

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF101822\  
 Data File : BF130700.D  
 Acq On : 18 Oct 2022 16:12  
 Operator : CG\JU  
 Sample : N5164-02  
 Misc :  
 ALS Vial : 8 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 588A-2

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-BF101122.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130700.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         | 4.734       | 481           | 484         | 497          | rBV      | 176696         | 229104        | 7.56%           | 1.337%        |
| 2         | 5.181       | 557           | 560         | 582          | rBV      | 930952         | 1055504       | 34.81%          | 6.158%        |
| 3         | 6.228       | 735           | 738         | 757          | rBV      | 586998         | 635140        | 20.95%          | 3.706%        |
| 4         | 6.575       | 793           | 797         | 804          | rBV      | 624262         | 534869        | 17.64%          | 3.121%        |
| 5         | 7.145       | 890           | 894         | 897          | rBV      | 1738950        | 1673062       | 55.18%          | 9.762%        |
| 6         | 7.775       | 998           | 1001        | 1011         | rBV      | 211197         | 299281        | 9.87%           | 1.746%        |
| 7         | 7.857       | 1011          | 1015        | 1022         | rVB      | 831183         | 712834        | 23.51%          | 4.159%        |
| 8         | 8.934       | 1194          | 1198        | 1201         | rBV      | 3640269        | 3032170       | 100.00%         | 17.691%       |
| 9         | 9.057       | 1214          | 1219        | 1228         | rVB      | 33210          | 37199         | 1.23%           | 0.217%        |
| 10        | 9.604       | 1308          | 1312        | 1315         | rBV      | 908306         | 732935        | 24.17%          | 4.276%        |
| 11        | 10.392      | 1442          | 1446        | 1460         | rBV      | 1769152        | 1578441       | 52.06%          | 9.209%        |
| 12        | 11.081      | 1560          | 1563        | 1571         | rBV      | 639919         | 631330        | 20.82%          | 3.684%        |
| 13        | 11.151      | 1571          | 1575        | 1581         | rVB3     | 32564          | 44169         | 1.46%           | 0.258%        |
| 14        | 11.322      | 1600          | 1604        | 1611         | rBV      | 65472          | 92017         | 3.03%           | 0.537%        |
| 15        | 11.486      | 1629          | 1632        | 1635         | rBV      | 68288          | 52657         | 1.74%           | 0.307%        |
| 16        | 11.657      | 1657          | 1661        | 1664         | rVB      | 1513717        | 1215977       | 40.10%          | 7.095%        |
| 17        | 12.186      | 1748          | 1751        | 1754         | rVB      | 76900          | 65847         | 2.17%           | 0.384%        |
| 18        | 12.286      | 1763          | 1768        | 1776         | rBV      | 106092         | 150127        | 4.95%           | 0.876%        |
| 19        | 12.516      | 1801          | 1807        | 1814         | rBV      | 138073         | 186085        | 6.14%           | 1.086%        |
| 20        | 12.669      | 1829          | 1833        | 1836         | rBV      | 1791817        | 1511636       | 49.85%          | 8.820%        |
| 21        | 13.145      | 1909          | 1914        | 1919         | rBV      | 235524         | 225836        | 7.45%           | 1.318%        |
| 22        | 13.710      | 2004          | 2010        | 2013         | rBV2     | 662058         | 968337        | 31.94%          | 5.650%        |
| 23        | 13.739      | 2013          | 2015        | 2025         | rVV      | 302150         | 336980        | 11.11%          | 1.966%        |
| 24        | 13.816      | 2025          | 2028        | 2037         | rVB      | 53521          | 56774         | 1.87%           | 0.331%        |
| 25        | 14.227      | 2094          | 2098        | 2101         | rVB      | 39567          | 41271         | 1.36%           | 0.241%        |
| 26        | 14.316      | 2109          | 2113        | 2120         | rBV      | 183939         | 171089        | 5.64%           | 0.998%        |
| 27        | 14.716      | 2177          | 2181        | 2183         | rBV      | 125810         | 132808        | 4.38%           | 0.775%        |
| 28        | 14.739      | 2183          | 2185        | 2190         | rVB      | 101401         | 111063        | 3.66%           | 0.648%        |
| 29        | 15.039      | 2233          | 2236        | 2241         | rVB      | 45737          | 51223         | 1.69%           | 0.299%        |
| 30        | 15.092      | 2241          | 2245        | 2256         | rVB      | 488315         | 573609        | 18.92%          | 3.347%        |

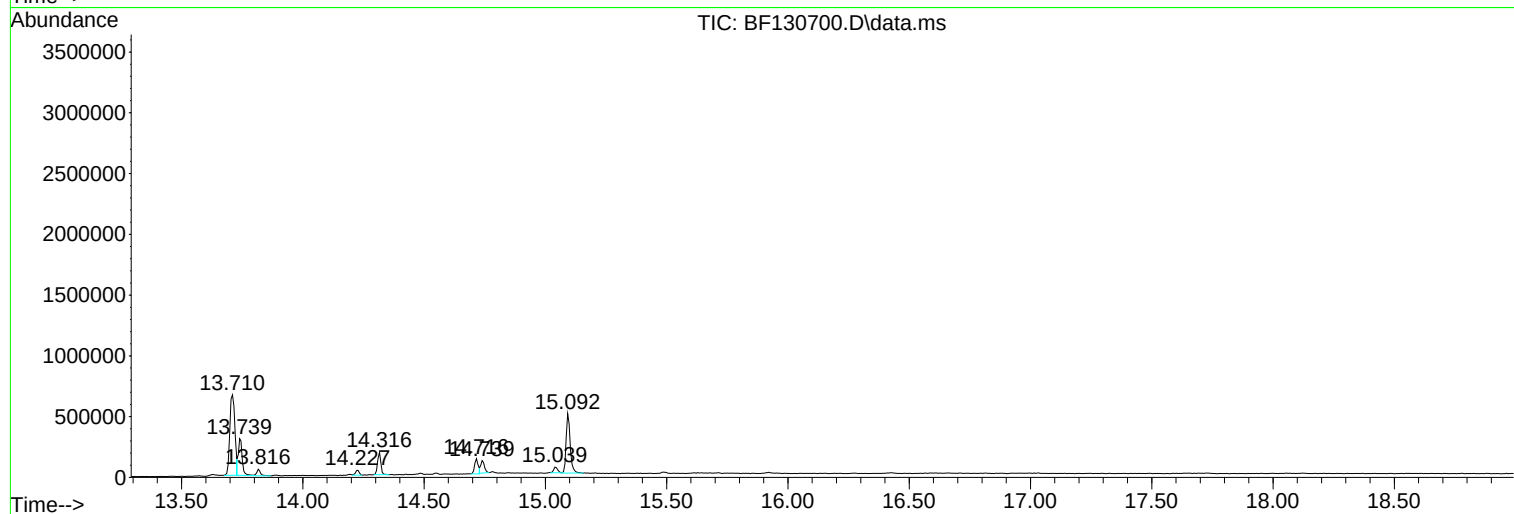
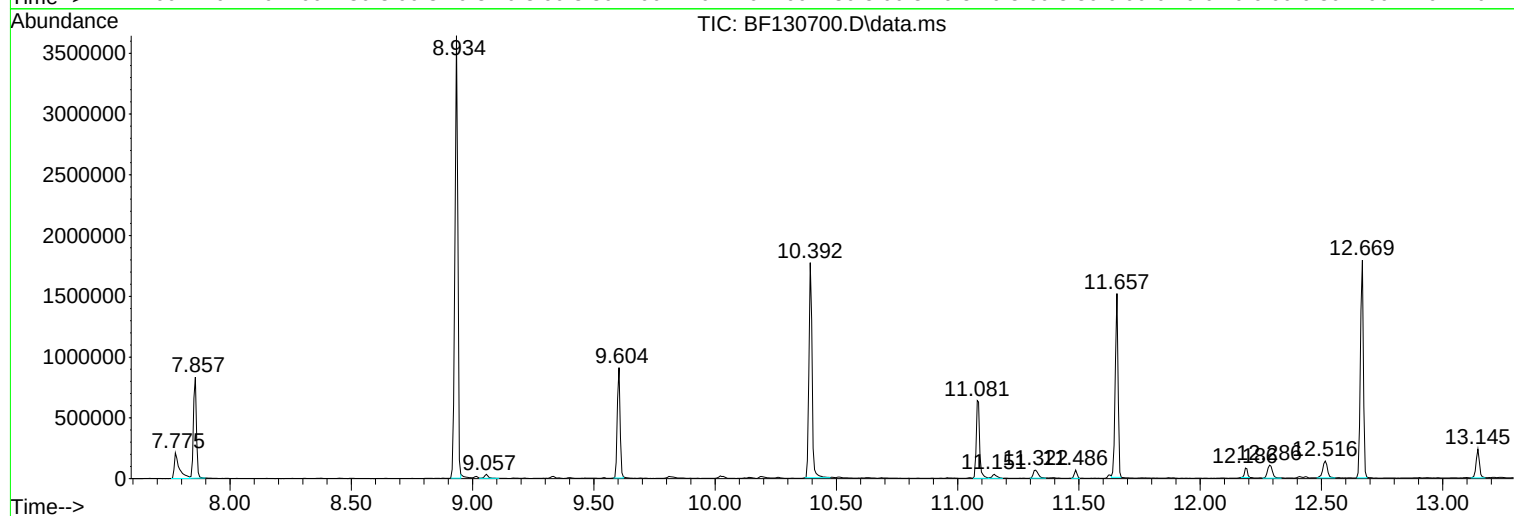
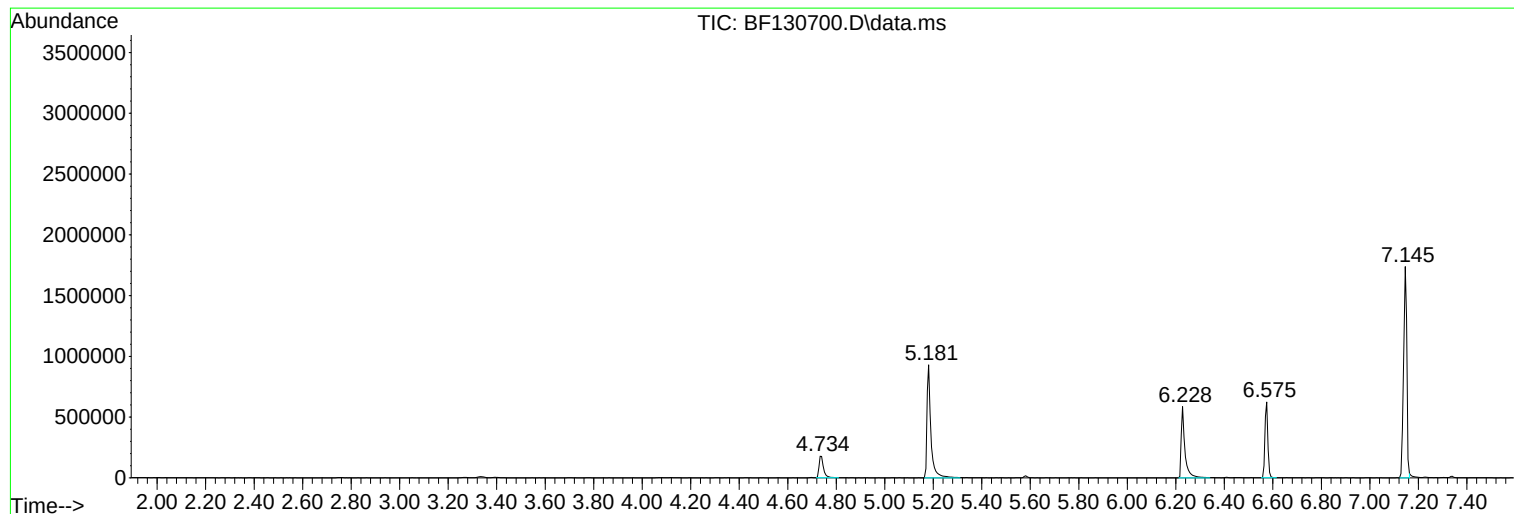
Sum of corrected areas: 17139374

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF101822\  
Data File : BF130700.D  
Acq On : 18 Oct 2022 16:12  
Operator : CG\JU  
Sample : N5164-02  
Misc :  
ALS Vial : 8 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
588A-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF101122.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\_F\Data\BF101822\  
Data File : BF130700.D  
Acq On : 18 Oct 2022 16:12  
Operator : CG\JU  
Sample : N5164-02  
Misc :  
ALS Vial : 8 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
588A-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF101122.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

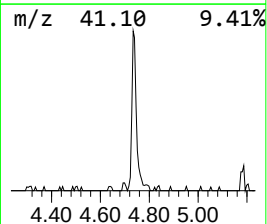
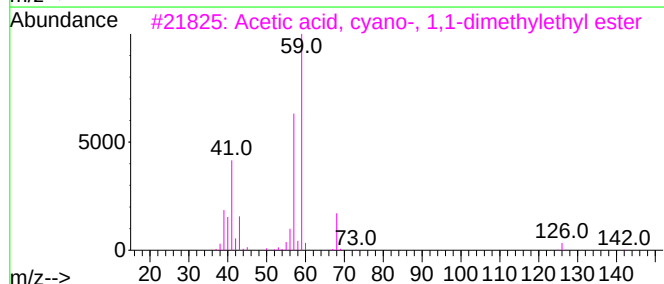
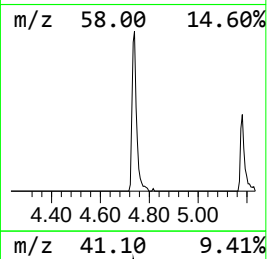
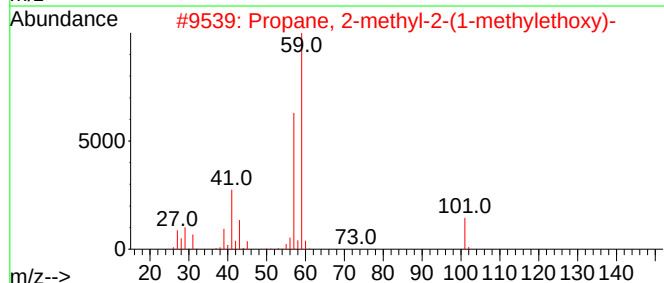
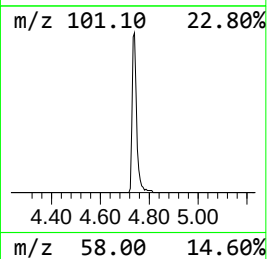
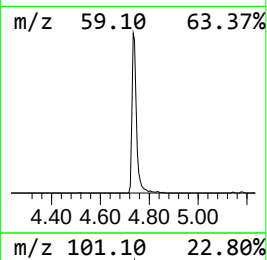
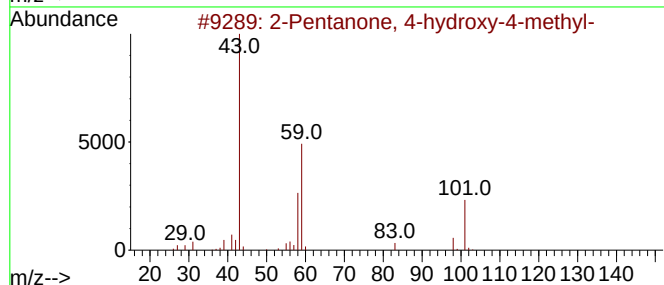
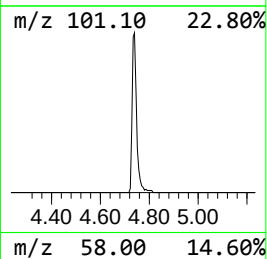
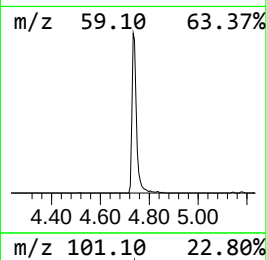
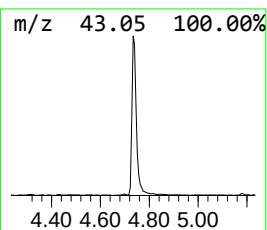
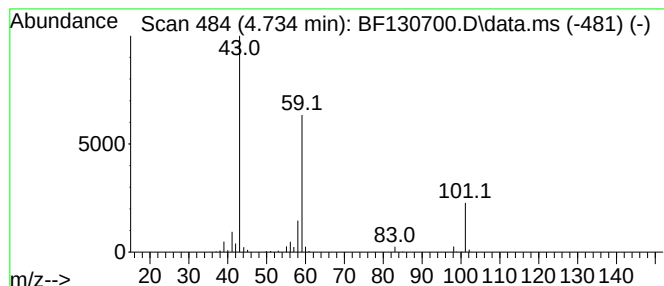
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*

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

| R.T.  | EstConc | Area   | Relative to ISTD       | R.T.  |
|-------|---------|--------|------------------------|-------|
| 4.734 | 8.57 ng | 229104 | 1,4-Dichlorobenzene-d4 | 6.575 |

| Hit# | of                                  | 5   | Tentative ID | MW          | MolForm | CAS# | Qual |
|------|-------------------------------------|-----|--------------|-------------|---------|------|------|
| 1    | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2      | 000123-42-2 | 64      |      |      |
| 2    | Propane, 2-methyl-2-(1-methyleth... | 116 | C7H16O       | 017348-59-3 | 53      |      |      |
| 3    | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2     | 001116-98-9 | 17      |      |      |
| 4    | 1-Propen-2-ol, acetate              | 100 | C5H8O2       | 000108-22-5 | 10      |      |      |
| 5    | Allyl acetate                       | 100 | C5H8O2       | 000591-87-7 | 9       |      |      |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF101822\  
Data File : BF130700.D  
Acq On : 18 Oct 2022 16:12  
Operator : CG\JU  
Sample : N5164-02  
Misc :  
ALS Vial : 8 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
588A-2

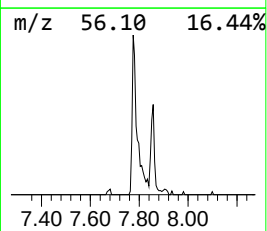
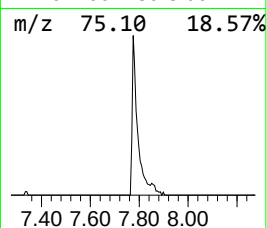
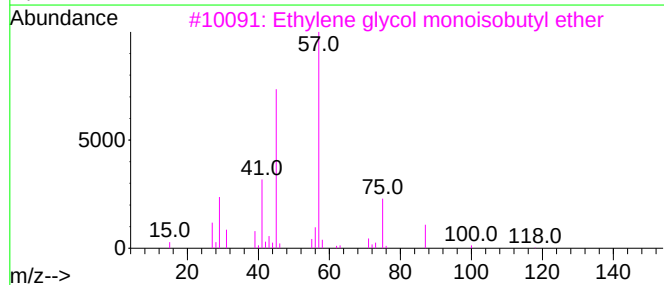
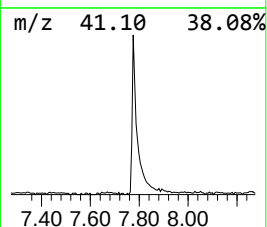
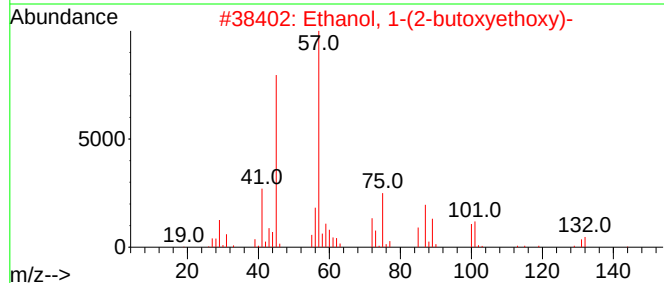
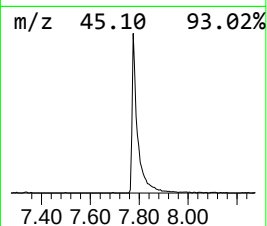
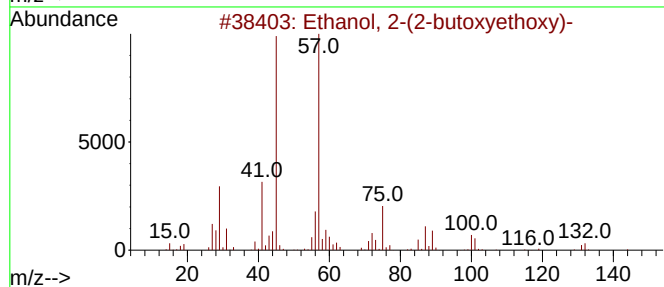
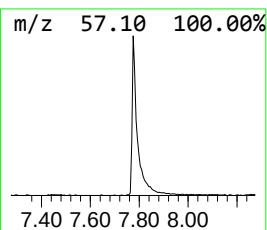
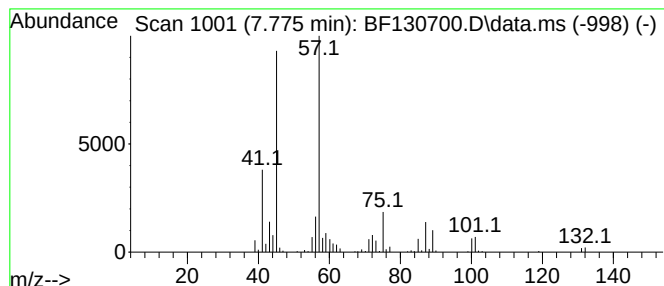
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF101122.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 7.775 | 8.40 ng | 299281 | Naphthalene-d8   | 7.857 |

| 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 | 64   |
| 4    |    |   | Butane, 1-(1-methylpropoxy)-       | 130 | C8H18O  | 000999-65-5 | 53   |
| 5    |    |   | Di-sec-Butyl ether                 | 130 | C8H18O  | 006863-58-7 | 53   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF101822\  
Data File : BF130700.D  
Acq On : 18 Oct 2022 16:12  
Operator : CG\JU  
Sample : N5164-02  
Misc :  
ALS Vial : 8 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
588A-2

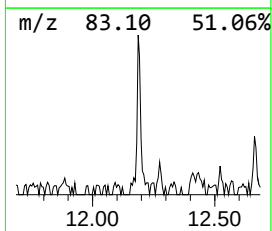
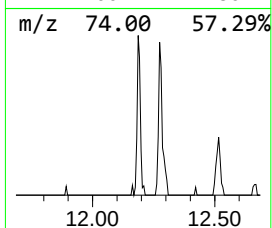
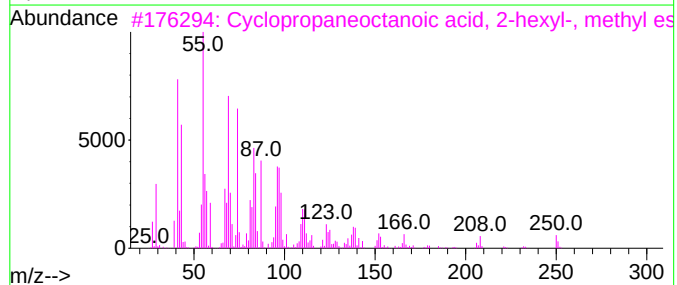
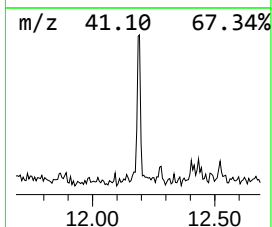
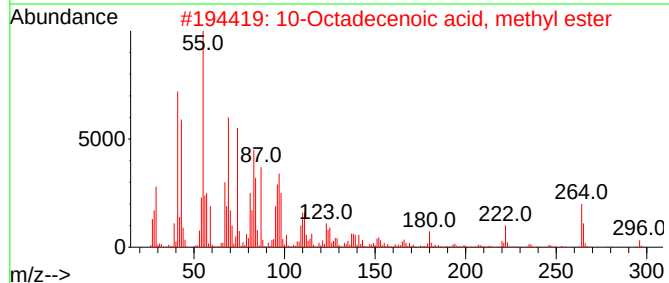
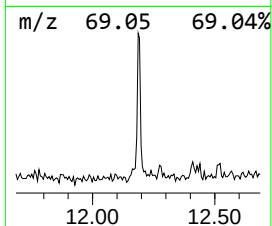
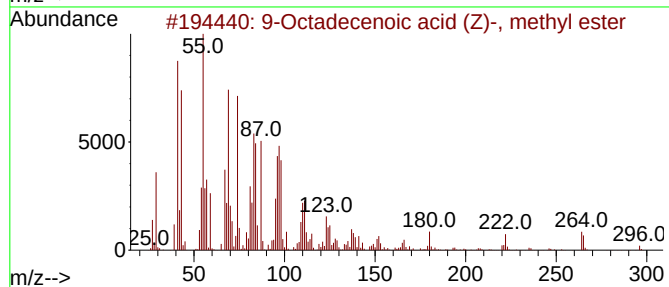
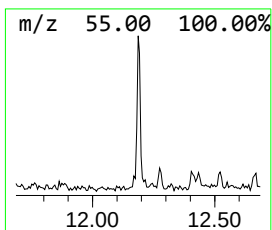
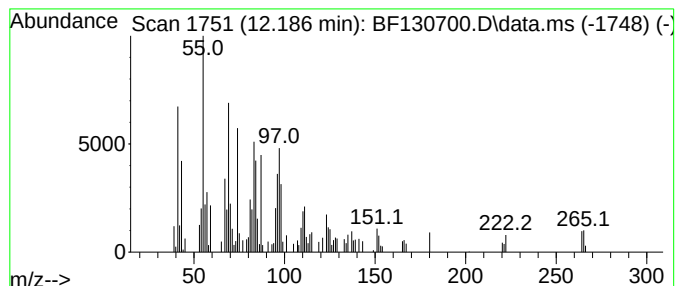
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF101122.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 3 9-Octadecenoic acid (Z)-, m... Concentration Rank 3

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 12.186 | 2.09 ng | 65847 | Phenanthrene-d10 | 11.086 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | 9-Octadecenoic acid (Z)-, methyl... | 296 | C19H36O2 | 000112-62-9 | 95   |
| 2    |    |   | 10-Octadecenoic acid, methyl ester  | 296 | C19H36O2 | 013481-95-3 | 91   |
| 3    |    |   | Cyclopropaneoctanoic acid, 2-hex... | 282 | C18H34O2 | 010152-61-1 | 90   |
| 4    |    |   | 16-Octadecenoic acid, methyl ester  | 296 | C19H36O2 | 056554-49-5 | 87   |
| 5    |    |   | 15-Octadecenoic acid, methyl ester  | 296 | C19H36O2 | 004764-72-1 | 87   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF101822\  
Data File : BF130700.D  
Acq On : 18 Oct 2022 16:12  
Operator : CG\JU  
Sample : N5164-02  
Misc :  
ALS Vial : 8 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
588A-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF101122.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-... | 4.734  | 8.6     | ng    | 229104   | 1                     | 6.575  | 534869 | 20.0 |
| Ethanol, 2-(2-b... | 7.775  | 8.4     | ng    | 299281   | 2                     | 7.857  | 712834 | 20.0 |
| 9-Octadecenoic ... | 12.186 | 2.1     | ng    | 65847    | 4                     | 11.086 | 631330 | 20.0 |