

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF011122\  
 Data File : BF126590.D  
 Acq On : 11 Jan 2022 14:19  
 Operator : JU/CG  
 Sample : N1054-04  
 Misc :  
 ALS Vial : 9 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 20220017-CAPE-4-COMP

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-BF122921.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126590.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         | 5.016       | 495           | 498         | 507          | rVB      | 27185          | 39075         | 1.24%           | 0.185%        |
| 2         | 5.398       | 557           | 563         | 566          | rBV      | 2651540        | 2886096       | 91.36%          | 13.655%       |
| 3         | 6.410       | 729           | 735         | 738          | rBV      | 2473374        | 3038938       | 96.20%          | 14.378%       |
| 4         | 6.598       | 765           | 767         | 776          | rBV      | 38638          | 38448         | 1.22%           | 0.182%        |
| 5         | 6.769       | 792           | 796         | 799          | rBV      | 614033         | 547315        | 17.33%          | 2.589%        |
| 6         | 7.334       | 886           | 892         | 895          | rBV      | 1795301        | 2038759       | 64.54%          | 9.646%        |
| 7         | 7.957       | 993           | 998         | 1009         | rBV      | 425561         | 408735        | 12.94%          | 1.934%        |
| 8         | 8.051       | 1009          | 1014        | 1017         | rVV      | 775279         | 785371        | 24.86%          | 3.716%        |
| 9         | 9.133       | 1191          | 1198        | 1201         | rBV      | 2741269        | 3159044       | 100.00%         | 14.946%       |
| 10        | 9.810       | 1307          | 1313        | 1316         | rBV      | 868253         | 848776        | 26.87%          | 4.016%        |
| 11        | 10.604      | 1440          | 1448        | 1451         | rBV      | 1868939        | 2001053       | 63.34%          | 9.467%        |
| 12        | 11.157      | 1538          | 1542        | 1553         | rVB2     | 38049          | 38044         | 1.20%           | 0.180%        |
| 13        | 11.292      | 1561          | 1565        | 1569         | rBV      | 918254         | 825392        | 26.13%          | 3.905%        |
| 14        | 11.833      | 1653          | 1657        | 1667         | rBV2     | 86517          | 101033        | 3.20%           | 0.478%        |
| 15        | 12.892      | 1831          | 1837        | 1840         | rBV      | 2673218        | 2749769       | 87.04%          | 13.010%       |
| 16        | 13.792      | 1986          | 1990        | 2007         | rBV2     | 109428         | 206116        | 6.52%           | 0.975%        |
| 17        | 13.939      | 2011          | 2015        | 2019         | rBV      | 770026         | 680507        | 21.54%          | 3.220%        |
| 18        | 14.039      | 2027          | 2032        | 2039         | rBV      | 33179          | 40641         | 1.29%           | 0.192%        |
| 19        | 15.068      | 2202          | 2207        | 2209         | rBV      | 30172          | 39120         | 1.24%           | 0.185%        |
| 20        | 15.115      | 2210          | 2215        | 2224         | rVB6     | 29824          | 70904         | 2.24%           | 0.335%        |
| 21        | 15.398      | 2258          | 2263        | 2267         | rBV      | 483822         | 593137        | 18.78%          | 2.806%        |

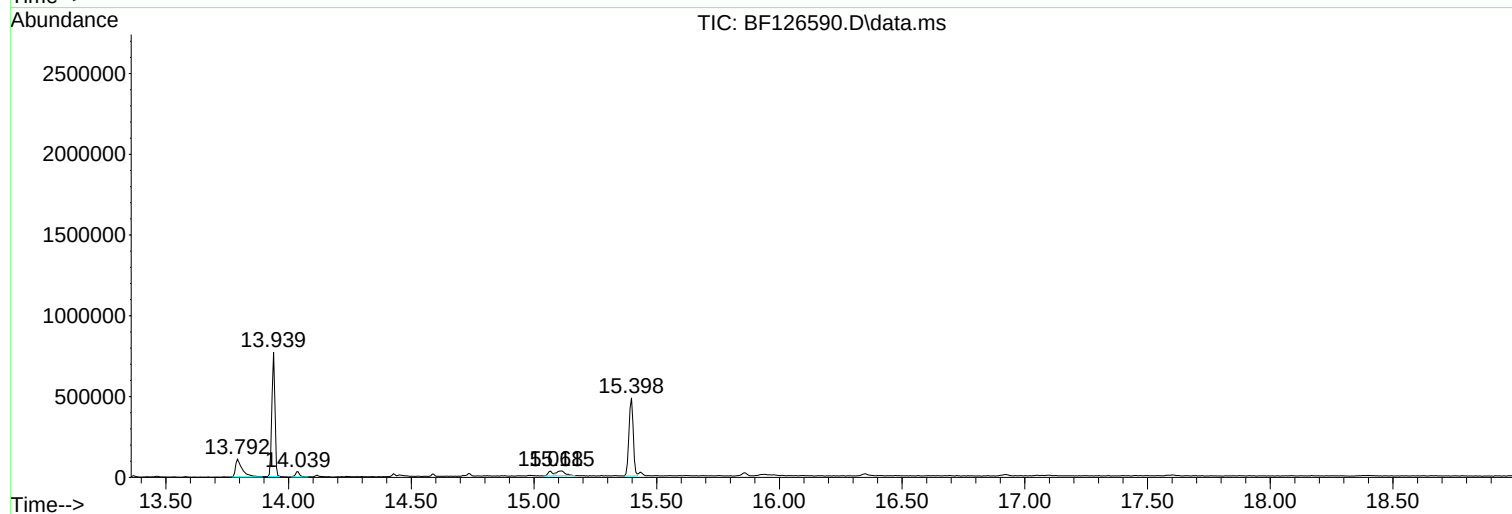
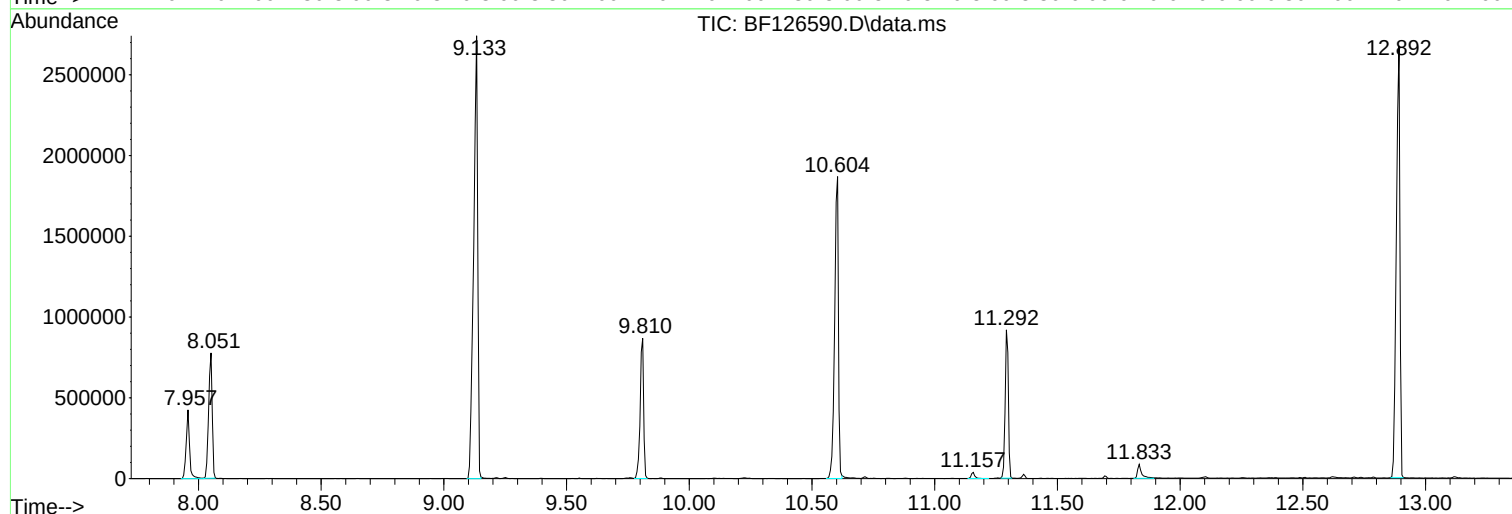
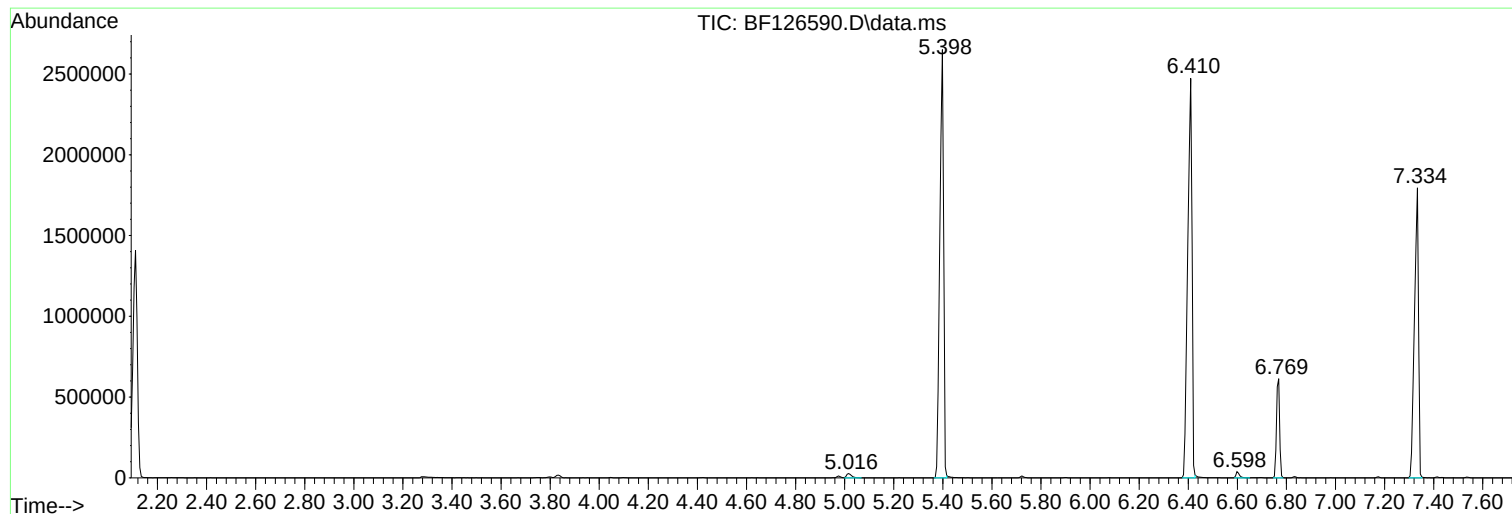
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Sample : N1054-04  
Misc :  
ALS Vial : 9 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
20220017-CAPE-4-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF122921.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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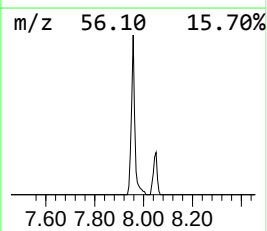
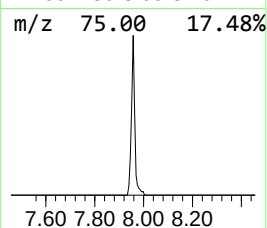
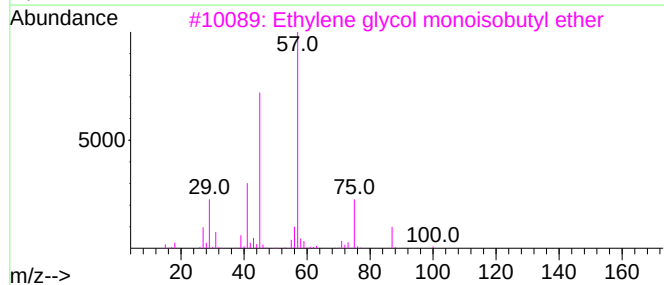
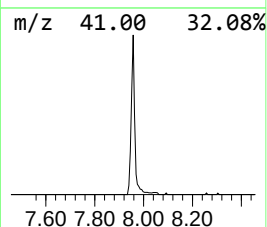
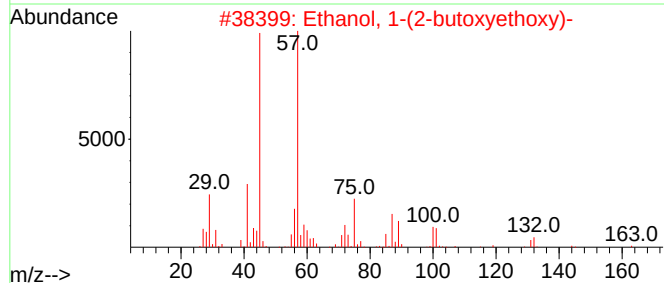
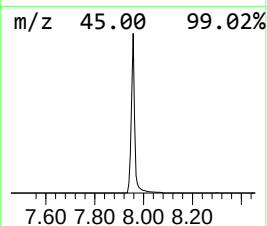
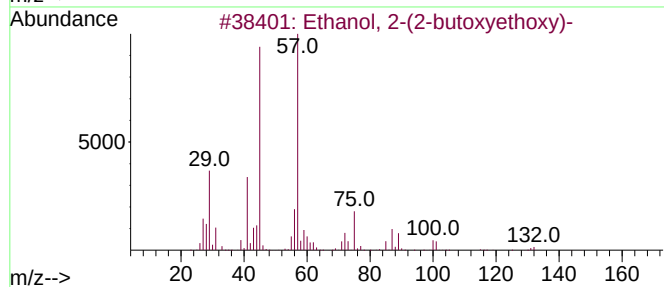
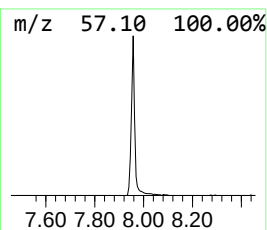
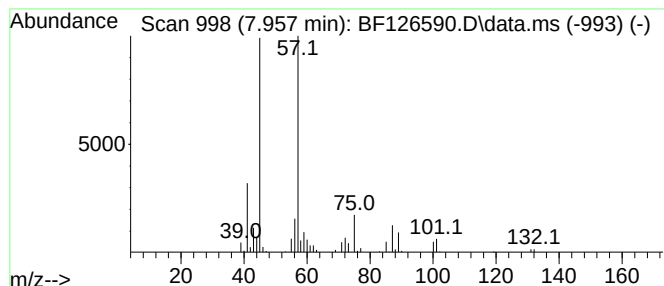
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF122921.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

| R.T.  | EstConc  | Area   | Relative to ISTD | R.T.  |
|-------|----------|--------|------------------|-------|
| 7.957 | 10.41 ng | 408735 | Naphthalene-d8   | 8.051 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|---------|-------------|------|
| 1    |    |   | Ethanol, 2-(2-butoxyethoxy)-        | 162 | C8H18O3 | 000112-34-5 | 90   |
| 2    |    |   | Ethanol, 1-(2-butoxyethoxy)-        | 162 | C8H18O3 | 054446-78-5 | 83   |
| 3    |    |   | Ethylene glycol monoisobutyl ether  | 118 | C6H14O2 | 004439-24-1 | 59   |
| 4    |    |   | Ethanol, 2-[2-(2-methylpropoxy)e... | 162 | C8H18O3 | 018912-80-6 | 56   |
| 5    |    |   | 3,3-Dimethylbutane-2-ol             | 102 | C6H14O  | 000464-07-3 | 53   |



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ClientSampleId :  
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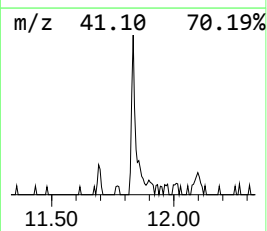
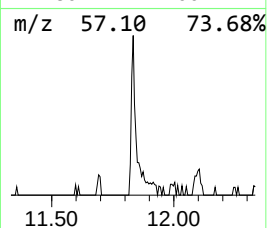
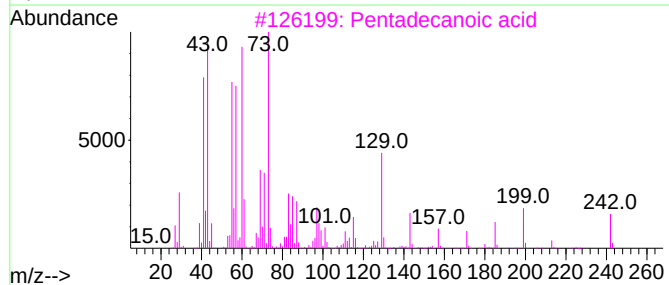
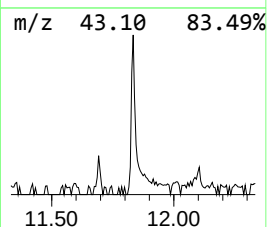
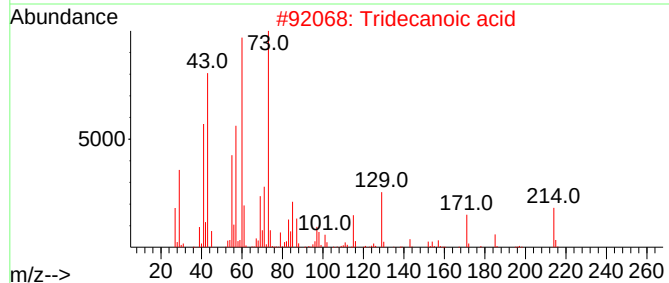
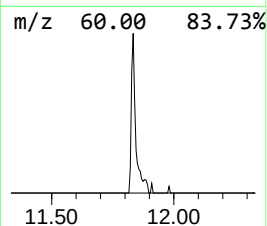
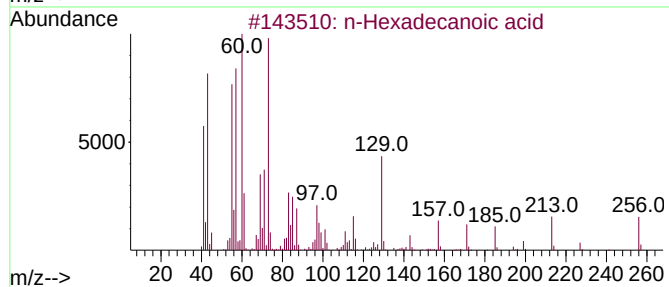
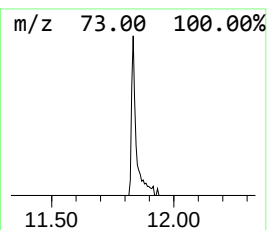
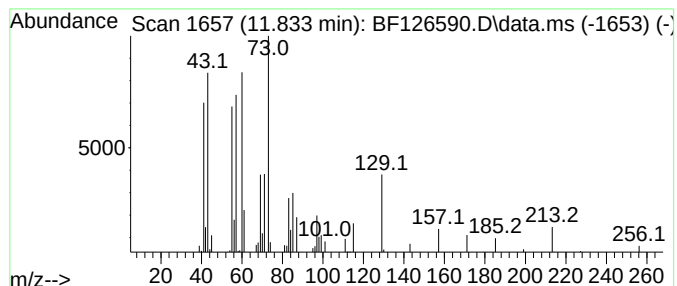
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF122921.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 11.833 | 2.45 ng | 101033 | Phenanthrene-d10 | 11.292 |

| 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  | 93   |
| 3    |    |   | Pentadecanoic acid                  | 242 | C15H30O2 | 001002-84-2  | 91   |
| 4    |    |   | Tetradecanoic acid                  | 228 | C14H28O2 | 000544-63-8  | 83   |
| 5    |    |   | Oxalic acid, allyl pentadecyl ester | 340 | C20H36O4 | 1000309-24-3 | 18   |



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Sample : N1054-04  
Misc :  
ALS Vial : 9 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
20220017-CAPE-4-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF122921.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

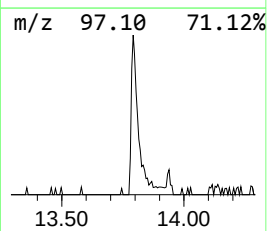
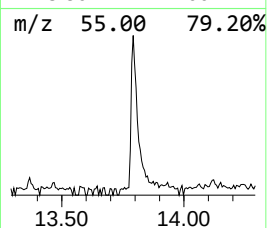
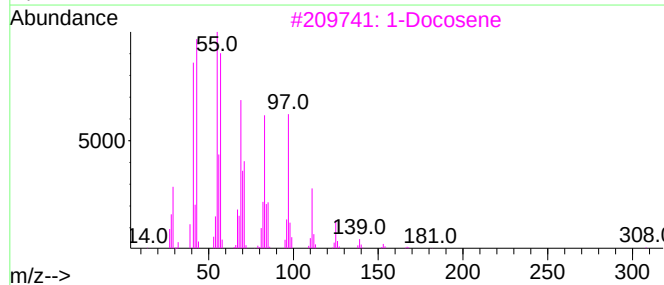
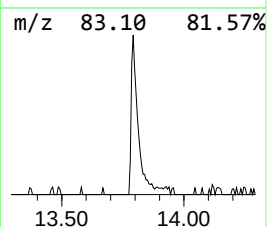
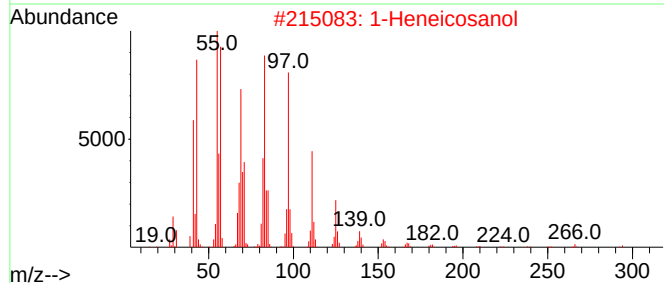
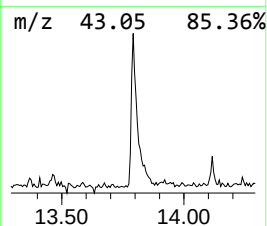
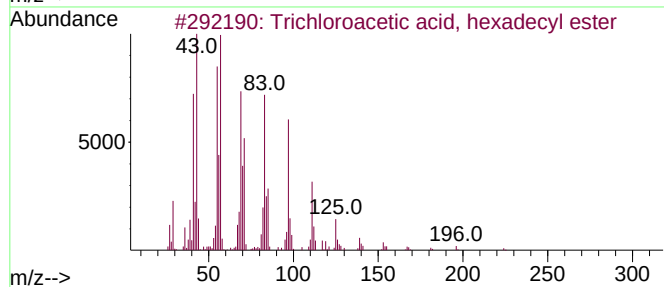
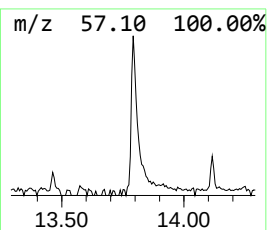
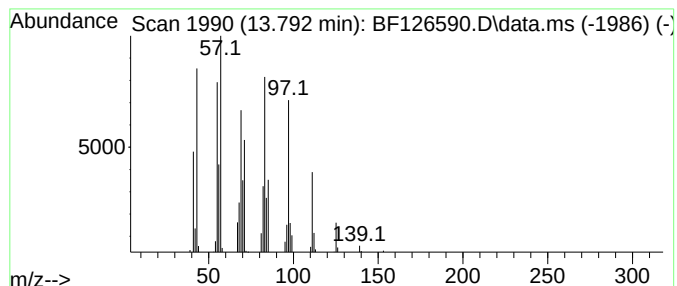
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 Trichloroacetic acid, hexad... Concentration Rank 2

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 13.792 | 6.06 ng | 206116 | Chrysene-d12     | 13.939 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm     | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|-------------|-------------|------|
| 1    |    |   | Trichloroacetic acid, hexadecyl ... | 386 | C18H33Cl3O2 | 074339-54-1 | 94   |
| 2    |    |   | 1-Heneicosanol                      | 312 | C21H44O     | 015594-90-8 | 93   |
| 3    |    |   | 1-Docosene                          | 308 | C22H44      | 001599-67-3 | 91   |
| 4    |    |   | Trifluoroacetoxy hexadecane         | 338 | C18H33F3O2  | 006222-03-3 | 91   |
| 5    |    |   | 1-Hexacosene                        | 364 | C26H52      | 018835-33-1 | 91   |



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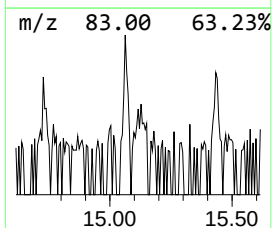
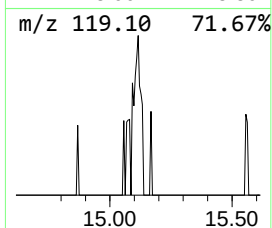
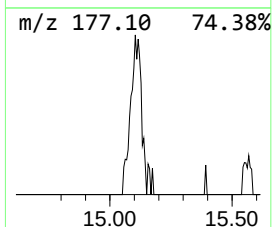
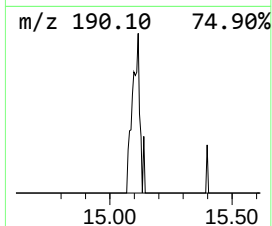
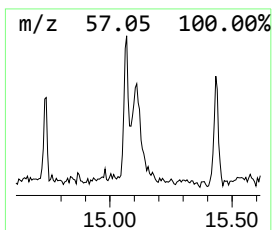
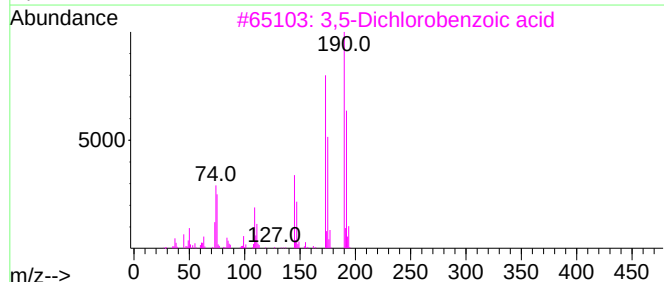
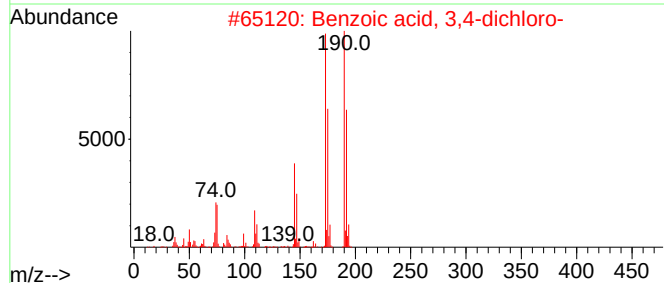
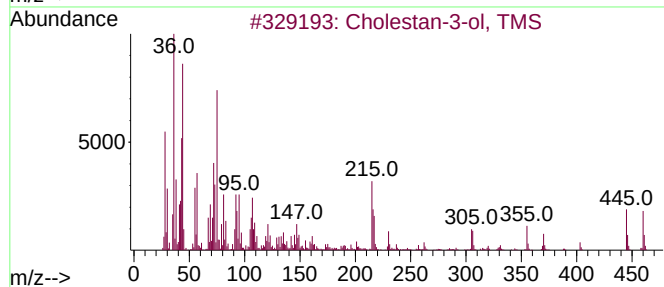
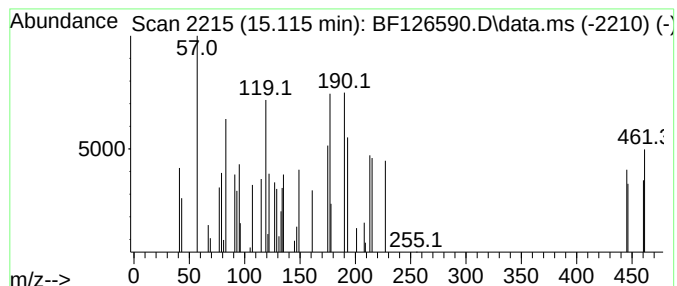
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L  
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Peak Number 4 unknown15.115 Concentration Rank 4

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 15.115 | 2.39 ng | 70904 | Perylene-d12     | 15.398 |

| Hit# | of | 5 | Tentative ID                         | MW  | MolForm    | CAS#        | Qual |
|------|----|---|--------------------------------------|-----|------------|-------------|------|
| 1    |    |   | Cholestan-3-ol, TMS                  | 460 | C30H56OSi  | 056907-47-2 | 10   |
| 2    |    |   | Benzoic acid, 3,4-dichloro-          | 190 | C7H4Cl2O2  | 000051-44-5 | 9    |
| 3    |    |   | 3,5-Dichlorobenzoic acid             | 190 | C7H4Cl2O2  | 000051-36-5 | 9    |
| 4    |    |   | Benzoic acid, 2,5-dichloro-          | 190 | C7H4Cl2O2  | 000050-79-3 | 9    |
| 5    |    |   | 4-Chloromethyl-2-(2-fluorophenyl)... | 225 | C11H9ClFNO | 671215-76-2 | 9    |



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

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| Ethanol, 2-(2-b... | 7.957  | 10.4    | ng    | 408735   | 2                     | 8.051  | 785371 | 20.0 |
| n-Hexadecanoic ... | 11.833 | 2.5     | ng    | 101033   | 4                     | 11.292 | 825392 | 20.0 |
| Trichloroacetic... | 13.792 | 6.1     | ng    | 206116   | 5                     | 13.939 | 680507 | 20.0 |
| unknown15.115      | 15.115 | 2.4     | ng    | 70904    | 6                     | 15.398 | 593137 | 20.0 |