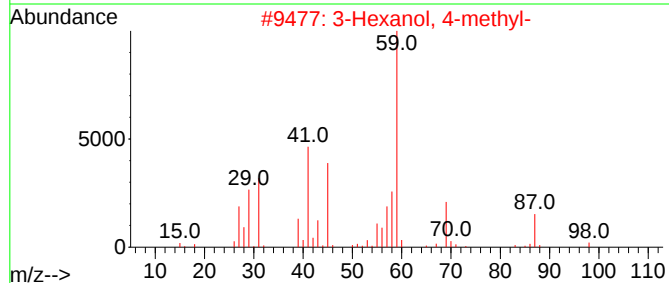
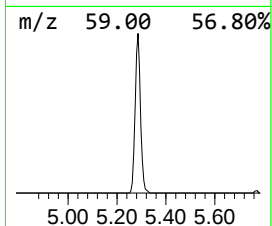
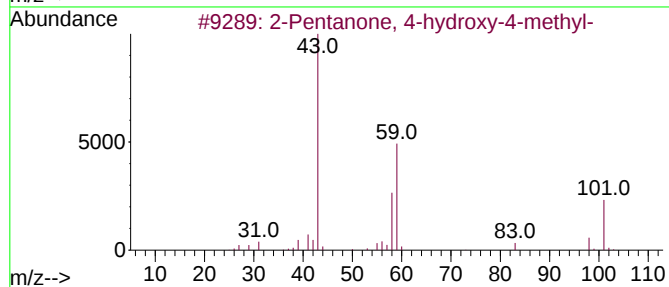
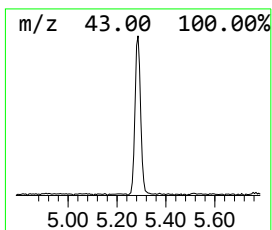
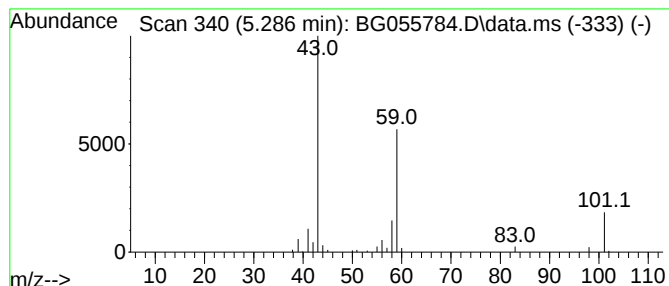
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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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.  |
|-------|---------|--------|------------------------|-------|
| 5.286 | 8.70 ng | 103582 | 1,4-Dichlorobenzene-d4 | 8.235 |

| Hit# | of                               | 5   | Tentative ID | MW          | MolForm | CAS# | Qual |
|------|----------------------------------|-----|--------------|-------------|---------|------|------|
| 1    | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2      | 000123-42-2 | 64      |      |      |
| 2    | 3-Hexanol, 4-methyl-             | 116 | C7H16O       | 000615-29-2 | 33      |      |      |
| 3    | 3-Pentanol, 2-methyl-            | 102 | C6H14O       | 000565-67-3 | 33      |      |      |
| 4    | 1-Propen-2-ol, acetate           | 100 | C5H8O2       | 000108-22-5 | 10      |      |      |
| 5    | 4-Penten-2-one, 4-methyl-        | 98  | C6H10O       | 003744-02-3 | 9       |      |      |



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ClientSampleId :  
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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG11622.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

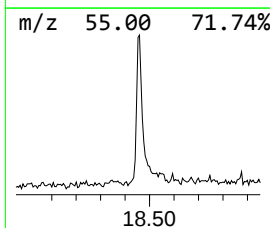
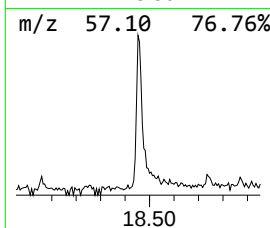
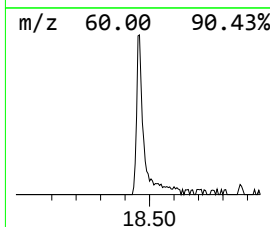
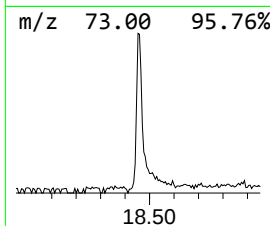
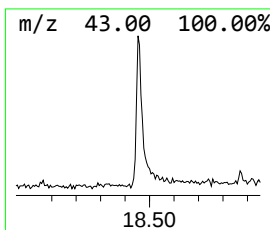
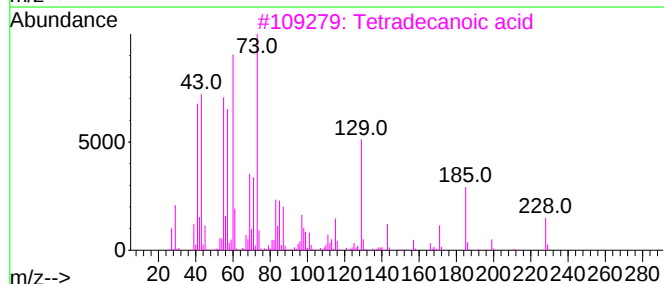
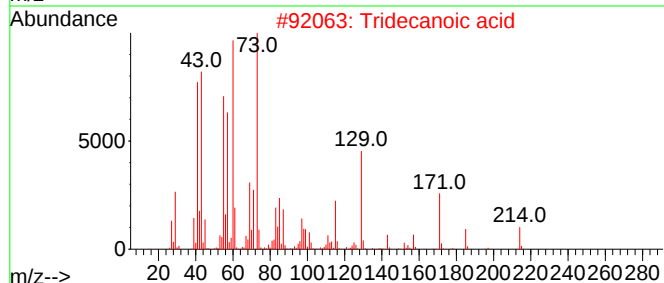
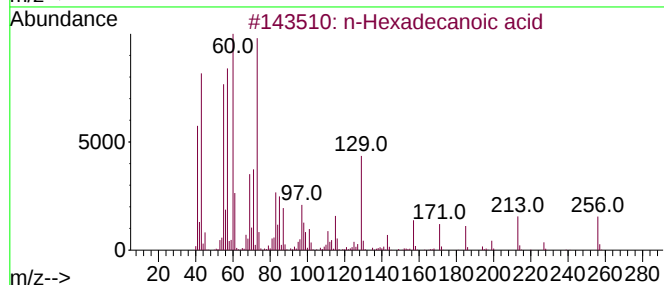
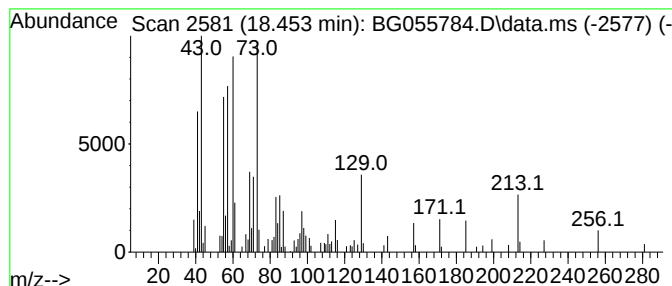
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 18.453 | 4.08 ng | 137824 | Phenanthrene-d10 | 17.601 |

| 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 | 91   |
| 3    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 74   |
| 4    |    |   | n-Decanoic acid     | 172 | C10H20O2 | 000334-48-5 | 64   |
| 5    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 64   |



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Misc :  
ALS Vial : 5 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
MW-18R

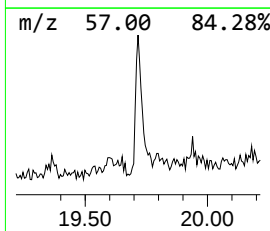
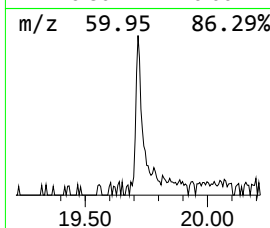
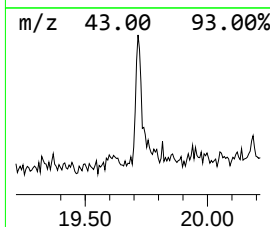
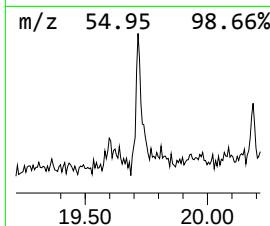
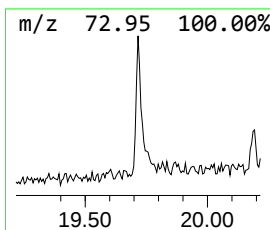
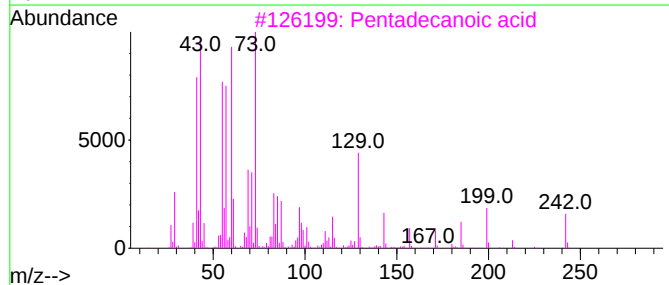
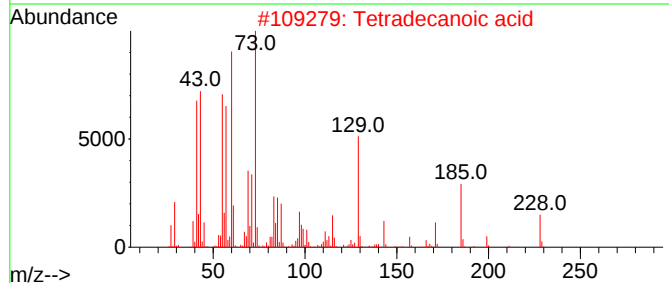
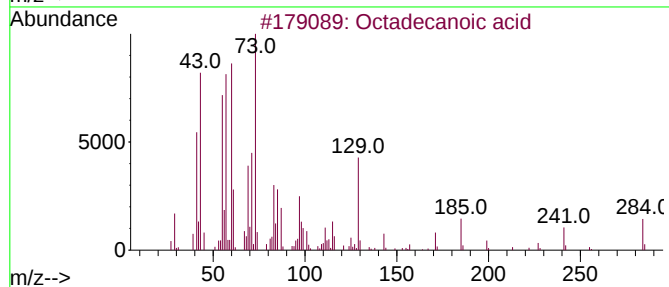
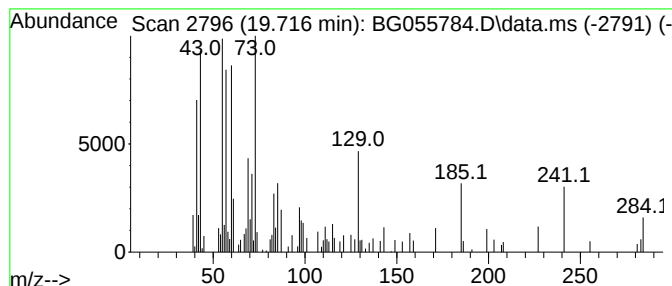
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG11622.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 3 Octadecanoic acid Concentration Rank 4

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 19.716 | 2.32 ng | 78486 | Phenanthrene-d10 | 17.601 |

| Hit# | of | 5 | Tentative ID       | MW  | MolForm  | CAS#        | Qual |
|------|----|---|--------------------|-----|----------|-------------|------|
| 1    |    |   | Octadecanoic acid  | 284 | C18H36O2 | 000057-11-4 | 99   |
| 2    |    |   | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 87   |
| 3    |    |   | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 72   |
| 4    |    |   | Tridecanoic acid   | 214 | C13H26O2 | 000638-53-9 | 72   |
| 5    |    |   | Dodecanoic acid    | 200 | C12H24O2 | 000143-07-7 | 59   |



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Misc :  
ALS Vial : 5 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
MW-18R

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG11622.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

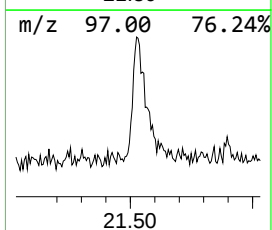
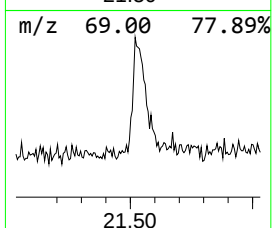
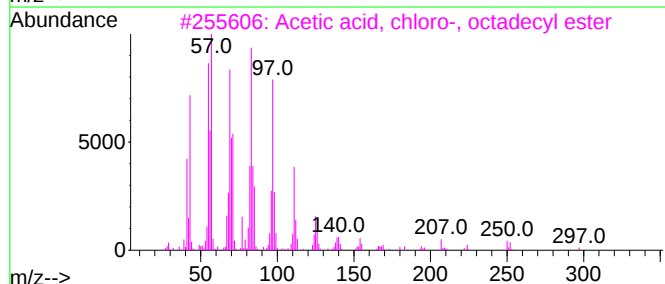
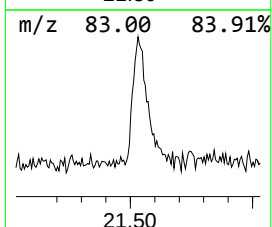
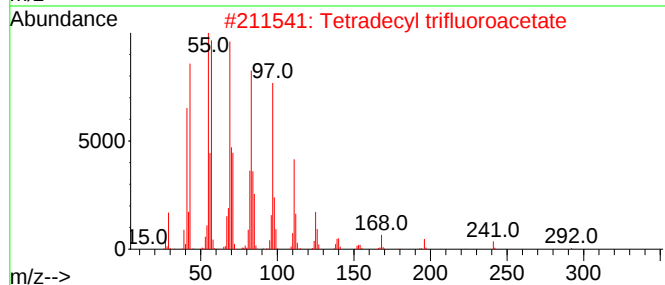
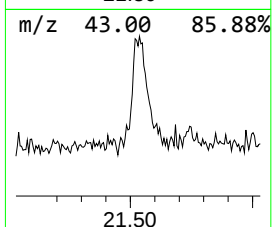
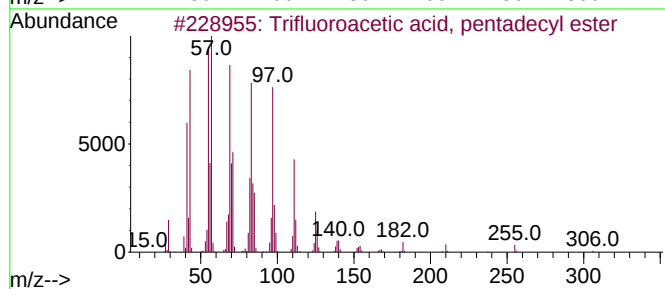
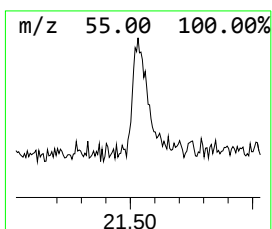
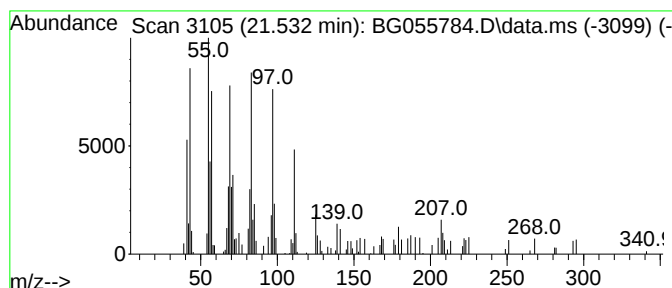
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 Trifluoroacetic acid, penta... Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 21.532 | 2.70 ng | 108130 | Chrysene-d12     | 21.896 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|------------|-------------|------|
| 1    |    |   | Trifluoroacetic acid, pentadecyl... | 324 | C17H31F3O2 | 959010-23-2 | 91   |
| 2    |    |   | Tetradecyl trifluoroacetate         | 310 | C16H29F3O2 | 006222-02-2 | 90   |
| 3    |    |   | Acetic acid, chloro-, octadecyl ... | 346 | C20H39ClO2 | 005348-82-3 | 86   |
| 4    |    |   | 1-Tricosene                         | 322 | C23H46     | 018835-32-0 | 86   |
| 5    |    |   | Pentafluoropropionic acid, dodec... | 332 | C15H25F5O2 | 006222-04-4 | 64   |



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| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| 2-Pentanone, 4-... | 5.286  | 8.7     | ng    | 103582   | 1                     | 8.235  | 238195 | 20.0 |
| n-Hexadecanoic ... | 18.453 | 4.1     | ng    | 137824   | 4                     | 17.601 | 675431 | 20.0 |
| Octadecanoic acid  | 19.716 | 2.3     | ng    | 78486    | 4                     | 17.601 | 675431 | 20.0 |
| Trifluoroacetic... | 21.532 | 2.7     | ng    | 108130   | 5                     | 21.896 | 801769 | 20.0 |