

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF122120\  
 Data File : BF122802.D  
 Acq On : 21 Dec 2020 16:11  
 Operator : JU/CG  
 Sample : L5160-04  
 Misc :  
 ALS Vial : 5 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 LLEXSITUTV-020-001-SO

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-BF120520.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122802.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         | 4.392       | 388           | 392         | 400          | rBV      | 75186          | 87868         | 2.75%           | 0.475%        |
| 2         | 5.022       | 494           | 499         | 512          | rBV      | 918272         | 969809        | 30.31%          | 5.247%        |
| 3         | 5.434       | 565           | 569         | 586          | rBV      | 1046003        | 971971        | 30.38%          | 5.259%        |
| 4         | 6.445       | 738           | 741         | 754          | rBV      | 1491976        | 1475087       | 46.10%          | 7.981%        |
| 5         | 6.816       | 801           | 804         | 808          | rBV      | 997828         | 751890        | 23.50%          | 4.068%        |
| 6         | 7.381       | 895           | 900         | 903          | rBV      | 1470473        | 1315314       | 41.11%          | 7.117%        |
| 7         | 8.104       | 1018          | 1023        | 1026         | rBV      | 1006407        | 954555        | 29.83%          | 5.165%        |
| 8         | 9.175       | 1201          | 1205        | 1209         | rBV      | 2666340        | 2552393       | 79.77%          | 13.810%       |
| 9         | 9.569       | 1268          | 1272        | 1281         | rVB      | 103056         | 99731         | 3.12%           | 0.540%        |
| 10        | 9.857       | 1316          | 1321        | 1332         | rBV      | 1273760        | 1137743       | 35.56%          | 6.156%        |
| 11        | 10.645      | 1451          | 1455        | 1466         | rVB      | 601905         | 613818        | 19.18%          | 3.321%        |
| 12        | 11.339      | 1569          | 1573        | 1581         | rBV      | 1254459        | 1220941       | 38.16%          | 6.606%        |
| 13        | 11.868      | 1658          | 1663        | 1672         | rBV2     | 194377         | 250103        | 7.82%           | 1.353%        |
| 14        | 12.168      | 1711          | 1714        | 1718         | rBV      | 124017         | 115532        | 3.61%           | 0.625%        |
| 15        | 12.557      | 1777          | 1780        | 1783         | rBV      | 47793          | 45011         | 1.41%           | 0.244%        |
| 16        | 12.657      | 1793          | 1797        | 1801         | rBV      | 104499         | 122120        | 3.82%           | 0.661%        |
| 17        | 12.927      | 1838          | 1843        | 1847         | rBV      | 3224358        | 3199695       | 100.00%         | 17.312%       |
| 18        | 13.839      | 1993          | 1998        | 2015         | rBV3     | 96168          | 256951        | 8.03%           | 1.390%        |
| 19        | 13.986      | 2018          | 2023        | 2033         | rBV      | 1032454        | 1112909       | 34.78%          | 6.022%        |
| 20        | 14.415      | 2093          | 2096        | 2099         | rBV      | 38689          | 43961         | 1.37%           | 0.238%        |
| 21        | 14.827      | 2163          | 2166        | 2170         | rVB      | 28949          | 32558         | 1.02%           | 0.176%        |
| 22        | 15.021      | 2195          | 2199        | 2206         | rBV      | 53741          | 81067         | 2.53%           | 0.439%        |
| 23        | 15.321      | 2246          | 2250        | 2254         | rVB      | 30159          | 40223         | 1.26%           | 0.218%        |
| 24        | 15.439      | 2266          | 2270        | 2282         | rBV      | 682174         | 941113        | 29.41%          | 5.092%        |
| 25        | 16.892      | 2512          | 2517        | 2524         | rBV2     | 20359          | 47632         | 1.49%           | 0.258%        |
| 26        | 18.374      | 2763          | 2769        | 2778         | rBV10    | 13151          | 42062         | 1.31%           | 0.228%        |

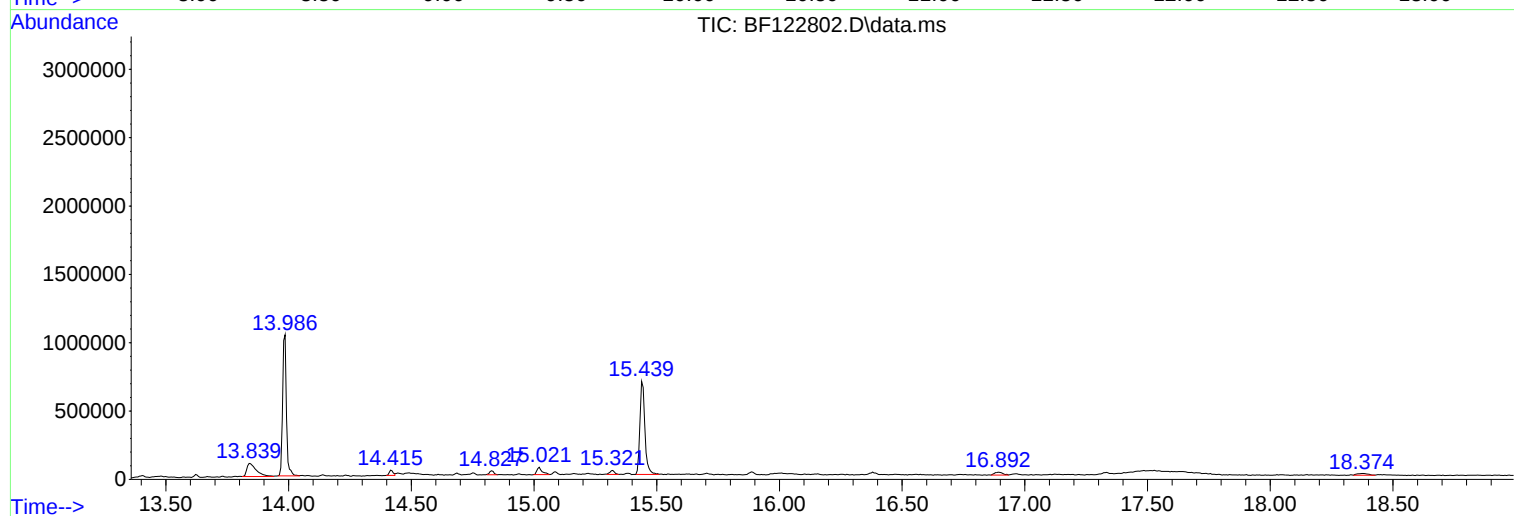
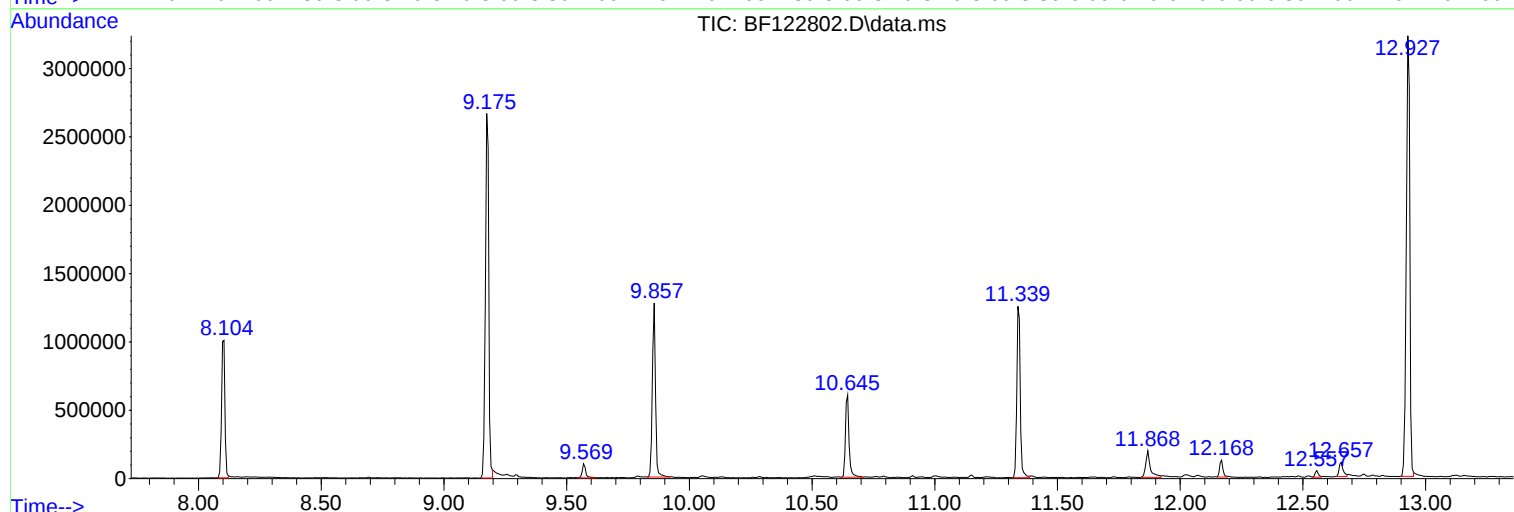
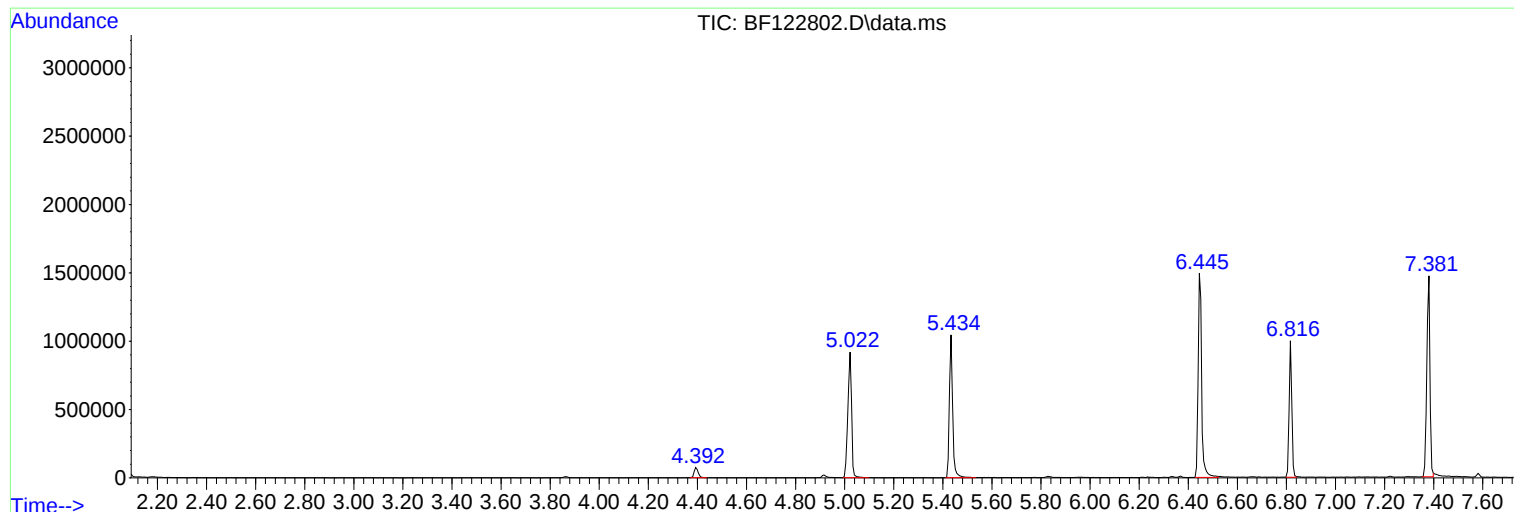
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Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF122120\  
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Sample : L5160-04  
Misc :  
ALS Vial : 5 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
LLEXSITUTV-020-001-SO

Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF120520.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF122120\  
Data File : BF122802.D  
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Misc :  
ALS Vial : 5 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
LLEXSITUTV-020-001-SO

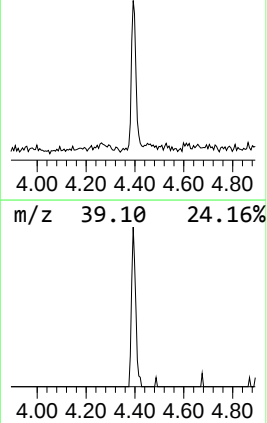
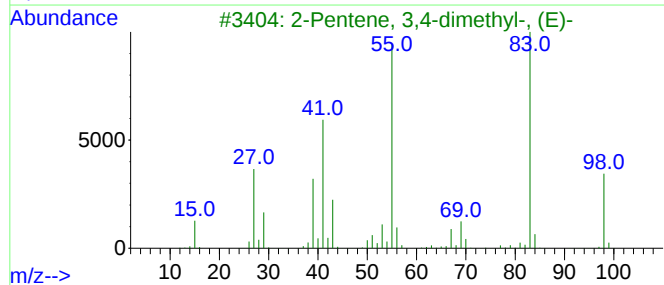
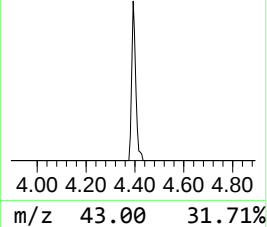
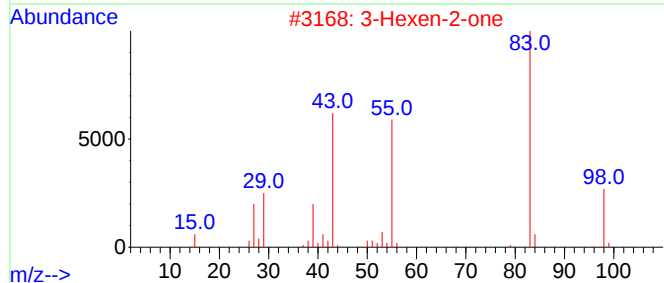
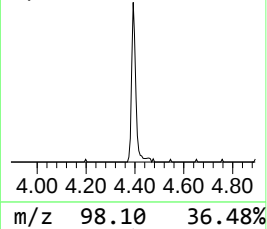
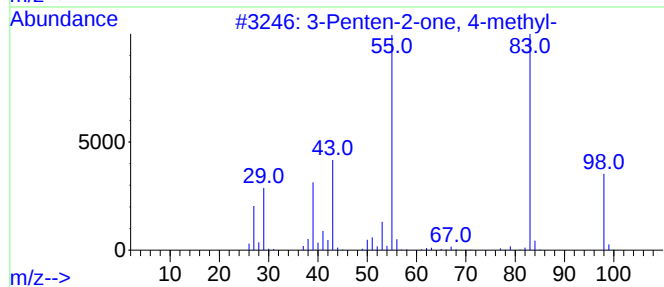
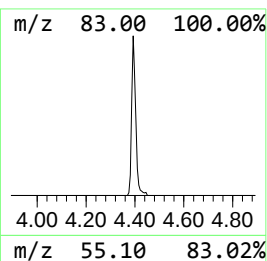
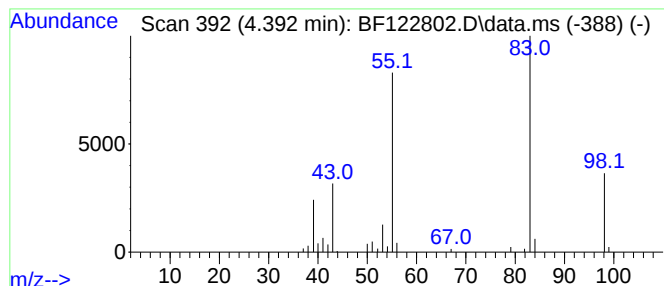
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

| R.T.  | EstConc | Area  | Relative to ISTD       | R.T.  |
|-------|---------|-------|------------------------|-------|
| 4.392 | 2.34 ng | 87868 | 1,4-Dichlorobenzene-d4 | 6.816 |

| Hit# | of | 5 | Tentative ID                   | MW | MolForm | CAS#        | Qual |
|------|----|---|--------------------------------|----|---------|-------------|------|
| 1    |    |   | 3-Penten-2-one, 4-methyl-      | 98 | C6H10O  | 000141-79-7 | 91   |
| 2    |    |   | 3-Hexen-2-one                  | 98 | C6H10O  | 000763-93-9 | 91   |
| 3    |    |   | 2-Pentene, 3,4-dimethyl-, (E)- | 98 | C7H14   | 004914-92-5 | 90   |
| 4    |    |   | 2-Pentene, 3,4-dimethyl-, (Z)- | 98 | C7H14   | 004914-91-4 | 86   |
| 5    |    |   | 2-Pentene, 4,4-dimethyl-, (E)- | 98 | C7H14   | 000690-08-4 | 86   |



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Sample : L5160-04  
Misc :  
ALS Vial : 5 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
LLEXSITUTV-020-001-SO

Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF120520.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

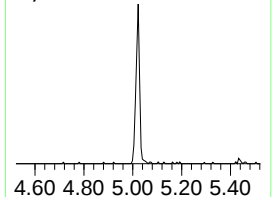
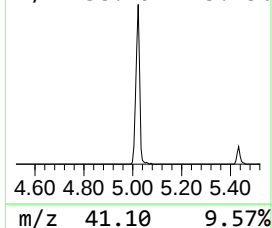
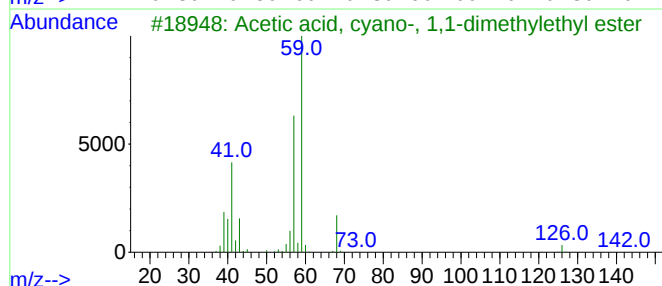
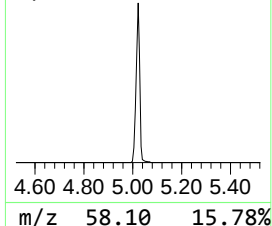
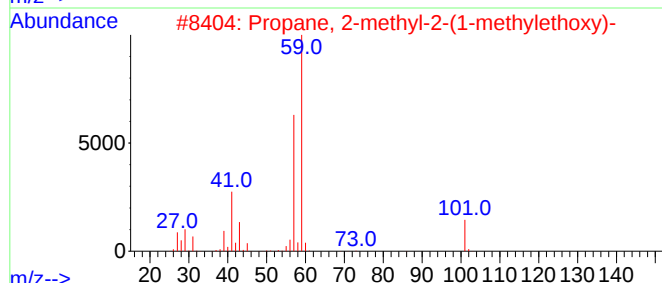
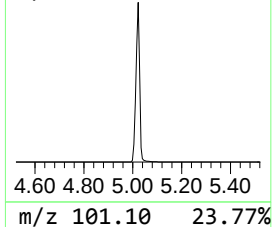
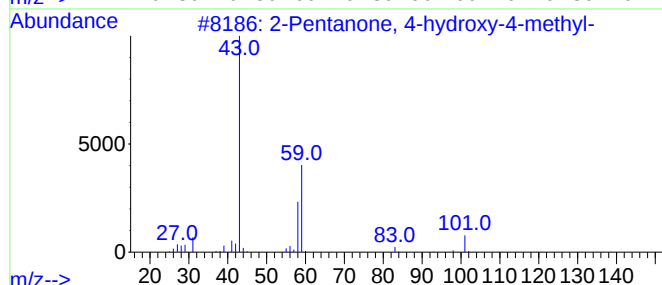
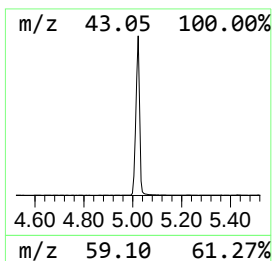
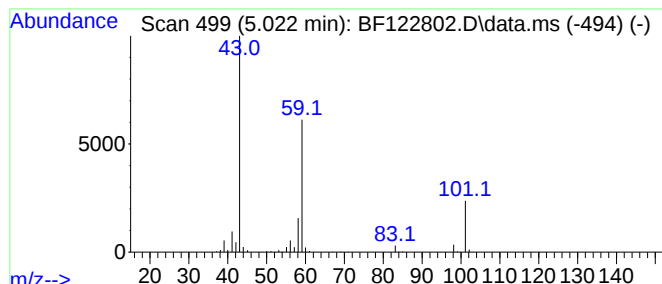
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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

| R.T.  | EstConc  | Area   | Relative to ISTD       | R.T.  |
|-------|----------|--------|------------------------|-------|
| 5.022 | 25.80 ng | 969809 | 1,4-Dichlorobenzene-d4 | 6.816 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2  | 000123-42-2 | 56   |
| 2    |    |   | Propane, 2-methyl-2-(1-methyleth... | 116 | C7H16O   | 017348-59-3 | 50   |
| 3    |    |   | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 25   |
| 4    |    |   | Morpholine, 4-methyl-               | 101 | C5H11NO  | 000109-02-4 | 9    |
| 5    |    |   | 5-Hexen-2-one                       | 98  | C6H10O   | 000109-49-9 | 9    |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF122120\  
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Sample : L5160-04  
Misc :  
ALS Vial : 5 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
LLEXSITUTV-020-001-SO

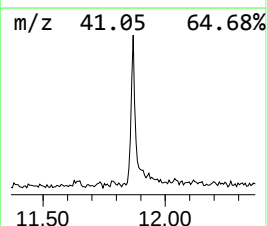
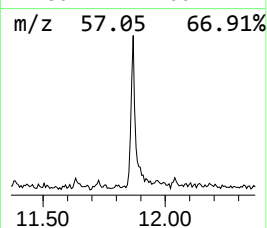
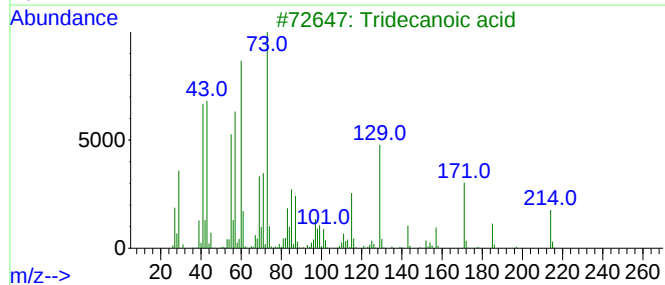
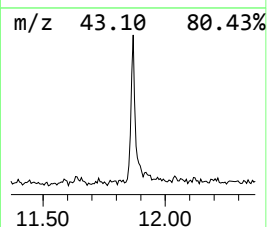
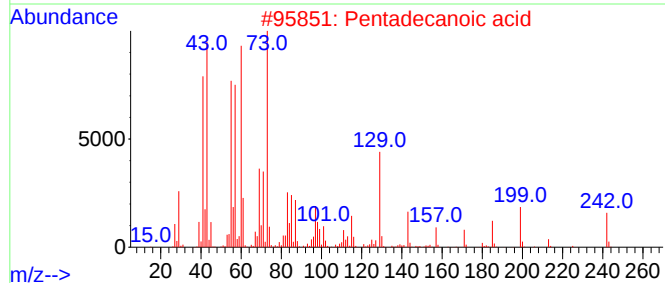
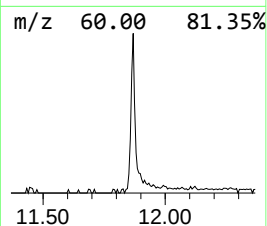
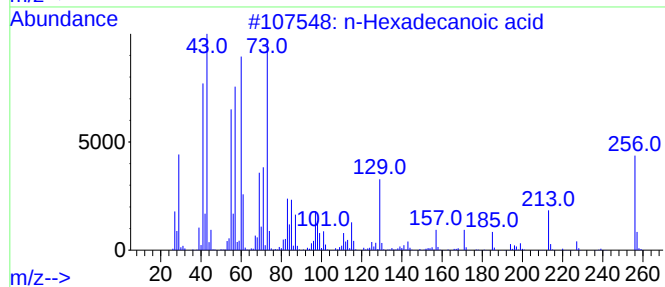
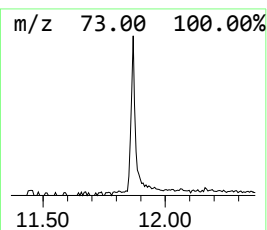
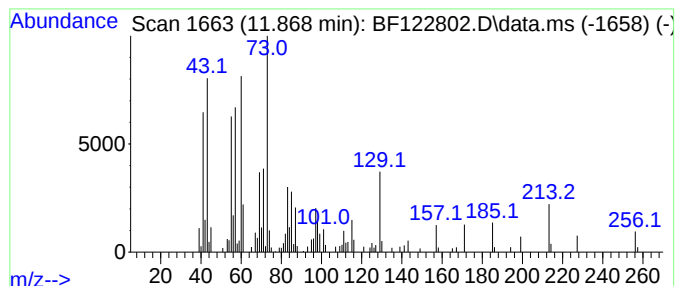
Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF120520.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 11.868 | 4.10 ng | 250103 | Phenanthrene-d10 | 11.339 |

| Hit# | of | 5 | Tentative ID                       | MW  | MolForm  | CAS#         | Qual |
|------|----|---|------------------------------------|-----|----------|--------------|------|
| 1    |    |   | n-Hexadecanoic acid                | 256 | C16H32O2 | 000057-10-3  | 99   |
| 2    |    |   | Pentadecanoic acid                 | 242 | C15H30O2 | 001002-84-2  | 91   |
| 3    |    |   | Tridecanoic acid                   | 214 | C13H26O2 | 000638-53-9  | 91   |
| 4    |    |   | Tetradecanoic acid                 | 228 | C14H28O2 | 000544-63-8  | 74   |
| 5    |    |   | Oxalic acid, allyl octadecyl ester | 382 | C23H42O4 | 1000309-24-5 | 20   |



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Misc :  
ALS Vial : 5 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
LLEXSITUTV-020-001-SO

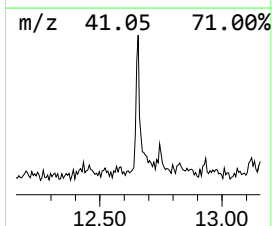
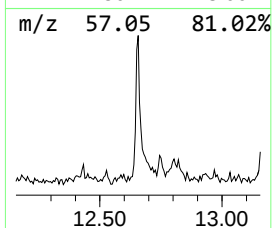
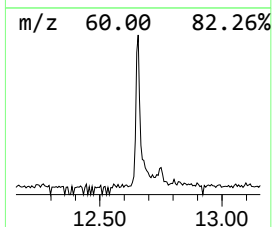
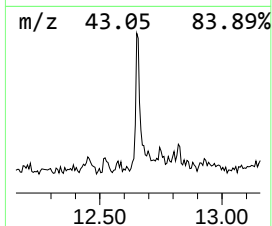
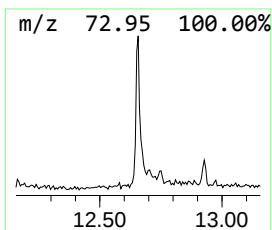
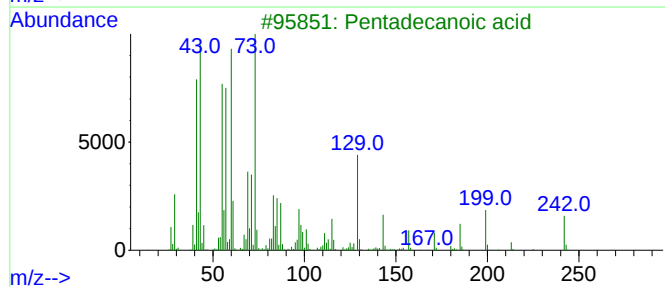
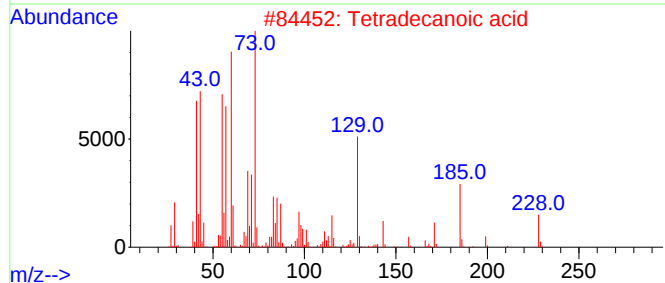
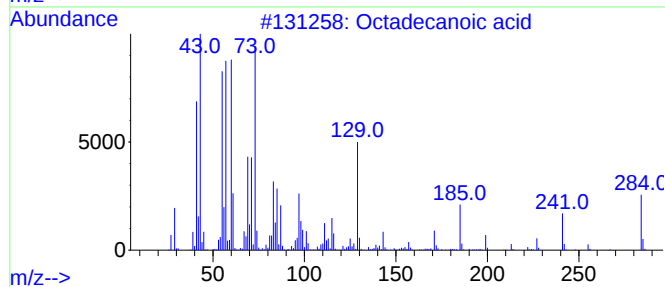
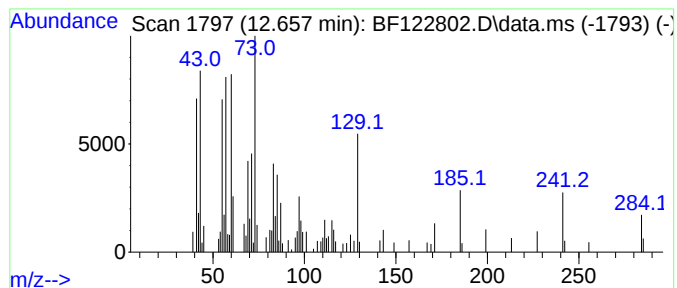
Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF120520.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 Octadecanoic acid Concentration Rank 5

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 12.657 | 2.00 ng | 122120 | Phenanthrene-d10 | 11.339 |

| 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 | 72   |
| 3    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 72   |
| 4    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 58   |
| 5    |    |   | n-Decanoic acid     | 172 | C10H20O2 | 000334-48-5 | 46   |



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Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF120520.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

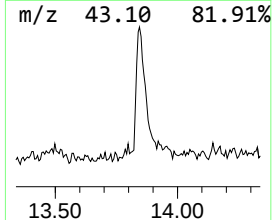
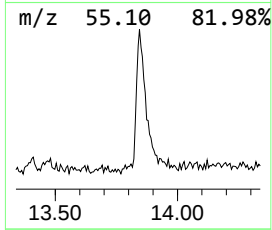
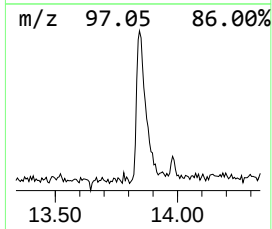
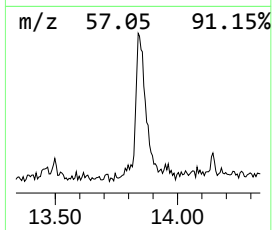
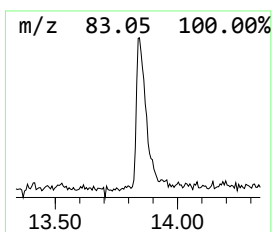
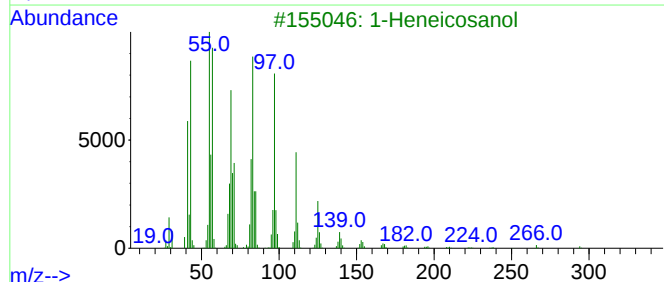
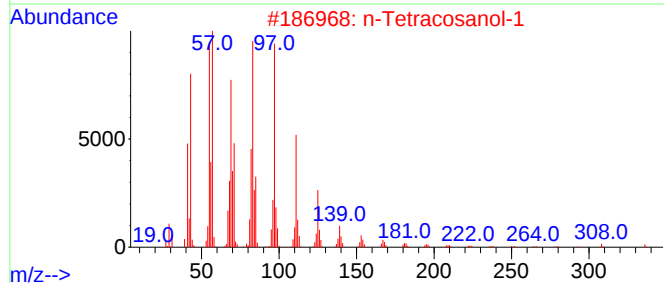
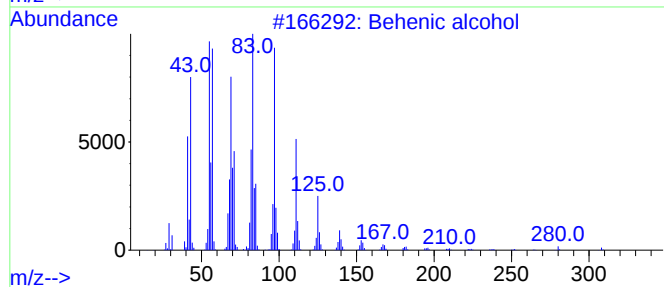
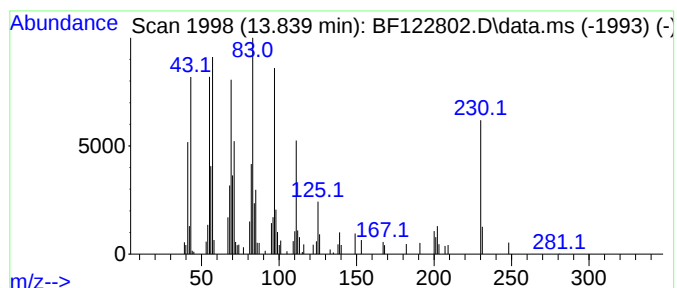
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 Behenic alcohol Concentration Rank 2

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 13.839 | 4.62 ng | 256951 | Chrysene-d12     | 13.986 |

| Hit# | of | 5 | Tentative ID                | MW  | MolForm    | CAS#         | Qual |
|------|----|---|-----------------------------|-----|------------|--------------|------|
| 1    |    |   | Behenic alcohol             | 326 | C22H46O    | 000661-19-8  | 93   |
| 2    |    |   | n-Tetracosanol-1            | 354 | C24H50O    | 000506-51-4  | 93   |
| 3    |    |   | 1-Heneicosanol              | 312 | C21H44O    | 015594-90-8  | 93   |
| 4    |    |   | 1-Heptacosanol              | 396 | C27H56O    | 002004-39-9  | 93   |
| 5    |    |   | Heptadecyl trifluoroacetate | 352 | C19H35F3O2 | 1000351-87-0 | 90   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF122120\  
Data File : BF122802.D  
Acq On : 21 Dec 2020 16:11  
Operator : JU/CG  
Sample : L5160-04  
Misc :  
ALS Vial : 5 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
LLEXSITUTV-020-001-SO

Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF120520.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |         |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|---------|------|
|                    |        |         |       |          | #                     | RT     | Resp    | Conc |
| 3-Penten-2-one,... | 4.392  | 2.3     | ng    | 87868    | 1                     | 6.816  | 751890  | 20.0 |
| 2-Pentanone, 4-... | 5.022  | 25.8    | ng    | 969809   | 1                     | 6.816  | 751890  | 20.0 |
| n-Hexadecanoic ... | 11.868 | 4.1     | ng    | 250103   | 4                     | 11.339 | 1220940 | 20.0 |
| Octadecanoic acid  | 12.657 | 2.0     | ng    | 122120   | 4                     | 11.339 | 1220940 | 20.0 |
| Behenic alcohol    | 13.839 | 4.6     | ng    | 256951   | 5                     | 13.986 | 1112910 | 20.0 |