

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF101824\  
 Data File : BF139860.D  
 Acq On : 18 Oct 2024 18:12  
 Operator : RC/JU  
 Sample : P4425-05  
 Misc :  
 ALS Vial : 18 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 TP-3

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-BF101824.M  
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139860.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         | 2.175       | 6             | 14          | 22           | rVB      | 1854846        | 2944727       | 100.00%         | 13.182%       |
| 2         | 5.104       | 504           | 512         | 521          | rVB      | 195735         | 290408        | 9.86%           | 1.300%        |
| 3         | 5.499       | 573           | 579         | 584          | rBV      | 2044426        | 2684327       | 91.16%          | 12.016%       |
| 4         | 6.504       | 743           | 750         | 765          | rVB      | 1977326        | 2738191       | 92.99%          | 12.257%       |
| 5         | 6.887       | 810           | 815         | 821          | rBV      | 695996         | 883008        | 29.99%          | 3.953%        |
| 6         | 6.945       | 821           | 825         | 833          | rVB      | 24281          | 30385         | 1.03%           | 0.136%        |
| 7         | 7.445       | 904           | 910         | 915          | rBV      | 1282717        | 1596620       | 54.22%          | 7.147%        |
| 8         | 7.698       | 949           | 953         | 958          | rBV      | 80028          | 94631         | 3.21%           | 0.424%        |
| 9         | 8.169       | 1028          | 1033        | 1038         | rBV      | 860332         | 1054784       | 35.82%          | 4.722%        |
| 10        | 9.245       | 1210          | 1216        | 1221         | rBV      | 2016648        | 2469671       | 83.87%          | 11.055%       |
| 11        | 9.922       | 1326          | 1331        | 1337         | rBV      | 768571         | 959277        | 32.58%          | 4.294%        |
| 12        | 10.633      | 1447          | 1452        | 1458         | rBV      | 289040         | 356000        | 12.09%          | 1.594%        |
| 13        | 10.710      | 1460          | 1465        | 1479         | rVB      | 951355         | 1195322       | 40.59%          | 5.351%        |
| 14        | 11.410      | 1579          | 1584        | 1591         | rBV      | 758320         | 928076        | 31.52%          | 4.154%        |
| 15        | 11.933      | 1666          | 1673        | 1684         | rBV2     | 47187          | 84677         | 2.88%           | 0.379%        |
| 16        | 12.457      | 1755          | 1762        | 1772         | rVB4     | 17187          | 35128         | 1.19%           | 0.157%        |
| 17        | 12.998      | 1848          | 1854        | 1859         | rBV      | 1820589        | 2338172       | 79.40%          | 10.466%       |
| 18        | 13.892      | 2001          | 2006        | 2022         | rBV      | 129459         | 233084        | 7.92%           | 1.043%        |
| 19        | 14.051      | 2027          | 2033        | 2040         | rVV      | 629463         | 869519        | 29.53%          | 3.892%        |
| 20        | 15.527      | 2278          | 2284        | 2289         | rBV      | 362796         | 553763        | 18.81%          | 2.479%        |

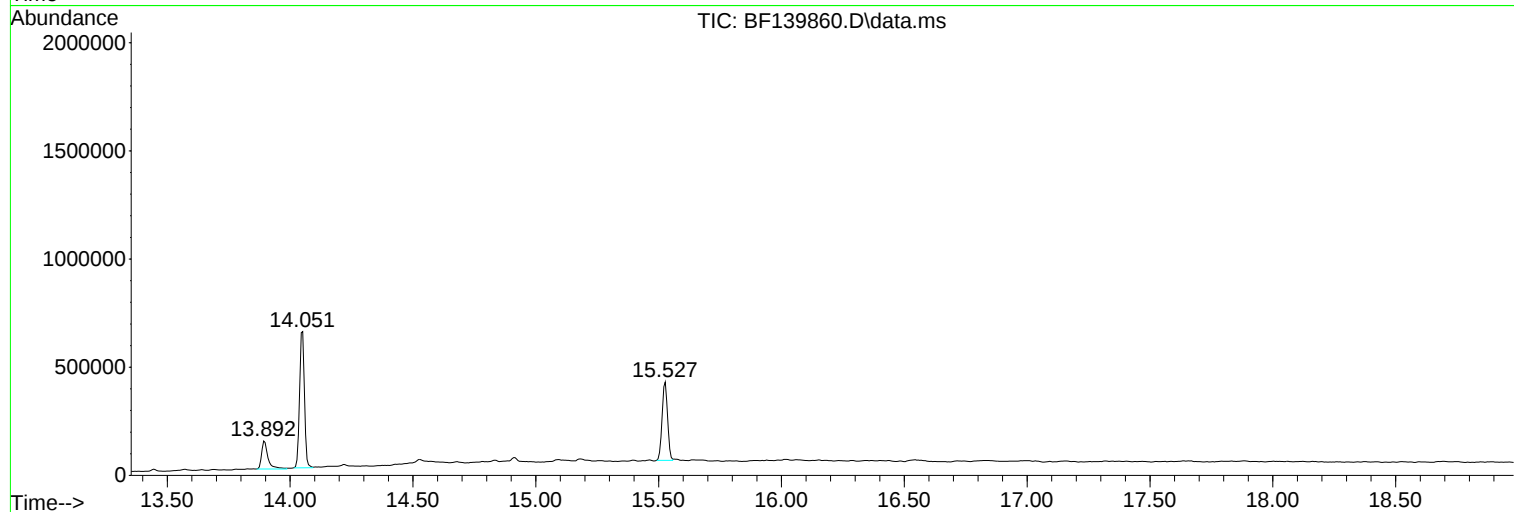
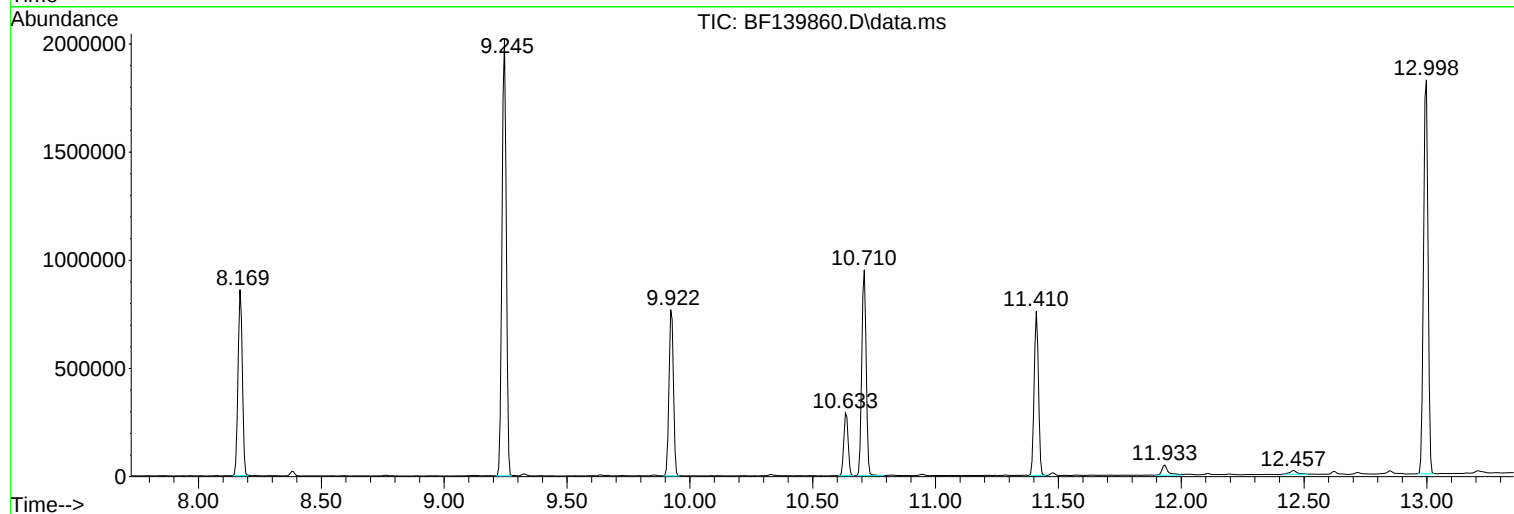
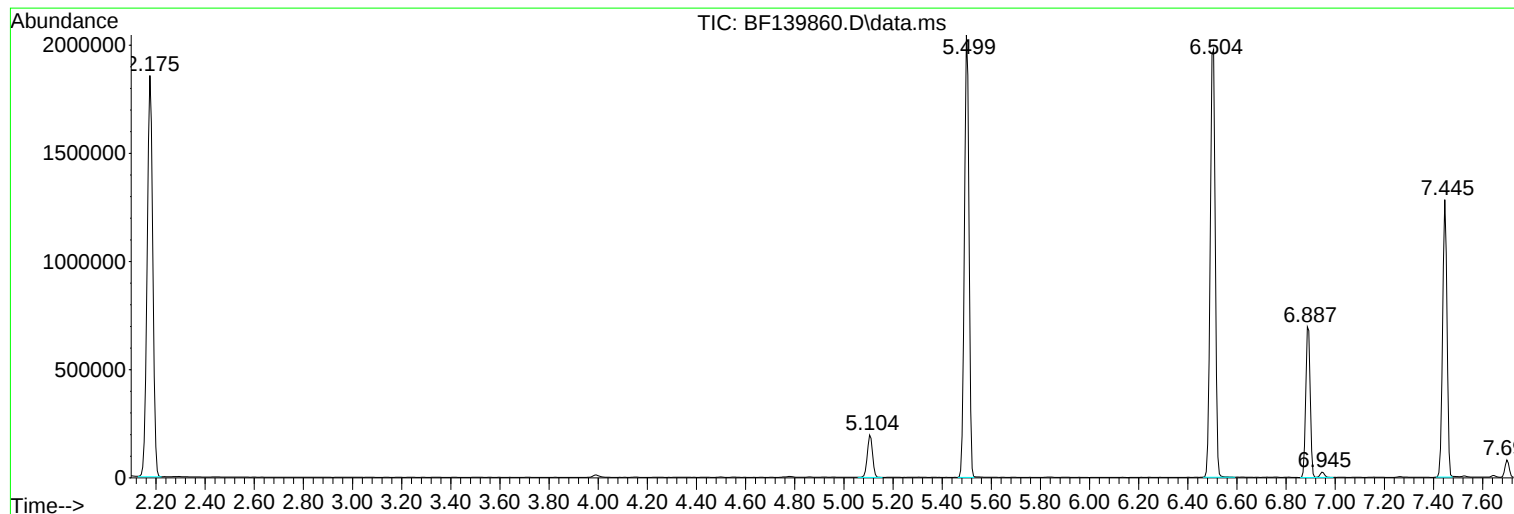
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ALS Vial : 18 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF101824.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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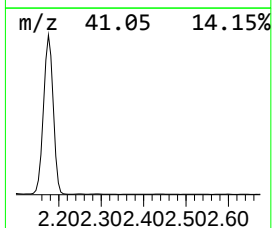
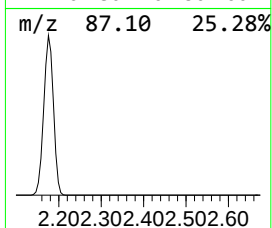
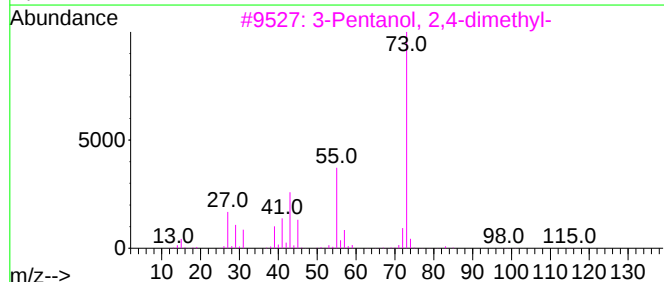
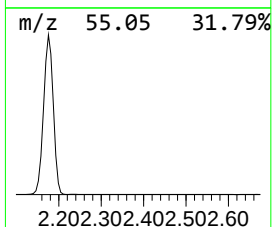
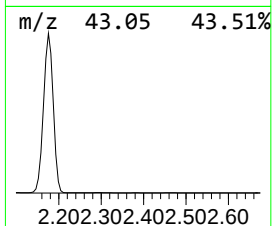
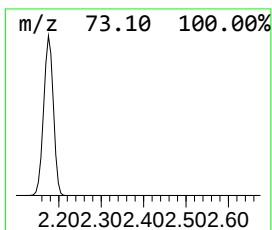
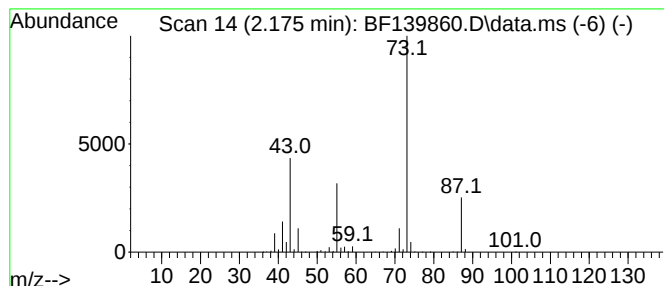
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Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

| R.T.  | EstConc  | Area    | Relative to ISTD       | R.T.  |
|-------|----------|---------|------------------------|-------|
| 2.175 | 66.70 ng | 2944730 | 1,4-Dichlorobenzene-d4 | 6.893 |

| 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 | 39   |
| 3    |    |   | 3-Pentanol, 2,4-dimethyl-        | 116 | C7H16O   | 000600-36-2 | 37   |
| 4    |    |   | 1,3-Dioxolane, 2-methyl-         | 88  | C4H8O2   | 000497-26-7 | 25   |
| 5    |    |   | Octanal, 7-methoxy-3,7-dimethyl- | 186 | C11H22O2 | 003613-30-7 | 17   |



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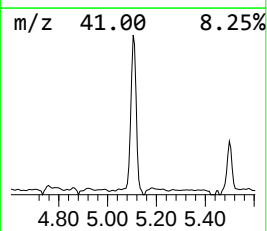
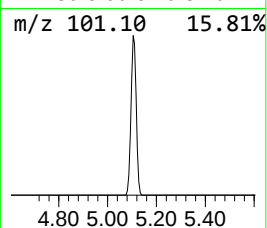
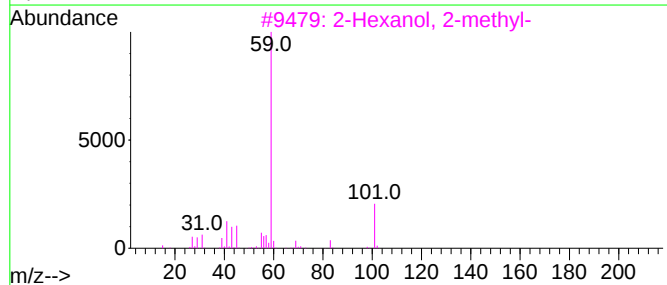
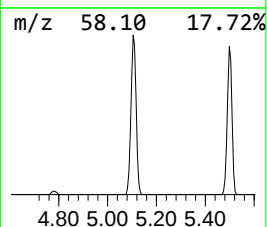
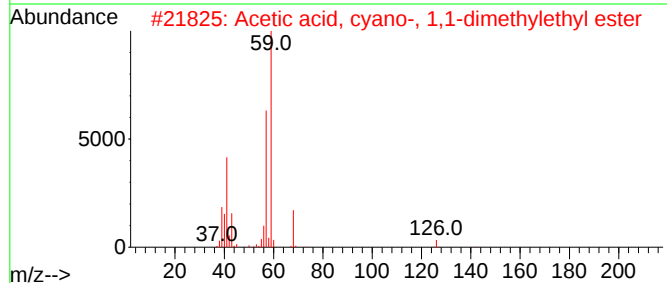
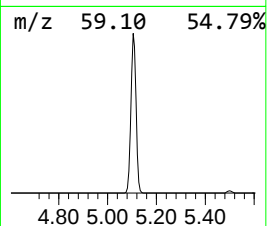
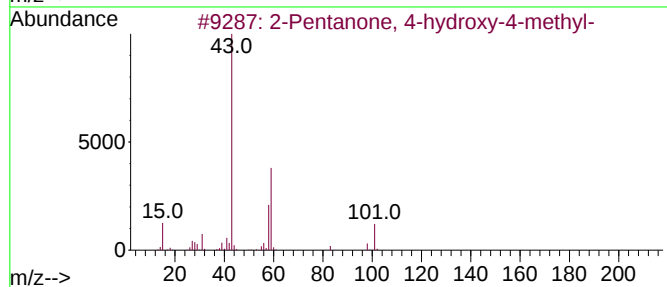
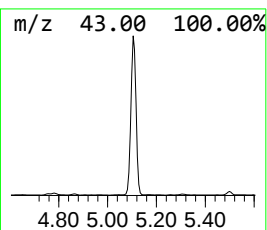
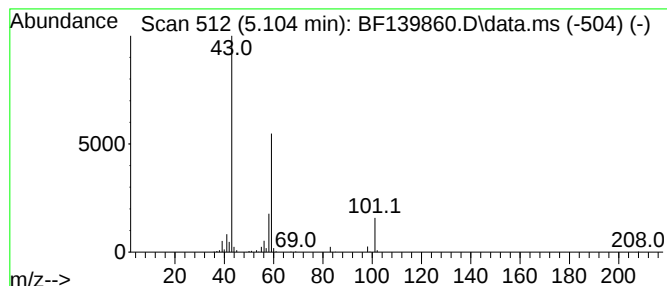
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF101824.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.  |
|-------|---------|--------|------------------------|-------|
| 5.104 | 6.58 ng | 290408 | 1,4-Dichlorobenzene-d4 | 6.893 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2  | 000123-42-2 | 59   |
| 2    |    |   | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 37   |
| 3    |    |   | 2-Hexanol, 2-methyl-                | 116 | C7H16O   | 000625-23-0 | 33   |
| 4    |    |   | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2  | 000540-88-5 | 17   |
| 5    |    |   | 2,3-Butanedione, monooxime          | 101 | C4H7NO2  | 000057-71-6 | 16   |



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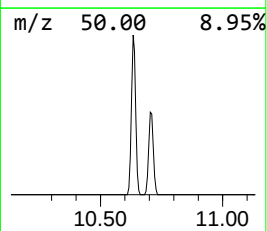
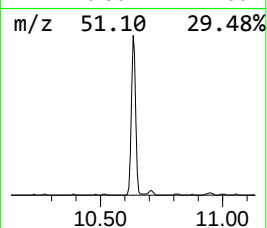
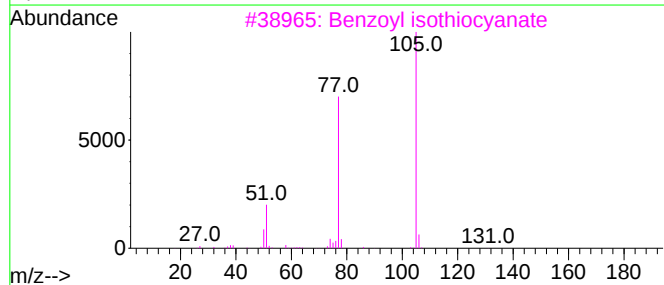
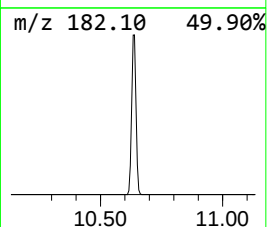
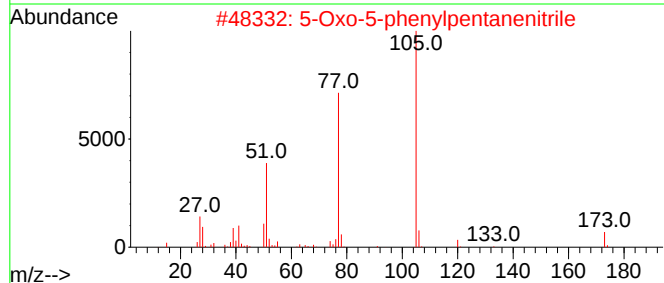
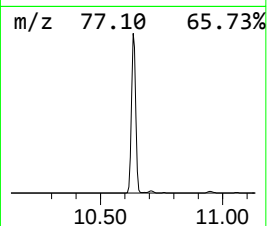
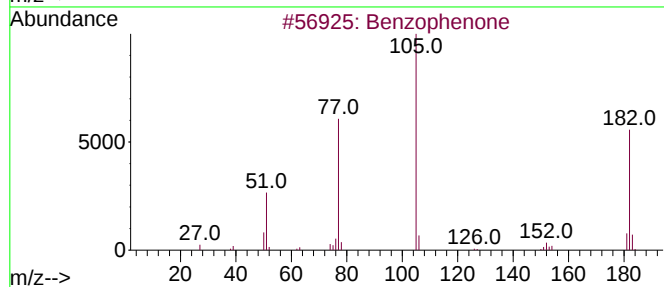
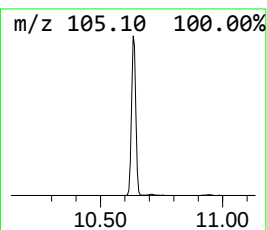
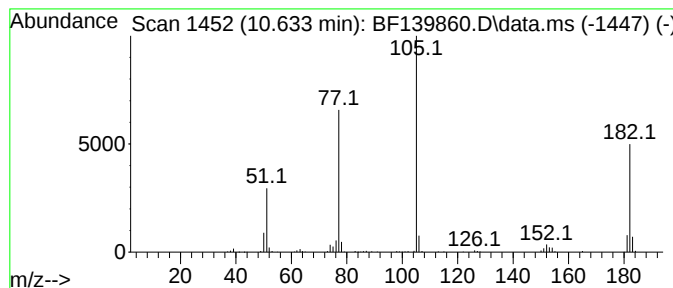
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF101824.M  
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TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 Benzophenone Concentration Rank 2

| R.T.      | EstConc                        | Area   | Relative to ISTD | R.T.         |      |
|-----------|--------------------------------|--------|------------------|--------------|------|
| 10.634    | 7.42 ng                        | 356000 | Acenaphthene-d10 | 9.922        |      |
| Hit# of 5 | Tentative ID                   | MW     | MolForm          | CAS#         | Qual |
| 1         | Benzophenone                   | 182    | C13H10O          | 000119-61-9  | 96   |
| 2         | 5-Oxo-5-phenylpentanenitrile   | 173    | C11H11NO         | 1000486-83-7 | 47   |
| 3         | Benzoyl isothiocyanate         | 163    | C8H5NOS          | 000532-55-8  | 47   |
| 4         | Benzilamide                    | 227    | C14H13NO2        | 004746-87-6  | 47   |
| 5         | Pentafluoroethyl phenyl ketone | 224    | C9H5F5O          | 000394-52-5  | 47   |



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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

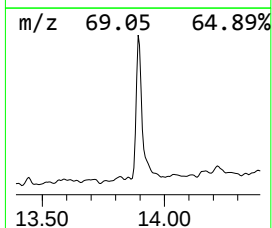
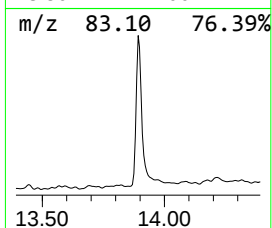
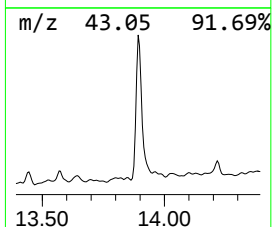
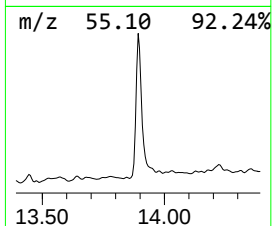
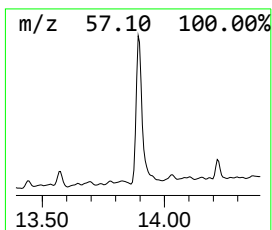
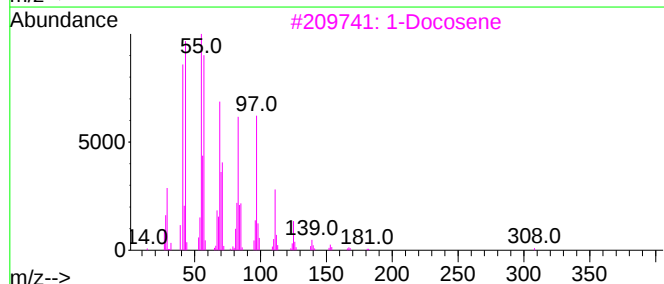
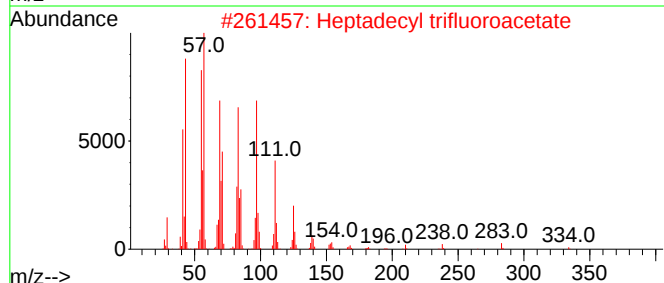
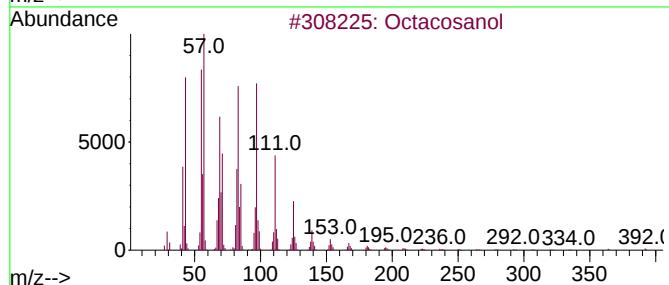
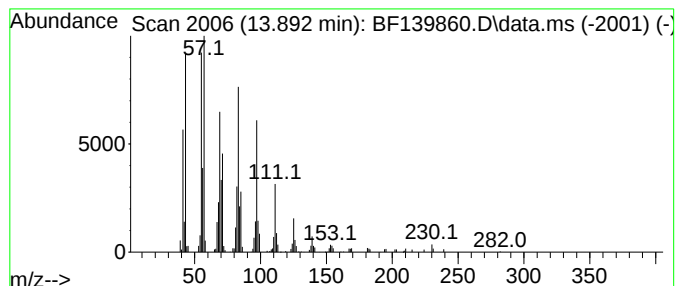
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 Octacosanol Concentration Rank 4

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 13.892 | 5.36 ng | 233084 | Chrysene-d12     | 14.051 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|------------|--------------|------|
| 1    |    |   | Octacosanol                         | 410 | C28H58O    | 000557-61-9  | 94   |
| 2    |    |   | Heptadecyl trifluoroacetate         | 352 | C19H35F3O2 | 1010351-87-0 | 94   |
| 3    |    |   | 1-Docosene                          | 308 | C22H44     | 001599-67-3  | 94   |
| 4    |    |   | Heptafluorobutyric acid, pentade... | 424 | C19H31F7O2 | 959261-23-5  | 94   |
| 5    |    |   | 1-Heptacosanol                      | 396 | C27H56O    | 002004-39-9  | 93   |



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| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| Butane, 2-metho... | 2.175  | 66.7    | ng    | 2944730  | 1                     | 6.893  | 883008 | 20.0 |
| 2-Pentanone, 4-... | 5.104  | 6.6     | ng    | 290408   | 1                     | 6.893  | 883008 | 20.0 |
| Benzophenone       | 10.634 | 7.4     | ng    | 356000   | 3                     | 9.922  | 959277 | 20.0 |
| Octacosanol        | 13.892 | 5.4     | ng    | 233084   | 5                     | 14.051 | 869519 | 20.0 |