

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF050223\  
 Data File : BF133187.D  
 Acq On : 02 May 2023 14:15  
 Operator : CG\JU  
 Sample : 02270-26  
 Misc :  
 ALS Vial : 10 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 SB-16-14-16-20230413

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\_F\Methods\8270-BF042123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133187.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         | 4.940       | 481           | 485         | 491          | rVB      | 159644         | 216027        | 3.35%           | 0.488%        |
| 2         | 5.351       | 549           | 555         | 558          | rBV      | 5038643        | 5584529       | 86.72%          | 12.614%       |
| 3         | 6.375       | 723           | 729         | 732          | rBV      | 5035967        | 5708357       | 88.65%          | 12.894%       |
| 4         | 6.728       | 786           | 789         | 792          | rBV      | 1668610        | 1308503       | 20.32%          | 2.956%        |
| 5         | 6.798       | 797           | 801         | 804          | rBV      | 108683         | 91461         | 1.42%           | 0.207%        |
| 6         | 7.298       | 880           | 886         | 889          | rBV      | 3894610        | 3735065       | 58.00%          | 8.437%        |
| 7         | 8.016       | 1004          | 1008        | 1011         | rVB      | 2018592        | 1754432       | 27.24%          | 3.963%        |
| 8         | 9.092       | 1185          | 1191        | 1194         | rBV      | 6792922        | 6247731       | 97.02%          | 14.113%       |
| 9         | 9.369       | 1234          | 1238        | 1246         | rBV      | 514783         | 436637        | 6.78%           | 0.986%        |
| 10        | 9.763       | 1302          | 1305        | 1309         | rVB      | 2272101        | 2000995       | 31.07%          | 4.520%        |
| 11        | 10.480      | 1423          | 1427        | 1430         | rBV      | 528946         | 417353        | 6.48%           | 0.943%        |
| 12        | 10.557      | 1435          | 1440        | 1443         | rBV      | 4028285        | 3923244       | 60.92%          | 8.862%        |
| 13        | 11.245      | 1553          | 1557        | 1561         | rBV      | 2231370        | 2007691       | 31.18%          | 4.535%        |
| 14        | 11.786      | 1645          | 1649        | 1664         | rBV      | 768911         | 765193        | 11.88%          | 1.728%        |
| 15        | 12.386      | 1748          | 1751        | 1758         | rBV      | 142834         | 116047        | 1.80%           | 0.262%        |
| 16        | 12.568      | 1779          | 1782        | 1795         | rBV2     | 159698         | 184773        | 2.87%           | 0.417%        |
| 17        | 12.839      | 1823          | 1828        | 1831         | rBV      | 6190782        | 6439467       | 100.00%         | 14.546%       |
| 18        | 13.745      | 1978          | 1982        | 1998         | rBV      | 256569         | 615499        | 9.56%           | 1.390%        |
| 19        | 13.880      | 2001          | 2005        | 2009         | rVV      | 1634719        | 1473125       | 22.88%          | 3.328%        |
| 20        | 14.215      | 2059          | 2062        | 2065         | rBV      | 106010         | 86791         | 1.35%           | 0.196%        |
| 21        | 14.368      | 2084          | 2088        | 2091         | rBV      | 68005          | 67509         | 1.05%           | 0.152%        |
| 22        | 15.304      | 2242          | 2247        | 2252         | rBV      | 905389         | 1090431       | 16.93%          | 2.463%        |

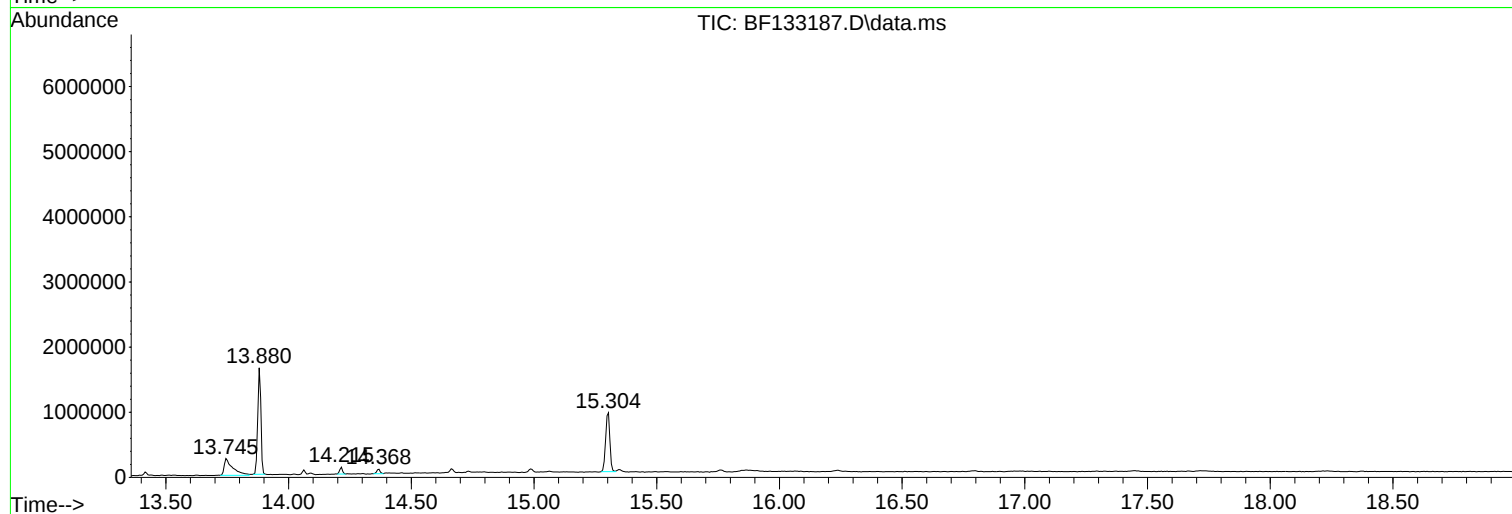
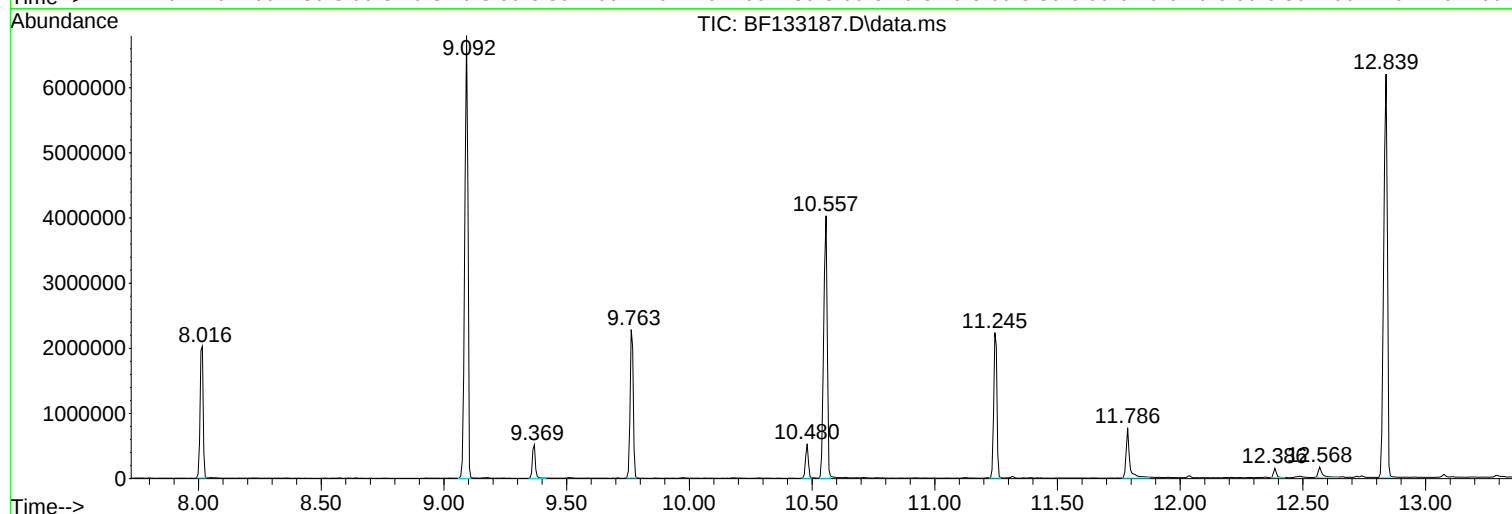
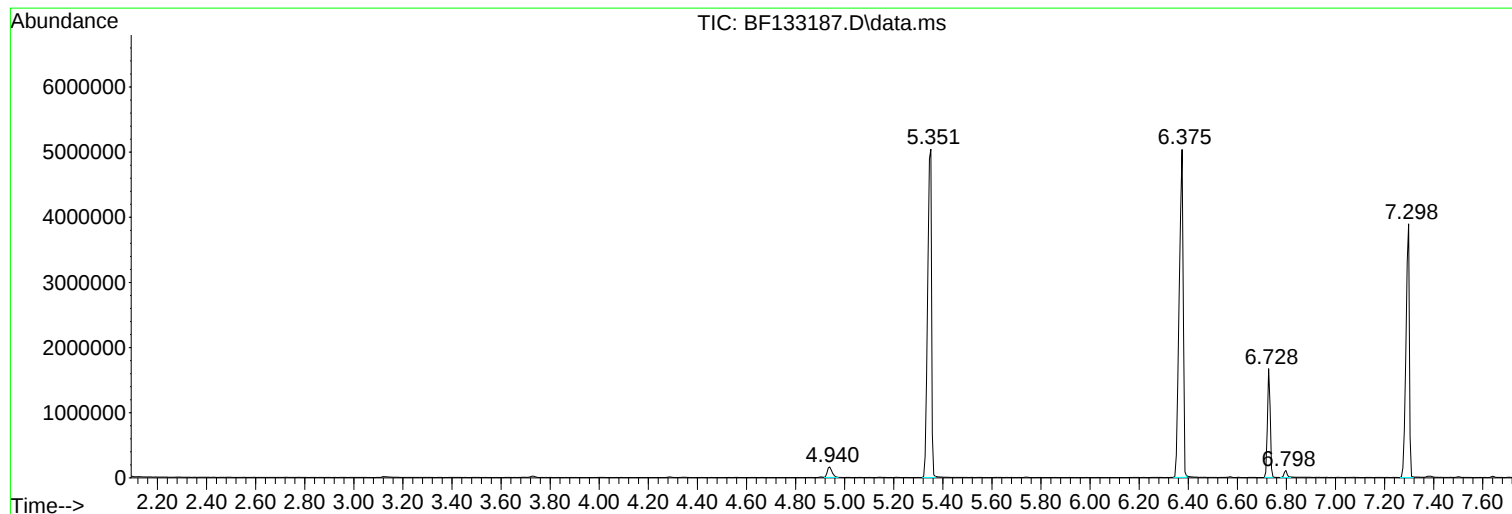
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ALS Vial : 10 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
SB-16-14-16-20230413

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF042123.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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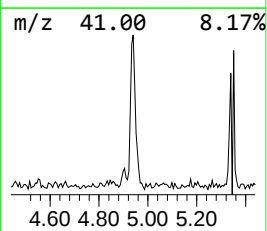
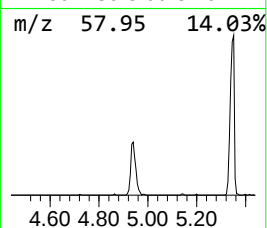
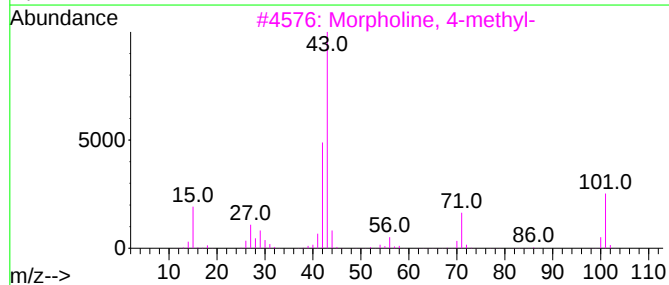
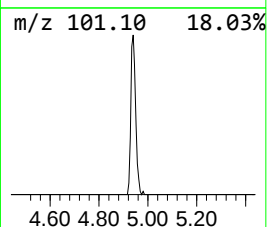
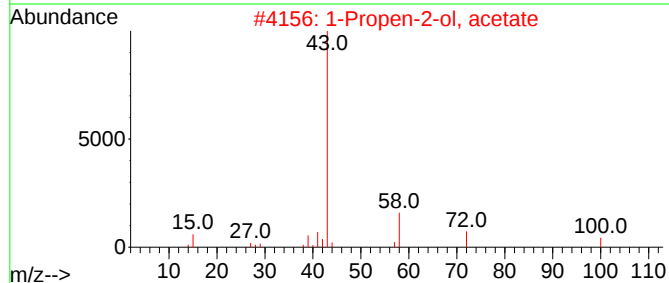
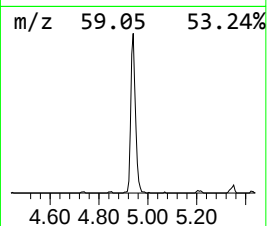
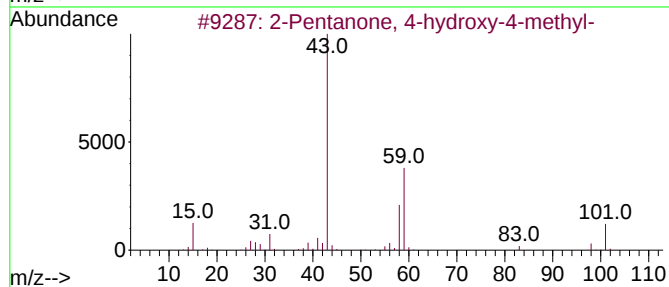
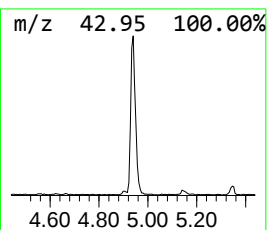
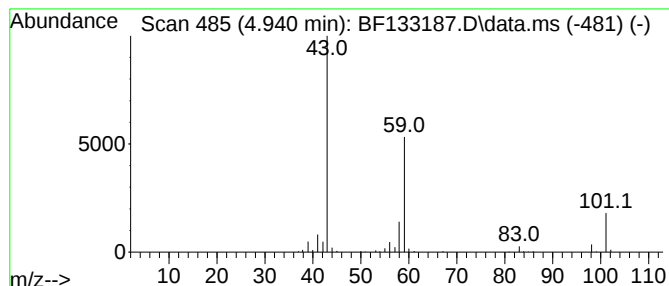
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF042123.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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 5

| R.T.  | EstConc | Area   | Relative to ISTD       | R.T.  |
|-------|---------|--------|------------------------|-------|
| 4.940 | 3.30 ng | 216027 | 1,4-Dichlorobenzene-d4 | 6.728 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|---------|--------------|------|
| 1    |    |   | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2 | 000123-42-2  | 53   |
| 2    |    |   | 1-Propen-2-ol, acetate              | 100 | C5H8O2  | 000108-22-5  | 12   |
| 3    |    |   | Morpholine, 4-methyl-               | 101 | C5H11NO | 000109-02-4  | 9    |
| 4    |    |   | 2,3-Butanedione, monooxime          | 101 | C4H7NO2 | 000057-71-6  | 9    |
| 5    |    |   | .alpha.-Hydroxyisobutyric acid, ... | 146 | C6H10O4 | 1000374-31-3 | 9    |



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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

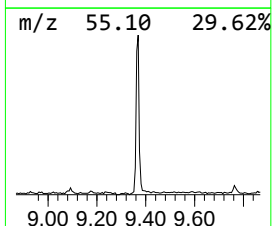
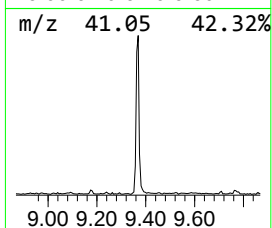
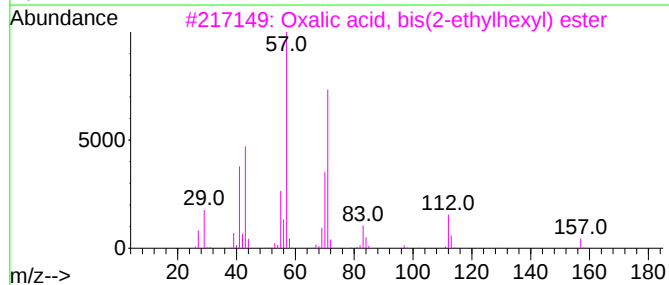
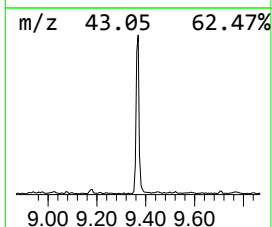
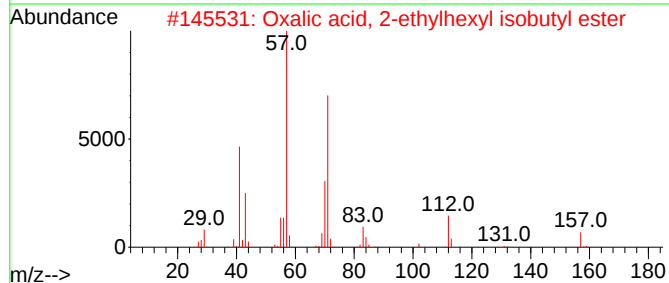
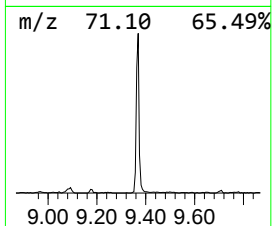
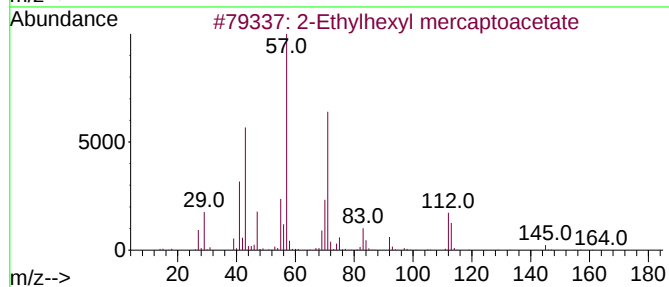
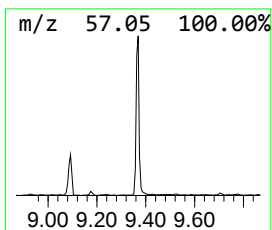
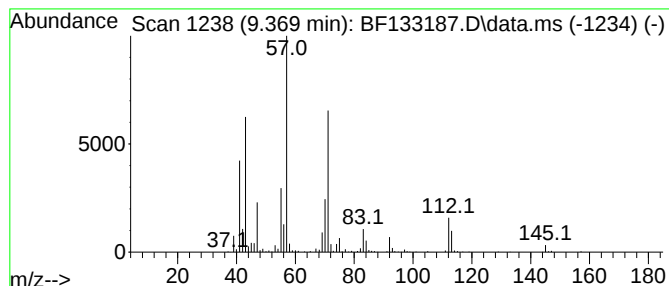
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 2-Ethylhexyl mercaptoacetate Concentration Rank 3

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 9.369 | 4.36 ng | 436637 | Acenaphthene-d10 | 9.763 |

| Hit# | of 5 | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|------|-------------------------------------|-----|-----------|--------------|------|
| 1    |      | 2-Ethylhexyl mercaptoacetate        | 204 | C10H20O2S | 007659-86-1  | 87   |
| 2    |      | Oxalic acid, 2-ethylhexyl isobut... | 258 | C14H26O4  | 1010309-38-5 | 64   |
| 3    |      | Oxalic acid, bis(2-ethylhexyl) e... | 314 | C18H34O4  | 1000309-39-0 | 52   |
| 4    |      | Undecane, 2,5-dimethyl-             | 184 | C13H28    | 017301-22-3  | 50   |
| 5    |      | Undecane, 3,6-dimethyl-             | 184 | C13H28    | 017301-28-9  | 47   |



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ALS Vial : 10 Sample Multiplier: 1

Instrument :  
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ClientSampleId :  
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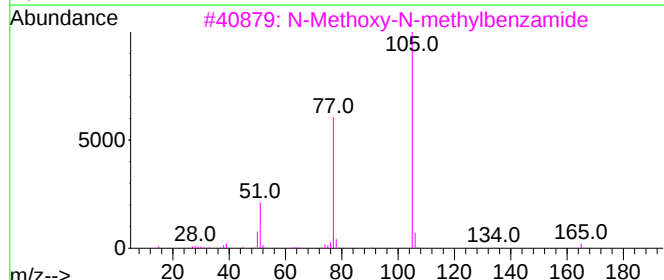
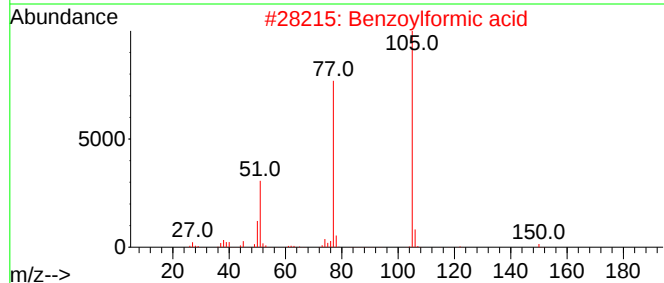
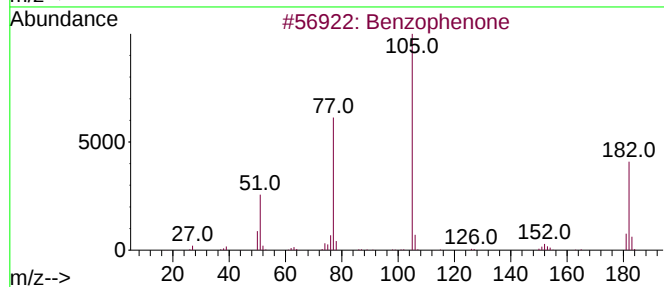
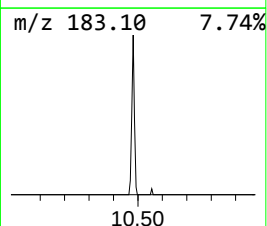
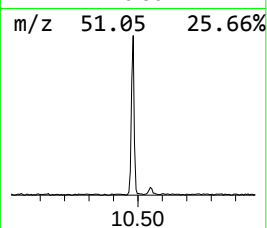
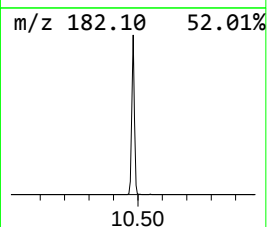
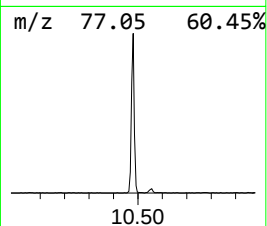
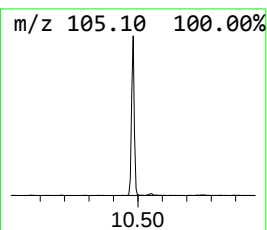
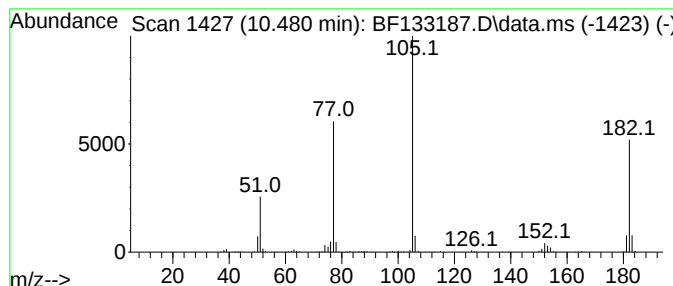
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF042123.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 3 Benzophenone Concentration Rank 4

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.  |
|--------|---------|--------|------------------|-------|
| 10.480 | 4.17 ng | 417353 | Acenaphthene-d10 | 9.763 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|----------|--------------|------|
| 1    |    |   | Benzophenone                        | 182 | C13H10O  | 000119-61-9  | 97   |
| 2    |    |   | Benzoylformic acid                  | 150 | C8H6O3   | 000611-73-4  | 47   |
| 3    |    |   | N-Methoxy-N-methylbenzamide         | 165 | C9H11NO2 | 006919-61-5  | 47   |
| 4    |    |   | 2-(2-Oxo-2-phenyl-ethyl)-malonon... | 184 | C11H8N2O | 1000296-76-9 | 47   |
| 5    |    |   | 1-Propanone, 2-bromo-1-phenyl-      | 212 | C9H9BrO  | 002114-00-3  | 47   |



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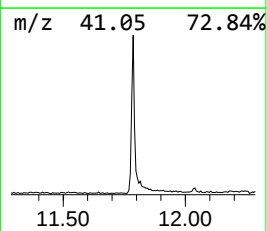
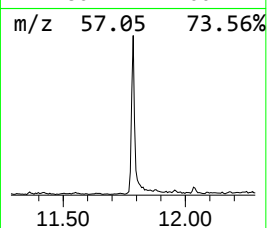
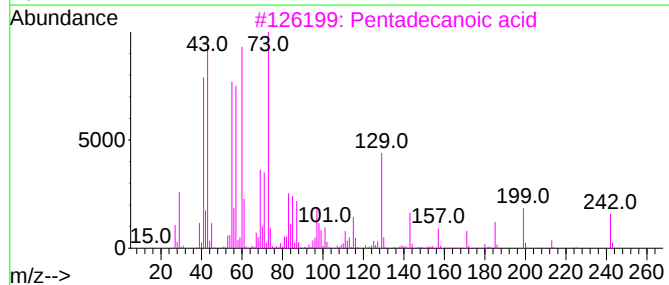
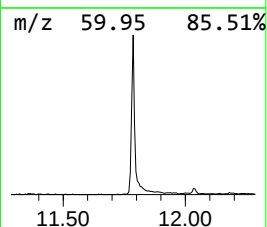
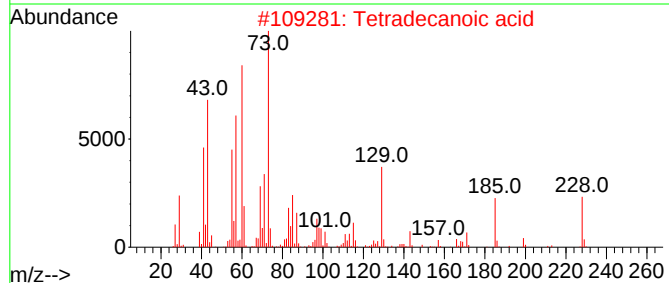
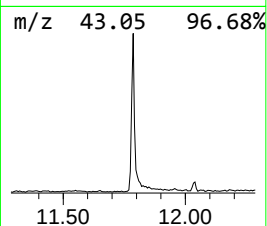
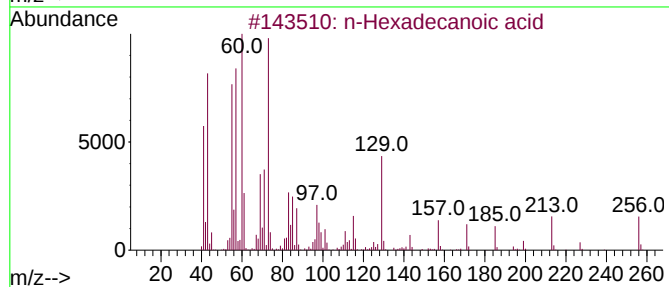
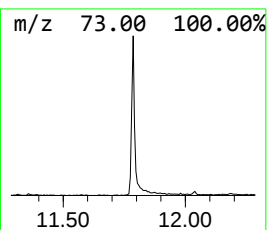
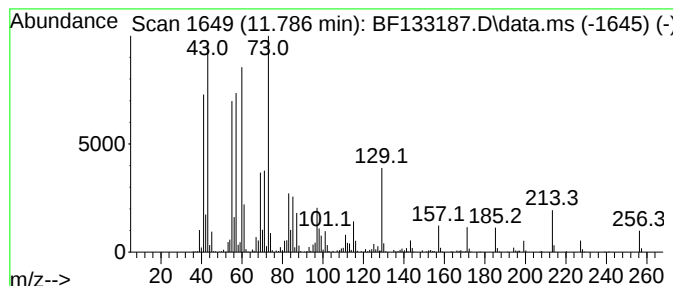
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

| R.T.      | EstConc             | Area   | Relative to ISTD |          | R.T.        |      |
|-----------|---------------------|--------|------------------|----------|-------------|------|
| 11.786    | 7.62 ng             | 765193 | Phenanthrene-d10 |          | 11.245      |      |
| 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 | 89   |
| 5         | Dodecanoic acid     |        | 200              | C12H24O2 | 000143-07-7 | 59   |



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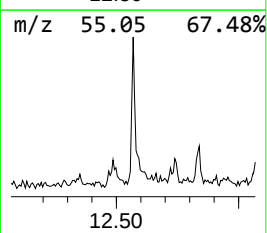
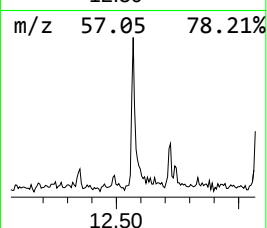
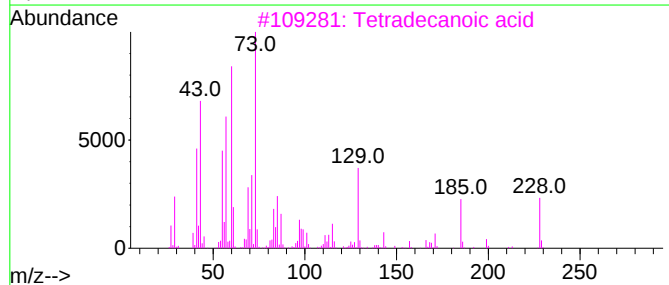
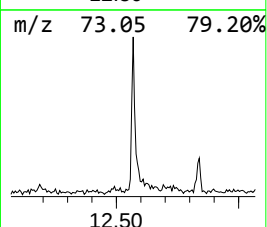
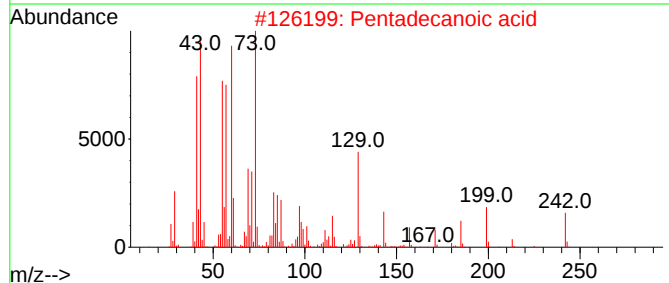
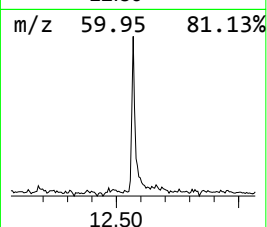
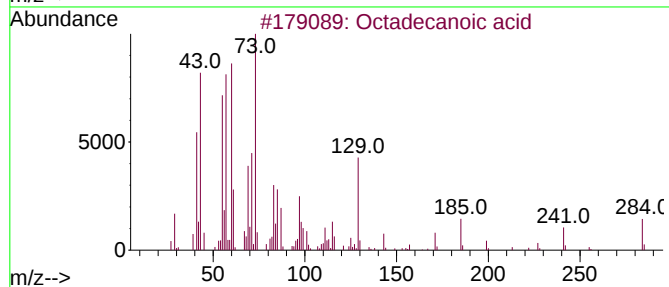
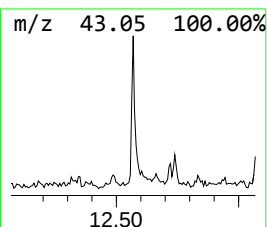
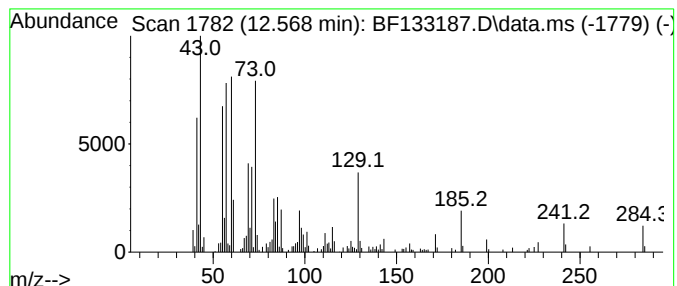
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF042123.M  
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TIC Library : C:\Database\NIST20.L  
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Peak Number 5 Octadecanoic acid Concentration Rank 6

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 12.568 | 2.51 ng | 184773 | Chrysene-d12     | 13.880 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | Octadecanoic acid   | 284 | C18H36O2 | 000057-11-4 | 99   |
| 2    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 90   |
| 3    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 83   |
| 4    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 81   |
| 5    |    |   | Undecanoic acid     | 186 | C11H22O2 | 000112-37-8 | 72   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF050223\  
Data File : BF133187.D  
Acq On : 02 May 2023 14:15  
Operator : CG\JU  
Sample : 02270-26  
Misc :  
ALS Vial : 10 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
SB-16-14-16-20230413

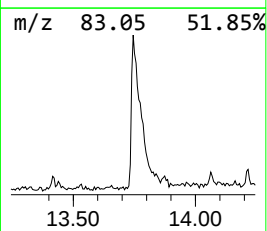
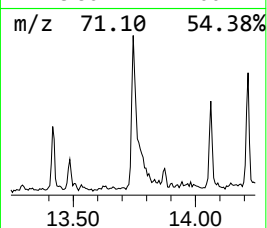
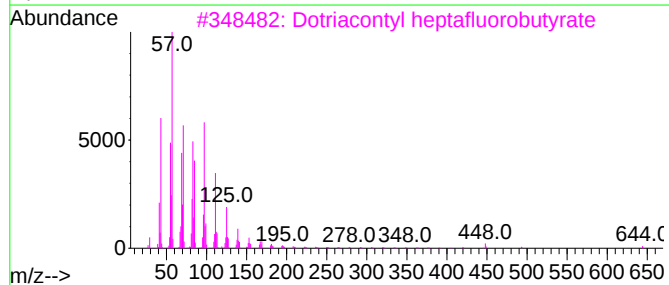
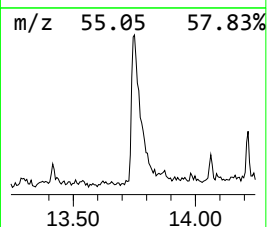
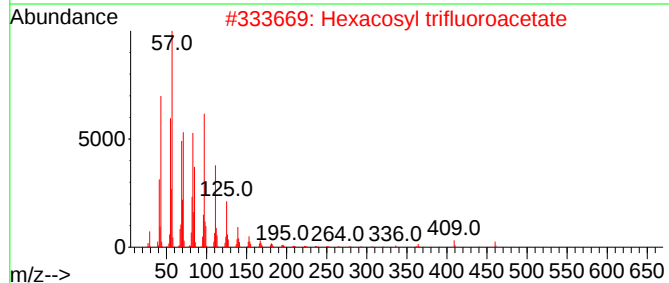
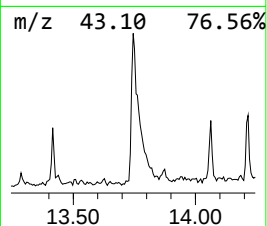
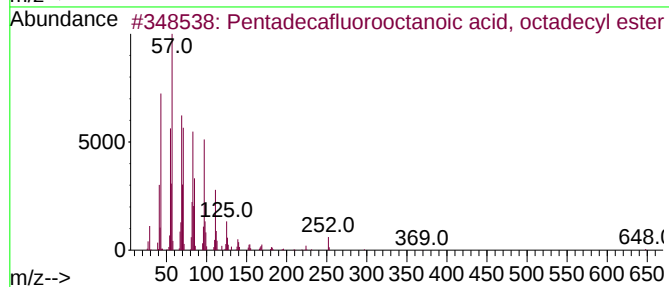
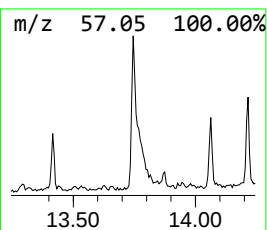
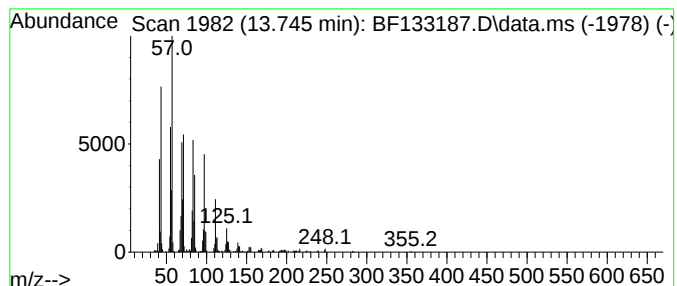
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 6 Pentadecafluorooctanoic aci... Concentration Rank 1

| R.T.      | EstConc                             | Area   | Relative to ISTD | R.T.         |      |
|-----------|-------------------------------------|--------|------------------|--------------|------|
| 13.745    | 8.36 ng                             | 615499 | Chrysene-d12     | 13.880       |      |
| Hit# of 5 | Tentative ID                        | MW     | MolForm          | CAS#         | Qual |
| 1         | Pentadecafluorooctanoic acid, oc... | 666    | C26H37F15O2      | 1000406-04-8 | 94   |
| 2         | Hexacosyl trifluoroacetate          | 478    | C28H53F3O2       | 1000351-75-0 | 91   |
| 3         | Dotriacontyl heptafluorobutyrate    | 662    | C36H65F7O2       | 1000351-84-2 | 91   |
| 4         | Tricosyl heptafluorobutyrate        | 536    | C27H47F7O2       | 1000351-83-4 | 91   |
| 5         | Dotriacontyl trifluoroacetate       | 562    | C34H65F3O2       | 1000351-75-4 | 91   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF050223\  
Data File : BF133187.D  
Acq On : 02 May 2023 14:15  
Operator : CG\JU  
Sample : 02270-26  
Misc :  
ALS Vial : 10 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
SB-16-14-16-20230413

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF042123.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |         |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|---------|------|
|                    |        |         |       |          | #                     | RT     | Resp    | Conc |
| 2-Pentanone, 4-... | 4.940  | 3.3     | ng    | 216027   | 1                     | 6.728  | 1308500 | 20.0 |
| 2-Ethylhexyl me... | 9.369  | 4.4     | ng    | 436637   | 3                     | 9.763  | 2001000 | 20.0 |
| Benzophenone       | 10.480 | 4.2     | ng    | 417353   | 3                     | 9.763  | 2001000 | 20.0 |
| n-Hexadecanoic ... | 11.786 | 7.6     | ng    | 765193   | 4                     | 11.245 | 2007690 | 20.0 |
| Octadecanoic acid  | 12.568 | 2.5     | ng    | 184773   | 5                     | 13.880 | 1473130 | 20.0 |
| Pentadecafluoro... | 13.745 | 8.4     | ng    | 615499   | 5                     | 13.880 | 1473130 | 20.0 |