

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF101921\  
 Data File : BF125901.D  
 Acq On : 19 Oct 2021 15:47  
 Operator : JU/CG  
 Sample : M4268-01  
 Misc :  
 ALS Vial : 11 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 P257-DITCH

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-BF100721.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125901.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         | 5.434       | 564           | 569         | 572          | rBV      | 2165364        | 1884017       | 41.30%          | 8.006%        |
| 2         | 6.445       | 737           | 741         | 744          | rBV      | 1512369        | 1217225       | 26.69%          | 5.172%        |
| 3         | 6.822       | 802           | 805         | 809          | rBV      | 1018554        | 789673        | 17.31%          | 3.355%        |
| 4         | 7.386       | 896           | 901         | 904          | rBV      | 2558322        | 2376953       | 52.11%          | 10.100%       |
| 5         | 8.004       | 1003          | 1006        | 1019         | rBV      | 894076         | 744371        | 16.32%          | 3.163%        |
| 6         | 8.104       | 1019          | 1023        | 1026         | rBV      | 1439619        | 1071959       | 23.50%          | 4.555%        |
| 7         | 9.180       | 1201          | 1206        | 1209         | rBV      | 5276286        | 4561351       | 100.00%         | 19.382%       |
| 8         | 9.292       | 1222          | 1225        | 1229         | rBV      | 277196         | 255382        | 5.60%           | 1.085%        |
| 9         | 9.857       | 1317          | 1321        | 1324         | rBV      | 1487095        | 1205160       | 26.42%          | 5.121%        |
| 10        | 10.639      | 1450          | 1454        | 1458         | rBV      | 2583196        | 2531648       | 55.50%          | 10.757%       |
| 11        | 10.739      | 1467          | 1471        | 1474         | rBV      | 245111         | 203386        | 4.46%           | 0.864%        |
| 12        | 11.339      | 1569          | 1573        | 1576         | rBV      | 1226543        | 1070431       | 23.47%          | 4.548%        |
| 13        | 11.733      | 1637          | 1640        | 1644         | rBV      | 118614         | 93549         | 2.05%           | 0.398%        |
| 14        | 11.863      | 1659          | 1662        | 1666         | rBV      | 129817         | 117171        | 2.57%           | 0.498%        |
| 15        | 12.521      | 1772          | 1774        | 1777         | rBV      | 88517          | 71023         | 1.56%           | 0.302%        |
| 16        | 12.921      | 1838          | 1842        | 1845         | rBV      | 3834214        | 3389154       | 74.30%          | 14.401%       |
| 17        | 13.821      | 1991          | 1995        | 2004         | rBV3     | 75251          | 126496        | 2.77%           | 0.538%        |
| 18        | 13.968      | 2016          | 2020        | 2024         | rBV      | 963805         | 931793        | 20.43%          | 3.959%        |
| 19        | 15.421      | 2262          | 2267        | 2271         | rBV      | 760486         | 893240        | 19.58%          | 3.796%        |

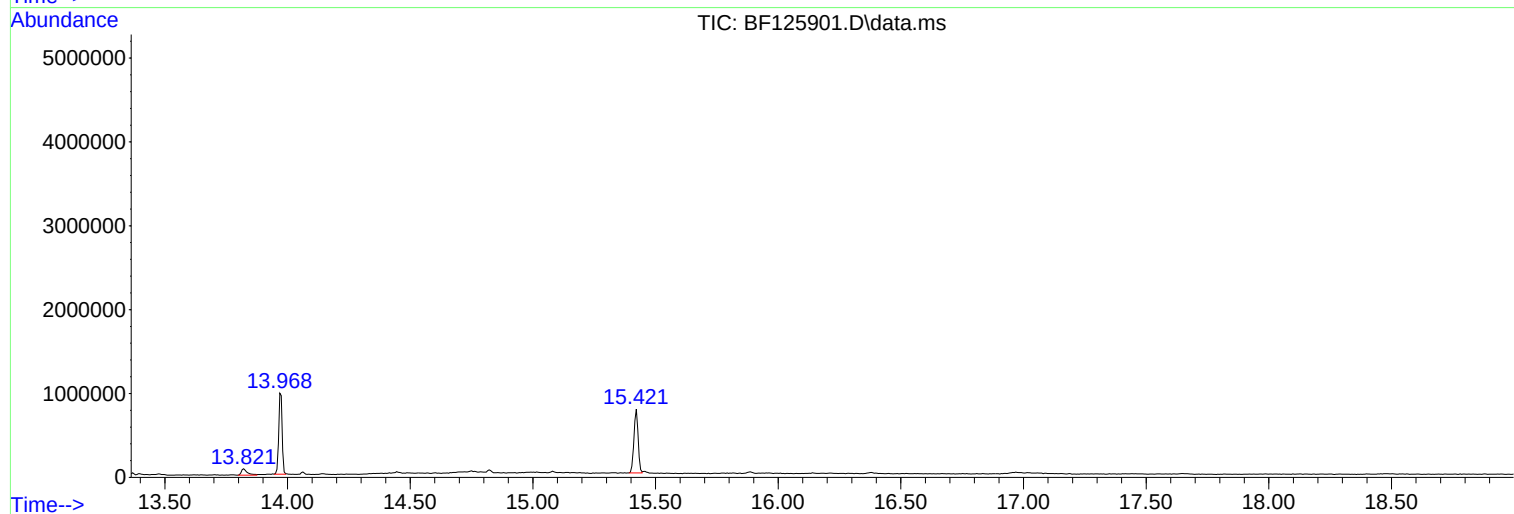
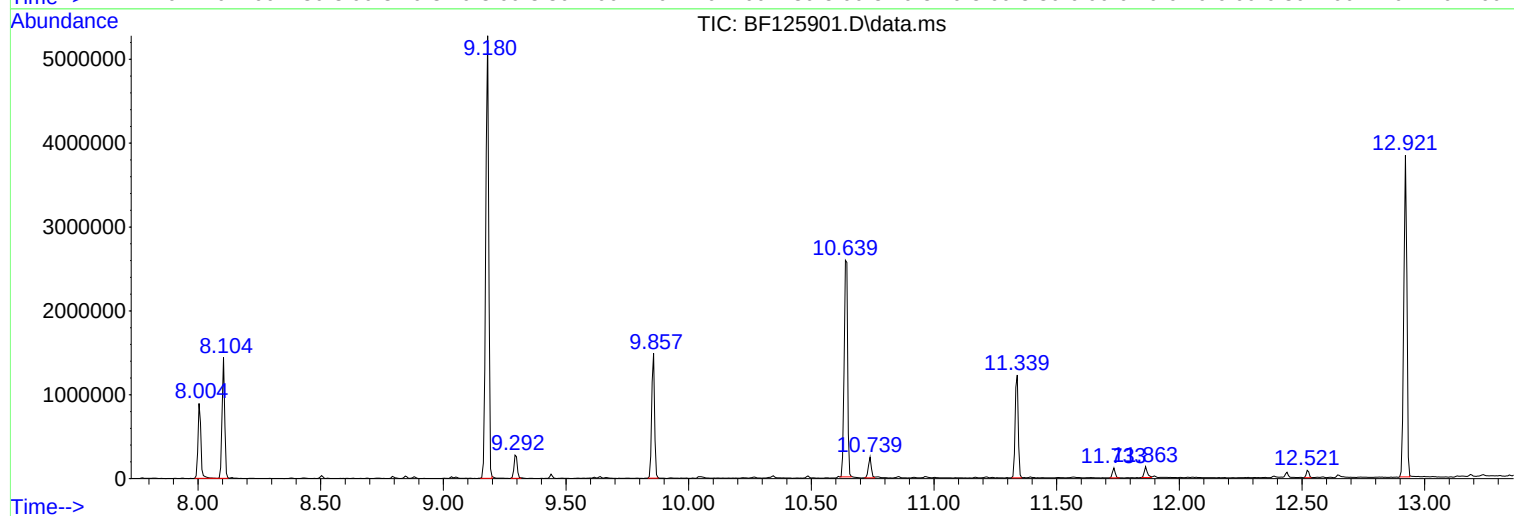
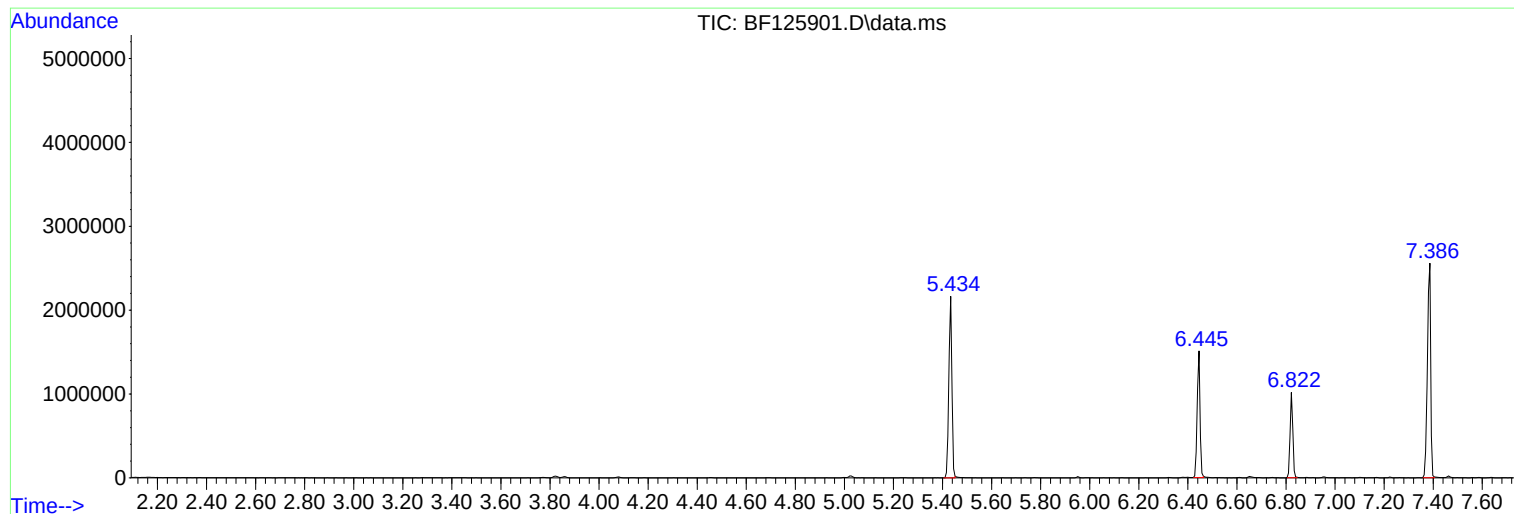
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Misc :  
ALS Vial : 11 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
P257-DITCH

Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF100721.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\BF101921\  
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P257-DITCH

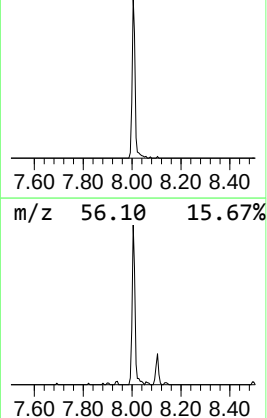
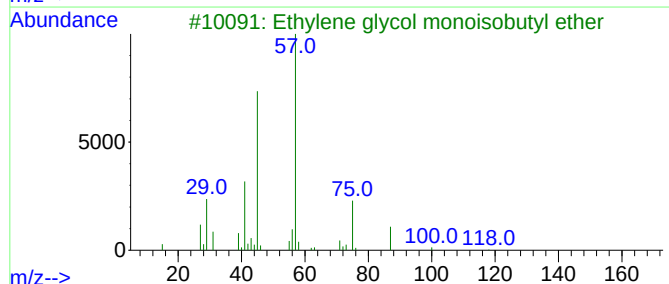
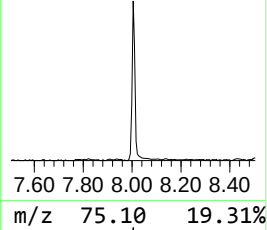
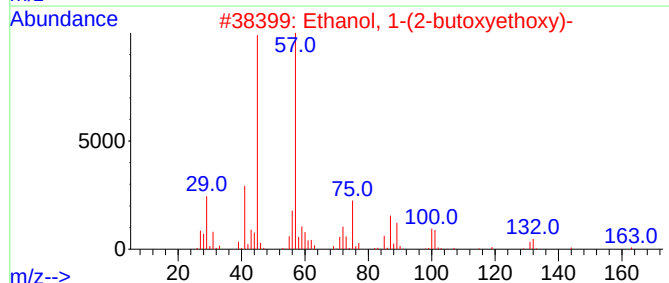
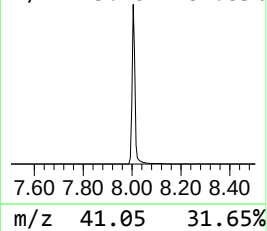
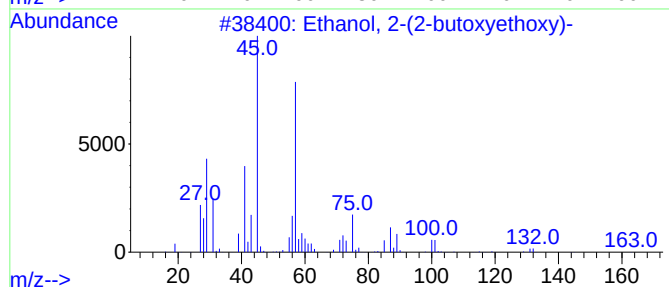
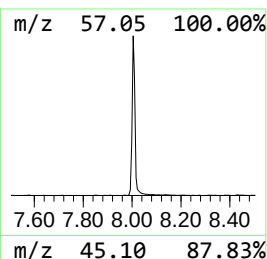
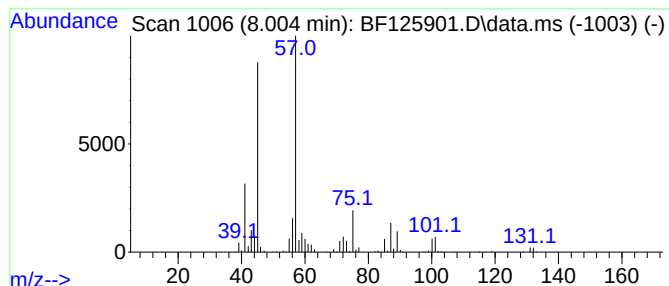
Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF100721.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.  |
|-------|----------|--------|------------------|-------|
| 8.004 | 13.89 ng | 744371 | Naphthalene-d8   | 8.104 |

| 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 | 78   |
| 3    |    |   | Ethylene glycol monoisobutyl ether | 118 | C6H14O2 | 004439-24-1 | 64   |
| 4    |    |   | 3,3-Dimethylbutane-2-ol            | 102 | C6H14O  | 000464-07-3 | 50   |
| 5    |    |   | Methoxyacetic acid, 2-butyl ester  | 146 | C7H14O3 | 070159-90-9 | 50   |



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Sample : M4268-01  
Misc :  
ALS Vial : 11 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
P257-DITCH

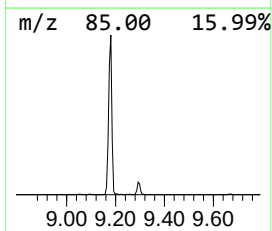
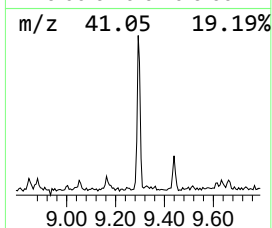
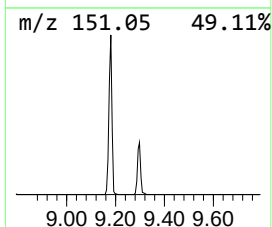
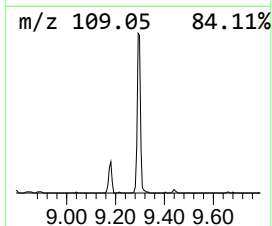
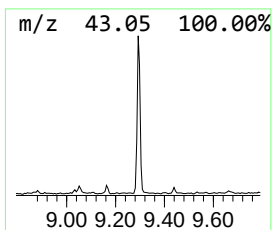
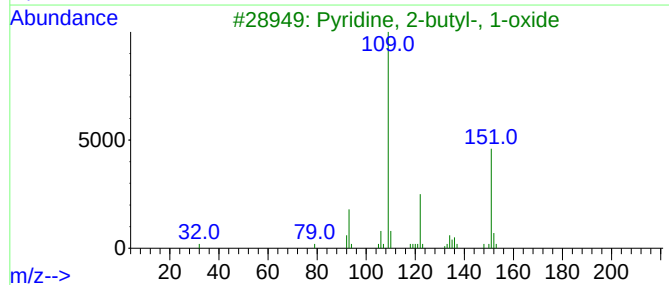
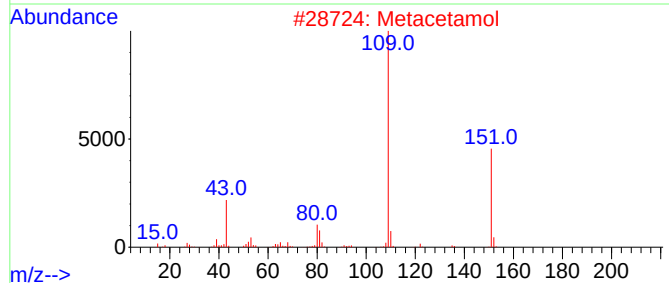
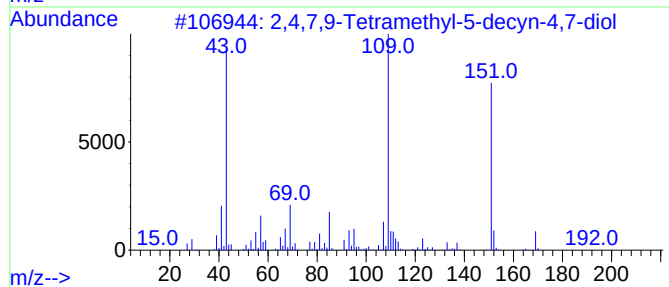
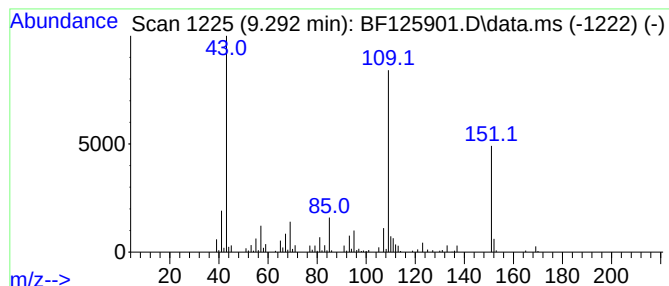
Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF100721.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 2 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 2

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 9.292 | 4.24 ng | 255382 | Acenaphthene-d10 | 9.857 |

| Hit# | of 5                                | Tentative ID | MW       | MolForm      | CAS# | Qual |
|------|-------------------------------------|--------------|----------|--------------|------|------|
| 1    | 2,4,7,9-Tetramethyl-5-decyn-4,7-... | 226          | C14H26O2 | 000126-86-3  | 91   |      |
| 2    | Metacetamol                         | 151          | C8H9NO2  | 000621-42-1  | 59   |      |
| 3    | Pyridine, 2-butyl-, 1-oxide         | 151          | C9H13NO  | 031396-32-4  | 59   |      |
| 4    | Cyclohexanol, 3,3,5-trimethyl-      | 142          | C9H18O   | 000116-02-9  | 47   |      |
| 5    | N-Cyclopropyl-p-fluorobenzylamine   | 165          | C10H12FN | 1000250-88-9 | 47   |      |



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Sample : M4268-01  
Misc :  
ALS Vial : 11 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
P257-DITCH

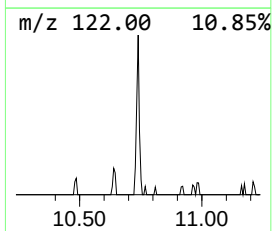
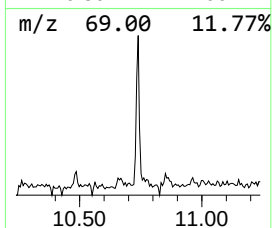
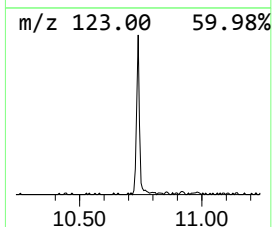
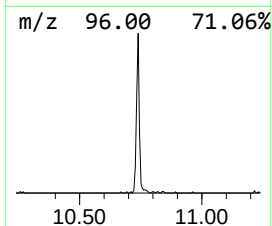
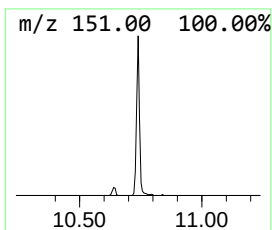
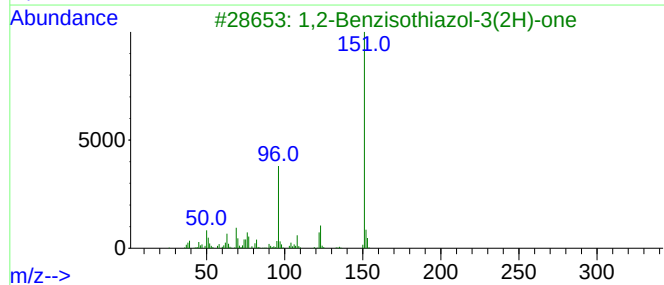
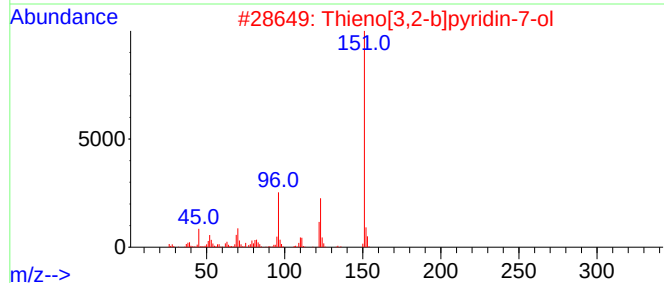
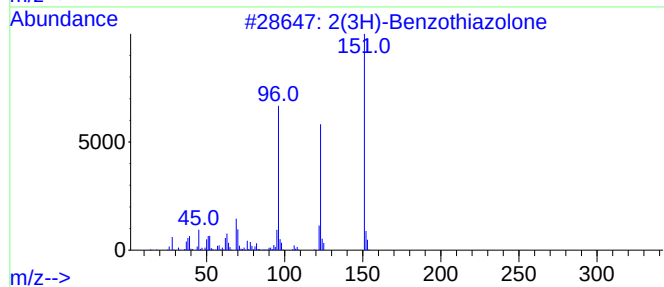
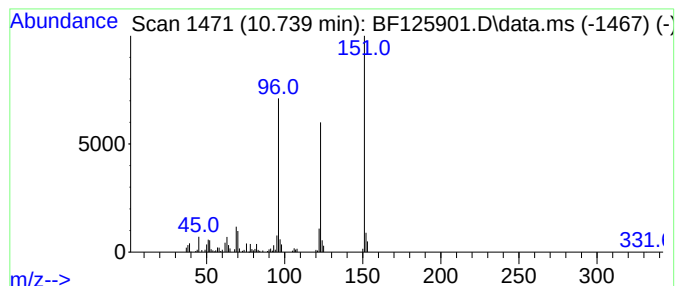
Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF100721.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 3 2(3H)-Benzothiazolone Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 10.739 | 3.80 ng | 203386 | Phenanthrene-d10 | 11.339 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|---------|-------------|------|
| 1    |    |   | 2(3H)-Benzothiazolone               | 151 | C7H5NOS | 000934-34-9 | 96   |
| 2    |    |   | Thieno[3,2-b]pyridin-7-ol           | 151 | C7H5NOS | 107818-20-2 | 64   |
| 3    |    |   | 1,2-Benzisothiazol-3(2H)-one        | 151 | C7H5NOS | 002634-33-5 | 52   |
| 4    |    |   | 6-Methyl-7-oxo-4,7-dihydro-triaz... | 151 | C5H5N5O | 057250-39-2 | 50   |
| 5    |    |   | 4-Mercaptoimidazo[4,5-c]pyridine    | 151 | C6H5N3S | 034550-51-1 | 38   |



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Sample : M4268-01  
Misc :  
ALS Vial : 11 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
P257-DITCH

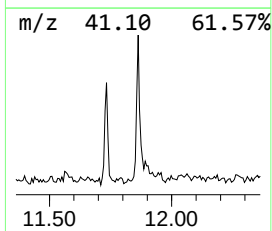
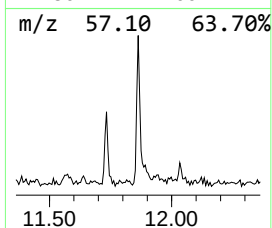
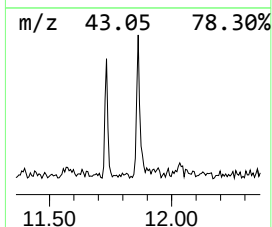
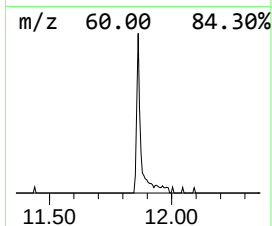
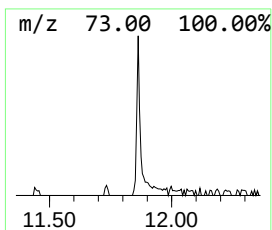
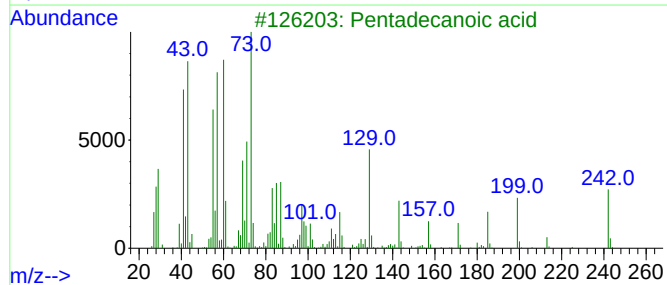
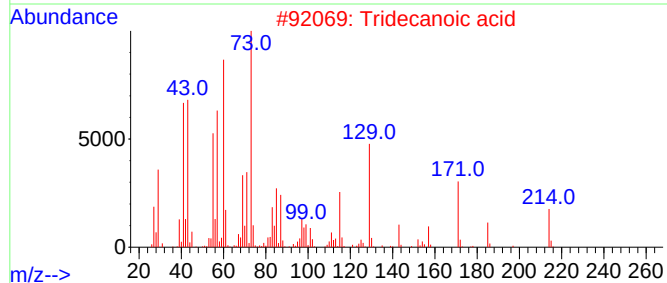
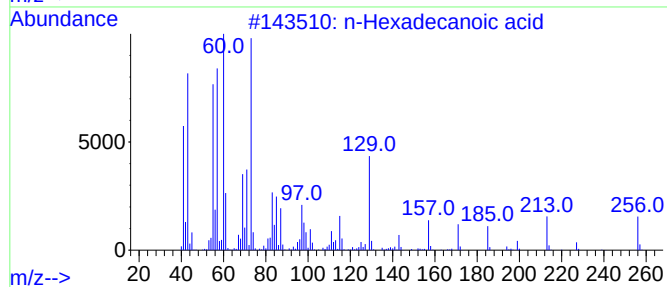
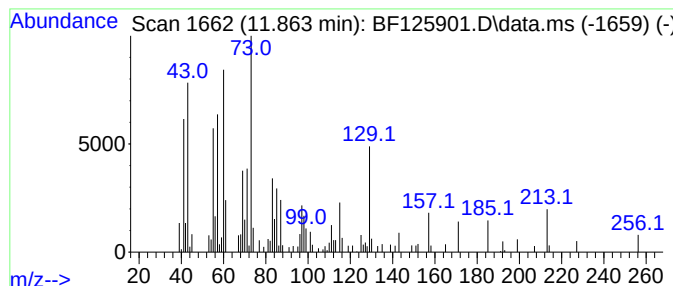
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TIC Library : C:\Database\NIST20.L  
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 11.863 | 2.19 ng | 117171 | Phenanthrene-d10 | 11.339 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 99   |
| 2    |    |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 87   |
| 3    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 87   |
| 4    |    |   | n-Decanoic acid     | 172 | C10H20O2 | 000334-48-5 | 64   |
| 5    |    |   | Nonanoic acid       | 158 | C9H18O2  | 000112-05-0 | 38   |



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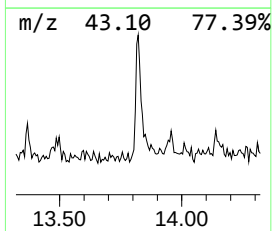
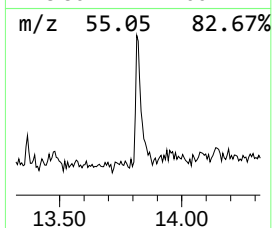
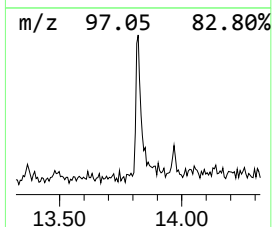
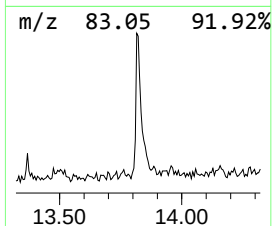
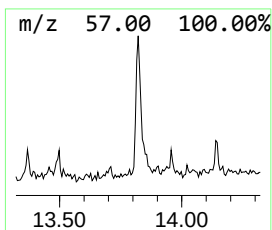
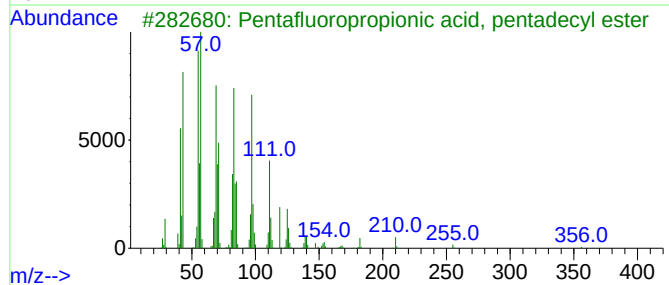
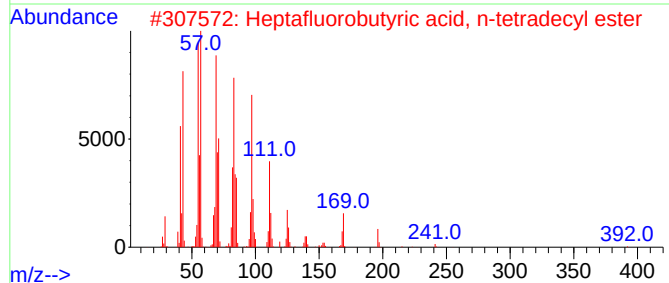
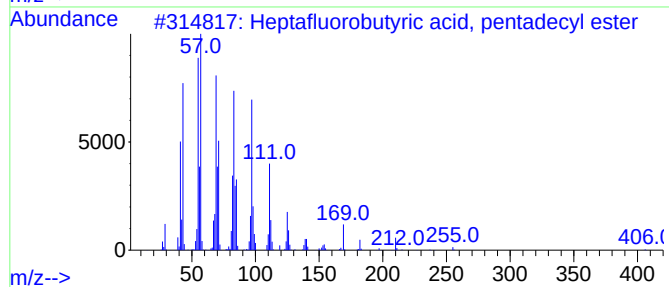
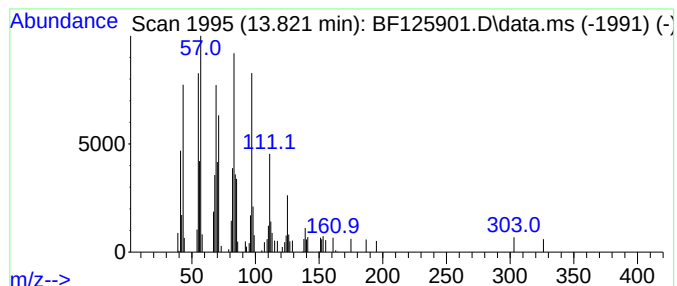
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 Heptafluorobutyric acid, pe... Concentration Rank 4

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 13.821 | 2.72 ng | 126496 | Chrysene-d12     | 13.974 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|------------|-------------|------|
| 1    |    |   | Heptafluorobutyric acid, pentade... | 424 | C19H31F7O2 | 959261-23-5 | 95   |
| 2    |    |   | Heptafluorobutyric acid, n-tetra... | 410 | C18H29F7O2 | 007365-36-8 | 95   |
| 3    |    |   | Pentafluoropropionic acid, penta... | 374 | C18H31F5O2 | 959092-08-1 | 95   |
| 4    |    |   | n-Nonadecanol-1                     | 284 | C19H40O    | 001454-84-8 | 94   |
| 5    |    |   | 1-Tetracosene                       | 336 | C24H48     | 010192-32-2 | 94   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF101921\  
Data File : BF125901.D  
Acq On : 19 Oct 2021 15:47  
Operator : JU/CG  
Sample : M4268-01  
Misc :  
ALS Vial : 11 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
P257-DITCH

Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF100721.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 |
| Ethanol, 2-(2-b... | 8.004  | 13.9    | ng    | 744371   | 2                     | 8.104  | 1071960 | 20.0 |
| 2,4,7,9-Tetrame... | 9.292  | 4.2     | ng    | 255382   | 3                     | 9.857  | 1205160 | 20.0 |
| 2(3H)-Benzothia... | 10.739 | 3.8     | ng    | 203386   | 4                     | 11.339 | 1070430 | 20.0 |
| n-Hexadecanoic ... | 11.863 | 2.2     | ng    | 117171   | 4                     | 11.339 | 1070430 | 20.0 |
| Heptafluorobuty... | 13.821 | 2.7     | ng    | 126496   | 5                     | 13.974 | 931793  | 20.0 |