

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF110921\  
 Data File : BF126093.D  
 Acq On : 9 Nov 2021 21:30  
 Operator : JU/CG  
 Sample : M4582-02  
 Misc :  
 ALS Vial : 12 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 VWE-B10-110621-10-20

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-BF110321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126093.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         | 2.157       | 4             | 12          | 18           | rBV      | 1807897        | 2350618       | 41.82%          | 6.131%        |
| 2         | 2.263       | 25            | 30          | 38           | rBV      | 65031          | 95003         | 1.69%           | 0.248%        |
| 3         | 5.069       | 503           | 507         | 515          | rVB      | 222282         | 282308        | 5.02%           | 0.736%        |
| 4         | 5.469       | 570           | 575         | 579          | rBV      | 4259410        | 4295166       | 76.42%          | 11.203%       |
| 5         | 6.481       | 741           | 747         | 750          | rBV      | 4426913        | 4380691       | 77.94%          | 11.426%       |
| 6         | 6.851       | 806           | 810         | 813          | rBV      | 1510924        | 1142739       | 20.33%          | 2.980%        |
| 7         | 7.416       | 900           | 906         | 908          | rBV      | 2903973        | 2935371       | 52.23%          | 7.656%        |
| 8         | 8.039       | 1007          | 1012        | 1024         | rBV      | 1159262        | 1167862       | 20.78%          | 3.046%        |
| 9         | 8.133       | 1024          | 1028        | 1031         | rBV      | 1867726        | 1439514       | 25.61%          | 3.755%        |
| 10        | 9.210       | 1206          | 1211        | 1214         | rBV      | 6999635        | 5620350       | 100.00%         | 14.659%       |
| 11        | 9.886       | 1322          | 1326        | 1329         | rBV      | 1982179        | 1635675       | 29.10%          | 4.266%        |
| 12        | 10.674      | 1456          | 1460        | 1463         | rBV      | 3386204        | 3158520       | 56.20%          | 8.238%        |
| 13        | 11.369      | 1574          | 1578        | 1581         | rBV      | 1841660        | 1543597       | 27.46%          | 4.026%        |
| 14        | 11.392      | 1581          | 1582        | 1586         | rVV      | 290230         | 168460        | 3.00%           | 0.439%        |
| 15        | 11.439      | 1586          | 1590        | 1594         | rVB3     | 97277          | 102666        | 1.83%           | 0.268%        |
| 16        | 11.763      | 1642          | 1645        | 1649         | rBV      | 170693         | 150415        | 2.68%           | 0.392%        |
| 17        | 12.468      | 1759          | 1765        | 1769         | rBV      | 253401         | 265855        | 4.73%           | 0.693%        |
| 18        | 12.580      | 1781          | 1784        | 1787         | rVB      | 341810         | 277648        | 4.94%           | 0.724%        |
| 19        | 12.810      | 1814          | 1823        | 1826         | rBV      | 272963         | 308205        | 5.48%           | 0.804%        |
| 20        | 12.957      | 1843          | 1848        | 1851         | rBV      | 4861599        | 4082611       | 72.64%          | 10.648%       |
| 21        | 13.857      | 1997          | 2001        | 2009         | rVB2     | 150361         | 211060        | 3.76%           | 0.550%        |
| 22        | 14.004      | 2021          | 2026        | 2029         | rBV      | 1196251        | 1159275       | 20.63%          | 3.024%        |
| 23        | 14.027      | 2029          | 2030        | 2037         | rVB      | 127329         | 105922        | 1.88%           | 0.276%        |
| 24        | 14.868      | 2169          | 2173        | 2179         | rBV      | 115304         | 142236        | 2.53%           | 0.371%        |
| 25        | 15.045      | 2199          | 2203        | 2205         | rBV      | 102271         | 149093        | 2.65%           | 0.389%        |
| 26        | 15.345      | 2251          | 2254        | 2260         | rVB2     | 77548          | 100469        | 1.79%           | 0.262%        |
| 27        | 15.404      | 2261          | 2264        | 2268         | rBV      | 74133          | 87234         | 1.55%           | 0.228%        |
| 28        | 15.468      | 2270          | 2275        | 2279         | rBV      | 803853         | 981981        | 17.47%          | 2.561%        |

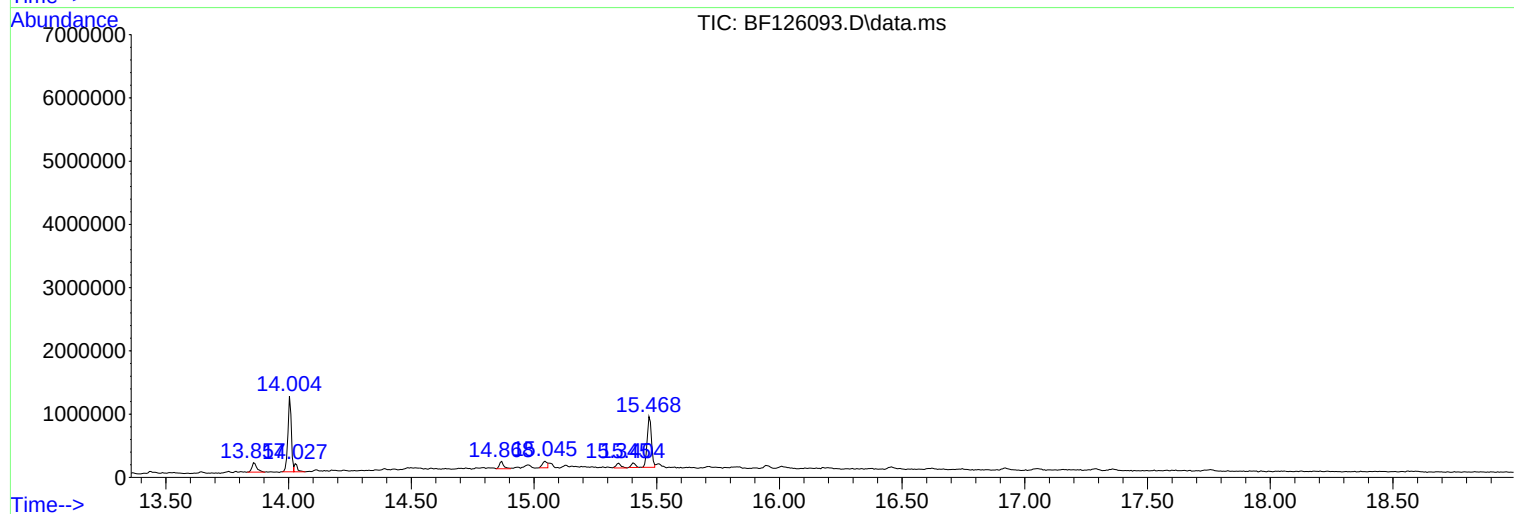
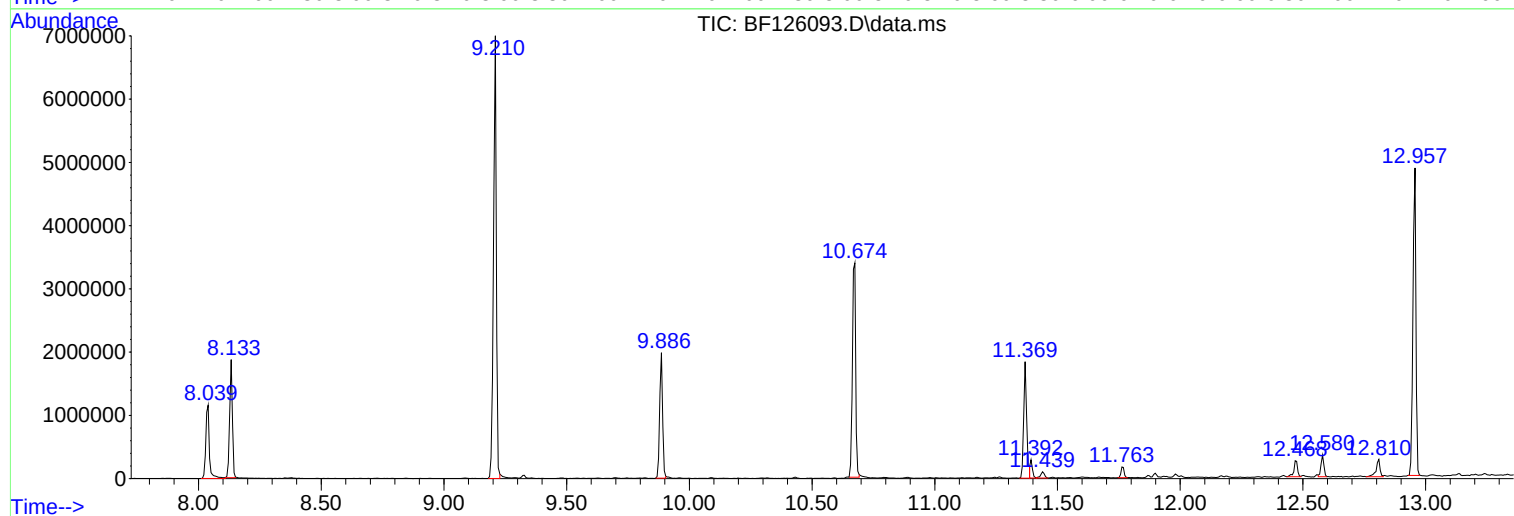
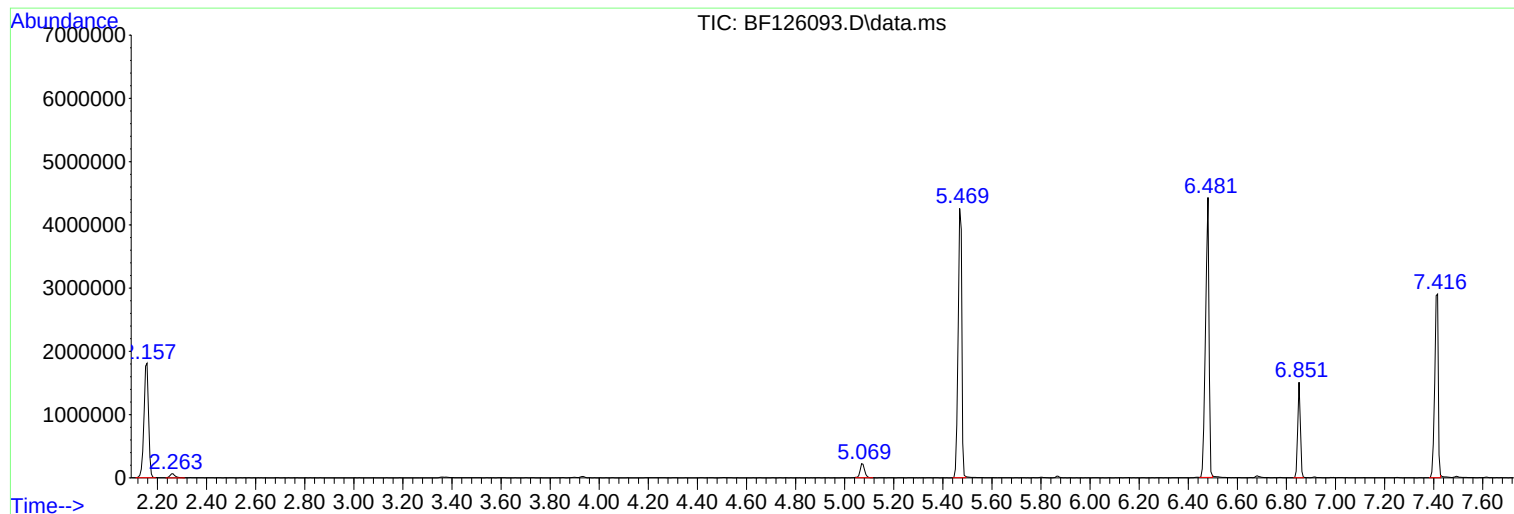
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Misc :  
ALS Vial : 12 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
VWE-B10-110621-10-20

Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF110321.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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ClientSampleId :  
VWE-B10-110621-10-20

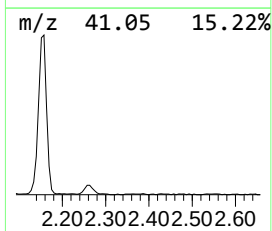
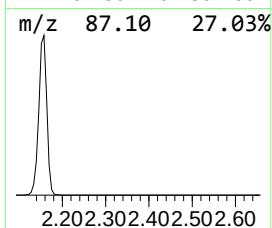
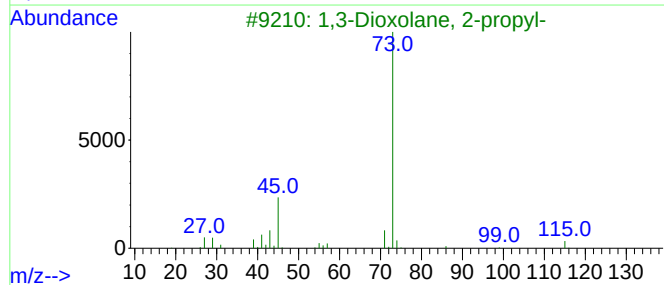
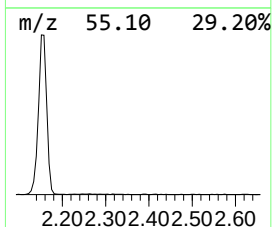
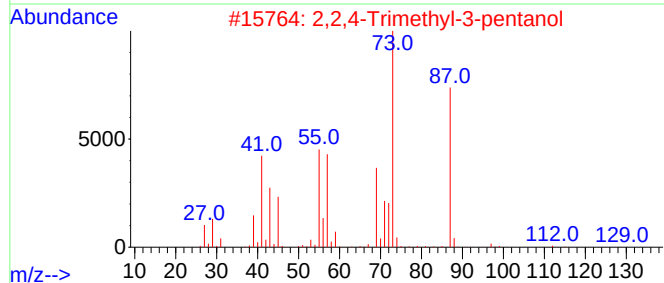
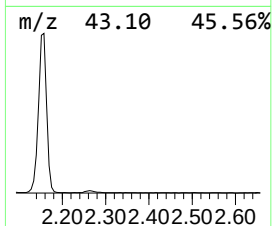
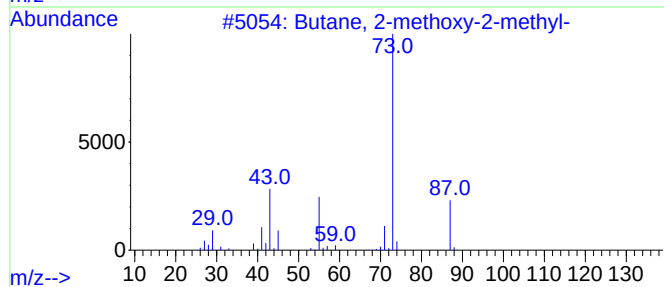
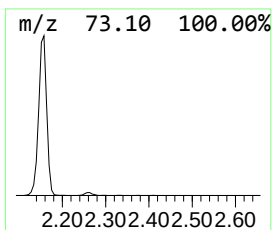
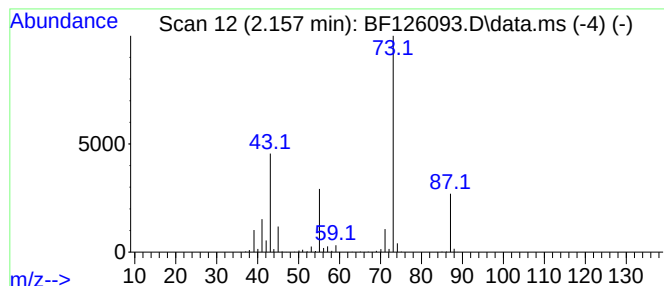
Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF110321.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

| R.T.  | EstConc  | Area    | Relative to ISTD       | R.T.  |
|-------|----------|---------|------------------------|-------|
| 2.157 | 41.14 ng | 2350620 | 1,4-Dichlorobenzene-d4 | 6.851 |

| Hit# | of | 5 | Tentative ID                | MW  | MolForm | CAS#        | Qual |
|------|----|---|-----------------------------|-----|---------|-------------|------|
| 1    |    |   | Butane, 2-methoxy-2-methyl- | 102 | C6H14O  | 000994-05-8 | 83   |
| 2    |    |   | 2,2,4-Trimethyl-3-pentanol  | 130 | C8H18O  | 005162-48-1 | 40   |
| 3    |    |   | 1,3-Dioxolane, 2-propyl-    | 116 | C6H12O2 | 003390-13-4 | 23   |
| 4    |    |   | Silane, tetramethyl-        | 88  | C4H12Si | 000075-76-3 | 17   |
| 5    |    |   | N-Ethylformamide            | 73  | C3H7NO  | 000627-45-2 | 9    |



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Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF110321.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

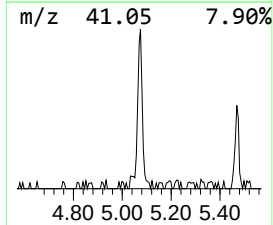
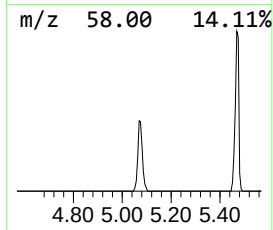
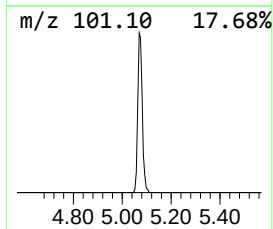
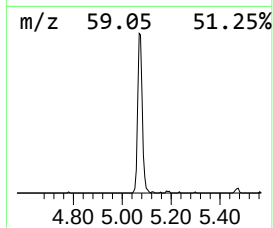
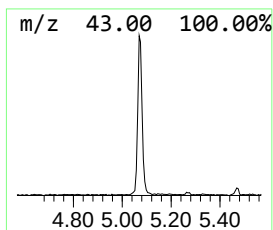
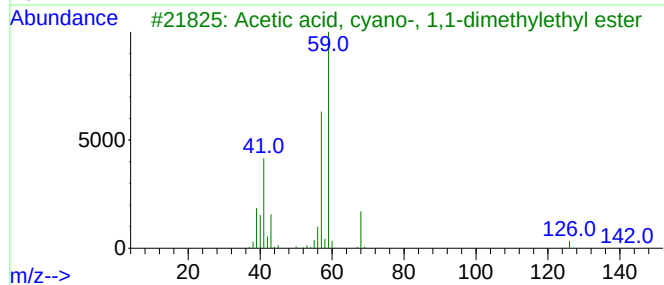
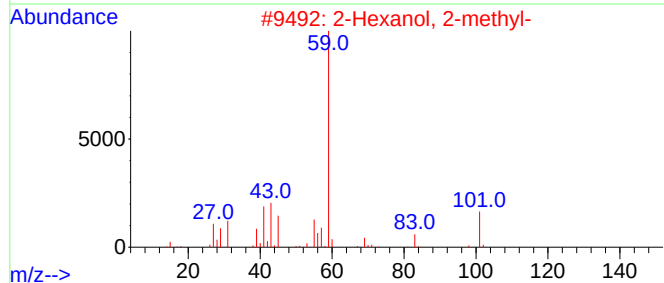
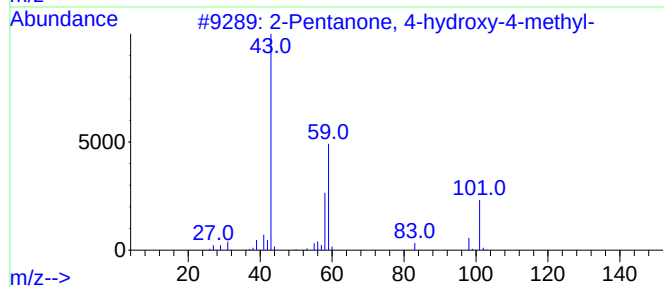
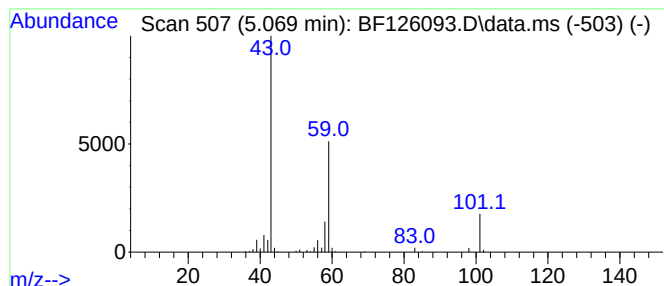
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T.  | EstConc | Area   | Relative to ISTD       | R.T.  |
|-------|---------|--------|------------------------|-------|
| 5.069 | 4.94 ng | 282308 | 1,4-Dichlorobenzene-d4 | 6.851 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2  | 000123-42-2 | 72   |
| 2    |    |   | 2-Hexanol, 2-methyl-                | 116 | C7H16O   | 000625-23-0 | 28   |
| 3    |    |   | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 25   |
| 4    |    |   | 2,3-Butanedione, monooxime          | 101 | C4H7NO2  | 000057-71-6 | 16   |
| 5    |    |   | 1-Propen-2-ol, acetate              | 100 | C5H8O2   | 000108-22-5 | 12   |



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Sample : M4582-02  
Misc :  
ALS Vial : 12 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
VWE-B10-110621-10-20

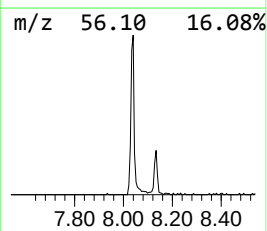
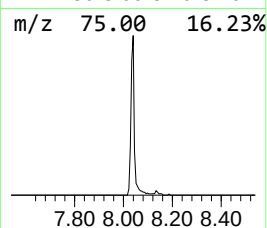
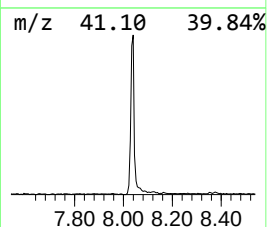
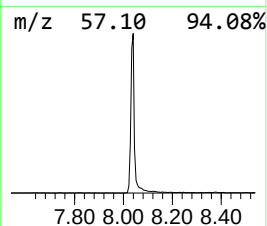
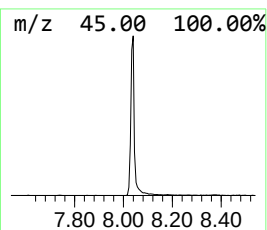
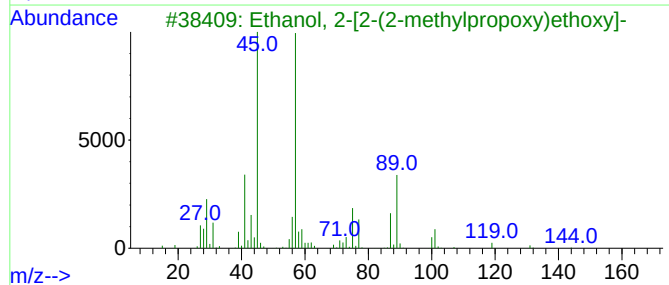
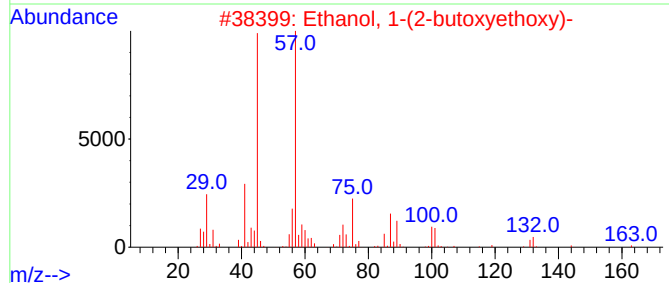
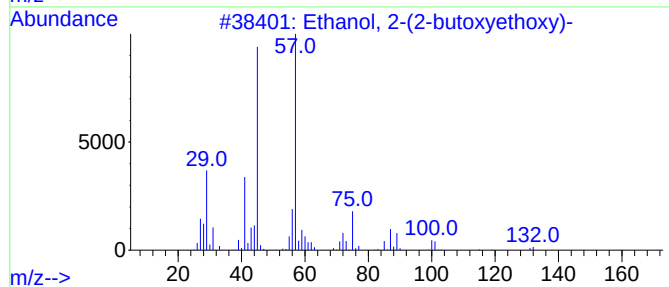
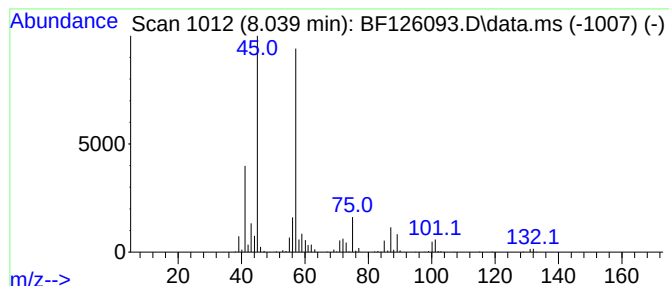
Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF110321.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

| R.T.  | EstConc  | Area    | Relative to ISTD | R.T.  |
|-------|----------|---------|------------------|-------|
| 8.039 | 16.23 ng | 1167860 | Naphthalene-d8   | 8.133 |

| 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    |    |   | Ethanol, 2-[2-(2-methylpropoxy)e... | 162 | C8H18O3 | 018912-80-6 | 78   |
| 4    |    |   | Di-sec-Butyl ether                  | 130 | C8H18O  | 006863-58-7 | 53   |
| 5    |    |   | 3,3-Dimethylbutane-2-ol             | 102 | C6H14O  | 000464-07-3 | 53   |



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Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF110321.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

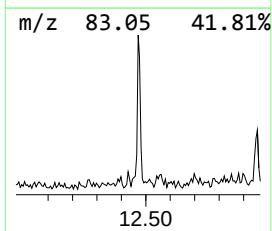
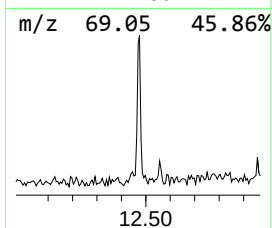
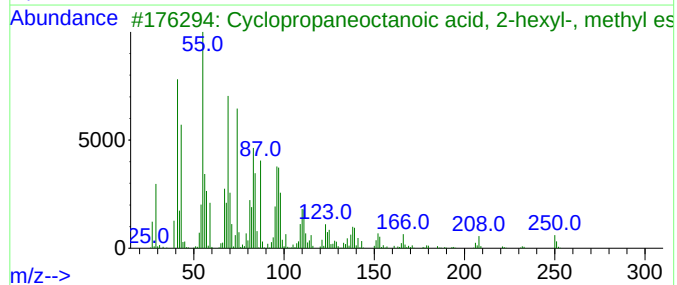
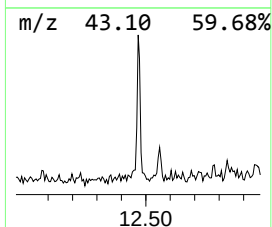
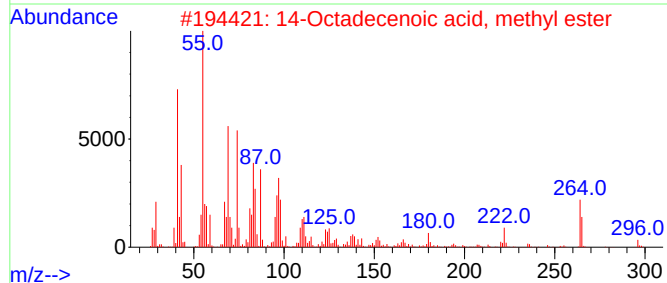
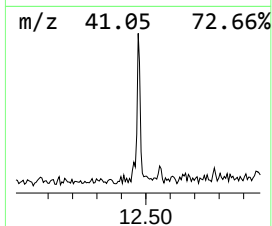
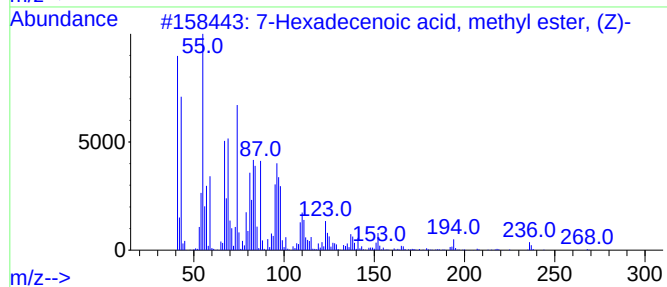
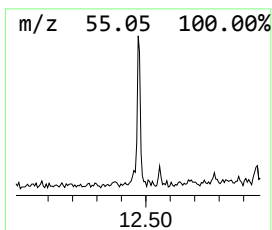
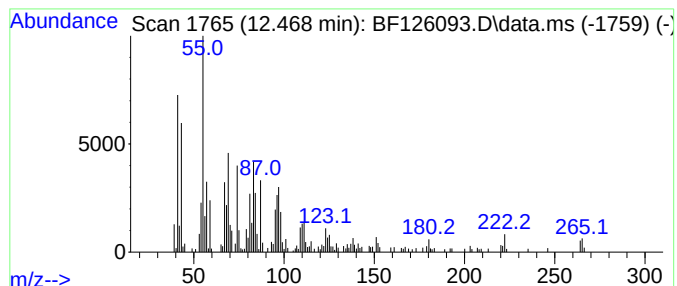
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 7-Hexadecenoic acid, methyl... Concentration Rank 5

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 12.468 | 3.44 ng | 265855 | Phenanthrene-d10 | 11.368 |

| Hit# | of 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|------|-------------------------------------|-----|----------|-------------|------|
| 1    |      | 7-Hexadecenoic acid, methyl este... | 268 | C17H32O2 | 056875-67-3 | 87   |
| 2    |      | 14-Octadecenoic acid, methyl ester  | 296 | C19H36O2 | 056554-48-4 | 87   |
| 3    |      | Cyclopropaneoctanoic acid, 2-hex... | 282 | C18H34O2 | 010152-61-1 | 83   |
| 4    |      | 13-Octadecenoic acid, methyl ester  | 296 | C19H36O2 | 056554-47-3 | 83   |
| 5    |      | 9-Octadecenoic acid (Z)-, methyl... | 296 | C19H36O2 | 000112-62-9 | 81   |



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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L  
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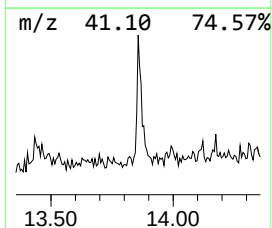
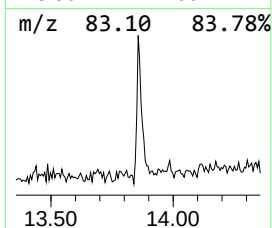
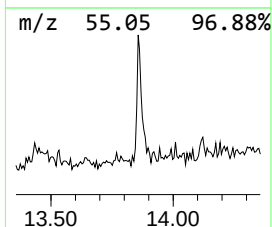
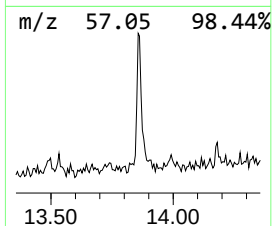
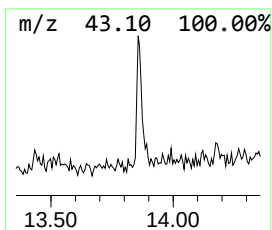
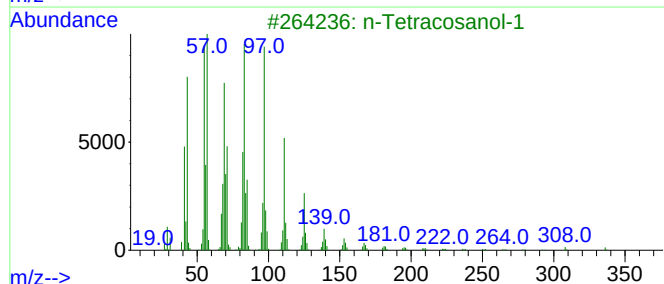
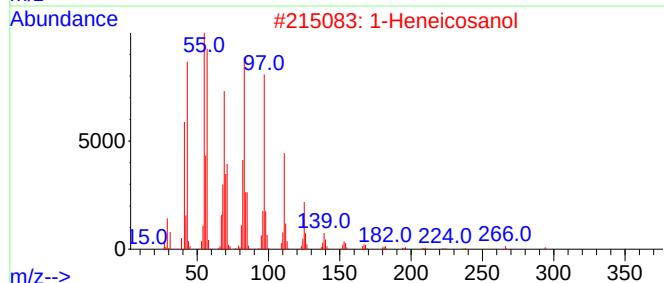
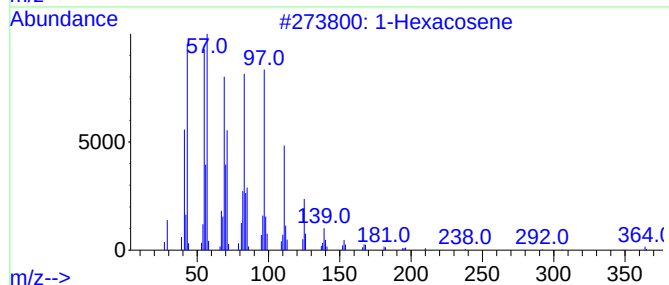
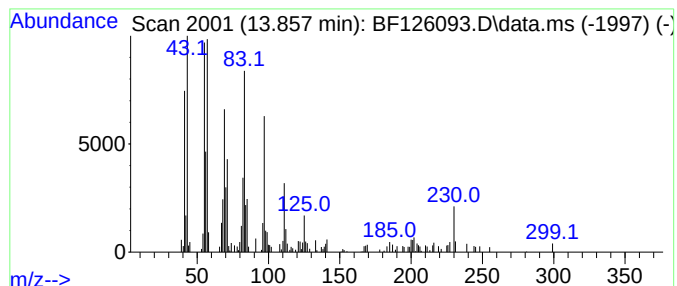
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Peak Number 5 1-Hexacosene Concentration Rank 4

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 13.857 | 3.64 ng | 211060 | Chrysene-d12     | 14.004 |

| Hit# | of 5 | Tentative ID   | MW  | MolForm | CAS#        | Qual |
|------|------|----------------|-----|---------|-------------|------|
| 1    | 1    | Hexacosene     | 364 | C26H52  | 018835-33-1 | 90   |
| 2    | 1    | Heneicosanol   | 312 | C21H44O | 015594-90-8 | 87   |
| 3    | n    | Tetracosanol-1 | 354 | C24H50O | 000506-51-4 | 87   |
| 4    | 1    | Pentadecene    | 210 | C15H30  | 013360-61-7 | 86   |
| 5    |      | Octacosanol    | 410 | C28H58O | 000557-61-9 | 83   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF110921\  
Data File : BF126093.D  
Acq On : 9 Nov 2021 21:30  
Operator : JU/CG  
Sample : M4582-02  
Misc :  
ALS Vial : 12 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
VWE-B10-110621-10-20

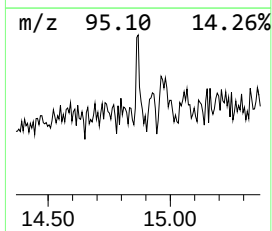
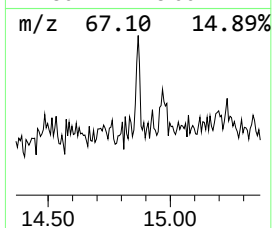
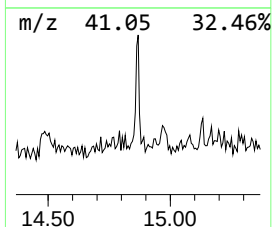
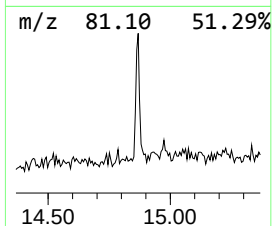
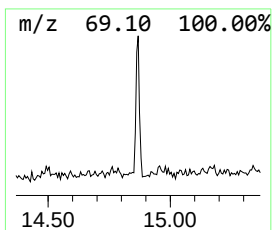
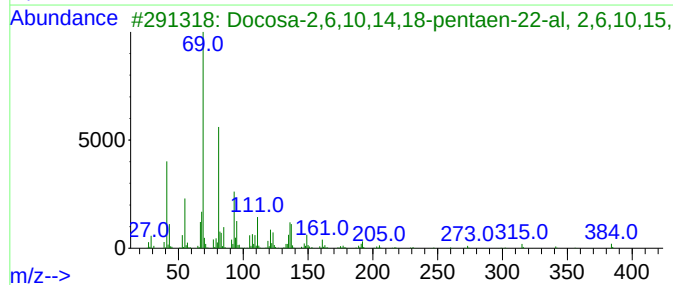
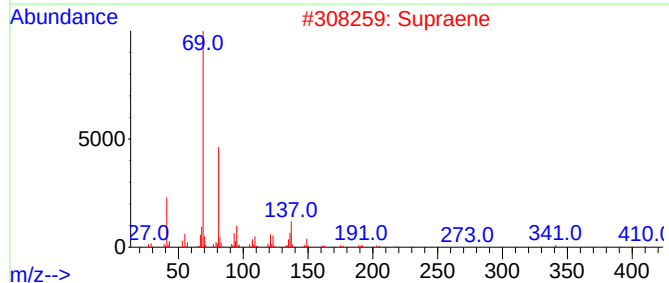
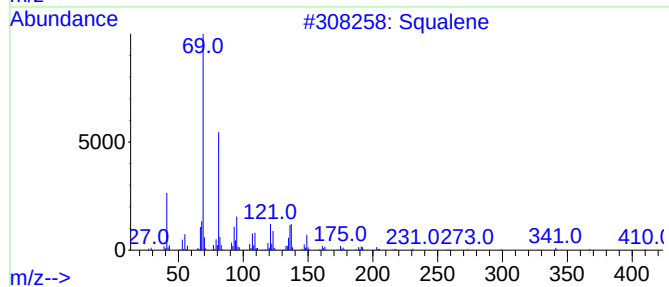
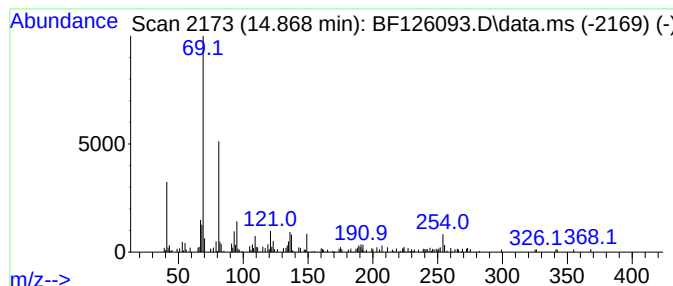
Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF110321.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 6 Squalene Concentration Rank 6

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 14.868 | 2.90 ng | 142236 | Perylene-d12     | 15.468 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|---------|--------------|------|
| 1    |    |   | Squalene                            | 410 | C30H50  | 000111-02-4  | 72   |
| 2    |    |   | Supraene                            | 410 | C30H50  | 007683-64-9  | 72   |
| 3    |    |   | Docosa-2,6,10,14,18-pentaen-22-a... | 384 | C27H44O | 1000163-04-7 | 72   |
| 4    |    |   | (3E,7E)-4,8,12-Trimethyltrideca...  | 218 | C16H26  | 062235-06-7  | 64   |
| 5    |    |   | Furan, 3-(4,8-dimethyl-3,7-nonad... | 218 | C15H22O | 023262-34-2  | 64   |





Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF110921\  
Data File : BF126093.D  
Acq On : 9 Nov 2021 21:30  
Operator : JU/CG  
Sample : M4582-02  
Misc :  
ALS Vial : 12 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
VWE-B10-110621-10-20

Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF110321.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 |
| Butane, 2-metho... | 2.157  | 41.1    | ng    | 2350620  | 1                     | 6.851  | 1142740 | 20.0 |
| 2-Pentanone, 4-... | 5.069  | 4.9     | ng    | 282308   | 1                     | 6.851  | 1142740 | 20.0 |
| Ethanol, 2-(2-b... | 8.039  | 16.2    | ng    | 1167860  | 2                     | 8.133  | 1439510 | 20.0 |
| 7-Hexadecenoic ... | 12.468 | 3.4     | ng    | 265855   | 4                     | 11.368 | 1543600 | 20.0 |
| 1-Hexacosene       | 13.857 | 3.6     | ng    | 211060   | 5                     | 14.004 | 1159280 | 20.0 |
| Squalene           | 14.868 | 2.9     | ng    | 142236   | 6                     | 15.468 | 981981  | 20.0 |