

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF102524\  
 Data File : BF140038.D  
 Acq On : 25 Oct 2024 15:32  
 Operator : RC/JU  
 Sample : P4467-01  
 Misc :  
 ALS Vial : 14 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 TP-1

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: BF140038.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         | 2.181       | 7             | 15          | 23           | rVB      | 1422883        | 2387868       | 86.75%          | 11.407%       |
| 2         | 5.116       | 504           | 514         | 520          | rBV2     | 16528          | 28104         | 1.02%           | 0.134%        |
| 3         | 5.504       | 574           | 580         | 585          | rBV      | 1706857        | 2267248       | 82.37%          | 10.831%       |
| 4         | 6.504       | 744           | 750         | 755          | rBV      | 1672241        | 2318202       | 84.22%          | 11.074%       |
| 5         | 6.887       | 810           | 815         | 820          | rBV      | 480235         | 580101        | 21.08%          | 2.771%        |
| 6         | 7.445       | 904           | 910         | 915          | rBV      | 1169738        | 1539074       | 55.92%          | 7.352%        |
| 7         | 8.169       | 1027          | 1033        | 1038         | rBV      | 605365         | 759500        | 27.59%          | 3.628%        |
| 8         | 9.245       | 1209          | 1216        | 1233         | rBV      | 1994171        | 2692249       | 97.81%          | 12.861%       |
| 9         | 9.922       | 1326          | 1331        | 1344         | rVB      | 694346         | 883622        | 32.10%          | 4.221%        |
| 10        | 10.633      | 1447          | 1452        | 1459         | rBV      | 302994         | 387858        | 14.09%          | 1.853%        |
| 11        | 10.710      | 1459          | 1465        | 1481         | rVV      | 1319413        | 1723574       | 62.62%          | 8.234%        |
| 12        | 11.410      | 1579          | 1584        | 1589         | rBV      | 764547         | 945298        | 34.34%          | 4.516%        |
| 13        | 11.475      | 1591          | 1595        | 1600         | rVB      | 35529          | 43125         | 1.57%           | 0.206%        |
| 14        | 11.933      | 1668          | 1673        | 1695         | rBV2     | 107640         | 187931        | 6.83%           | 0.898%        |
| 15        | 12.716      | 1801          | 1806        | 1816         | rBV2     | 16415          | 30163         | 1.10%           | 0.144%        |
| 16        | 12.998      | 1848          | 1854        | 1859         | rBV      | 2110567        | 2752440       | 100.00%         | 13.149%       |
| 17        | 13.898      | 2001          | 2007        | 2023         | rBV      | 58996          | 159700        | 5.80%           | 0.763%        |
| 18        | 14.051      | 2027          | 2033        | 2046         | rVB      | 473917         | 651102        | 23.66%          | 3.110%        |
| 19        | 15.527      | 2278          | 2284        | 2298         | rBV      | 355841         | 595663        | 21.64%          | 2.846%        |

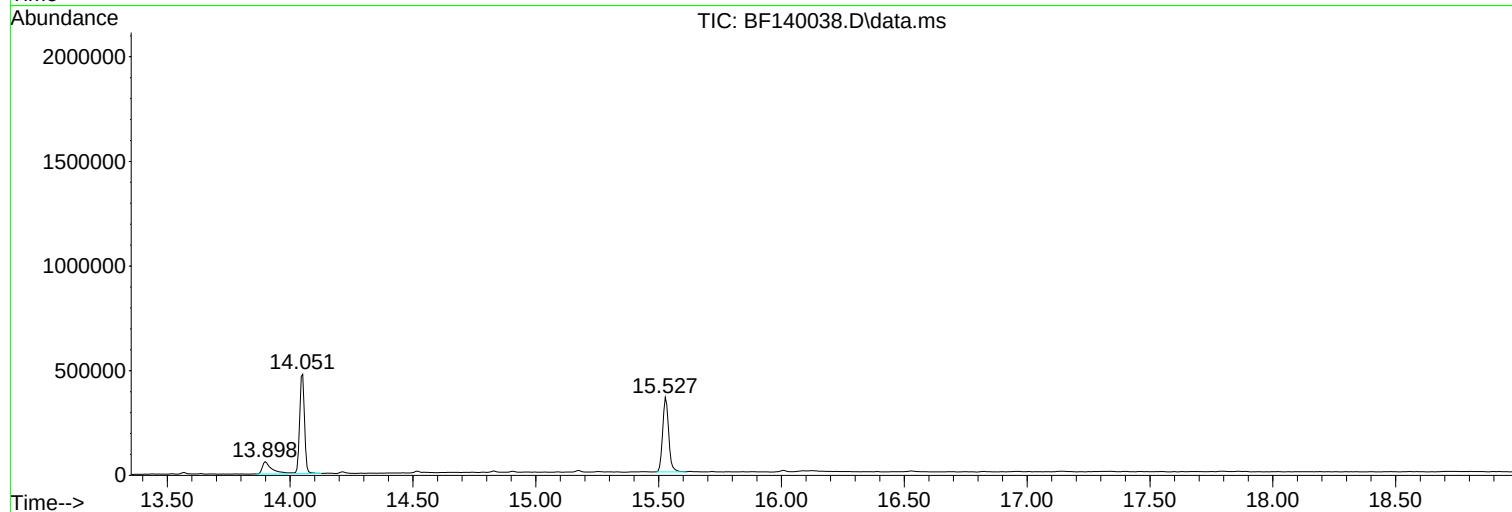
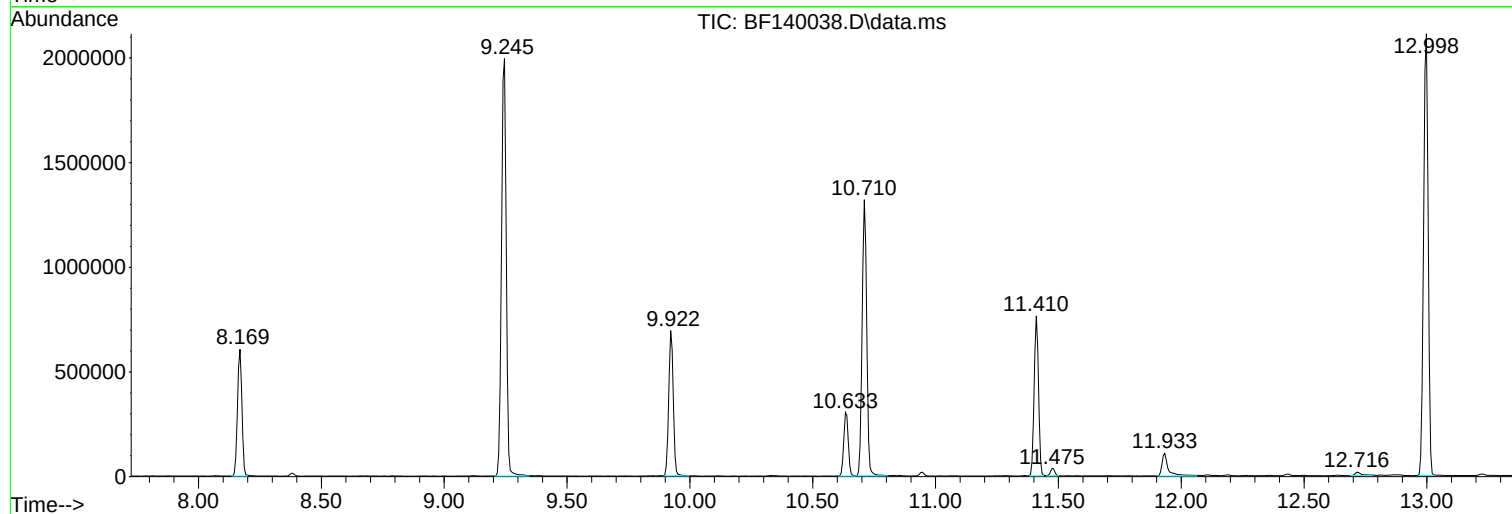
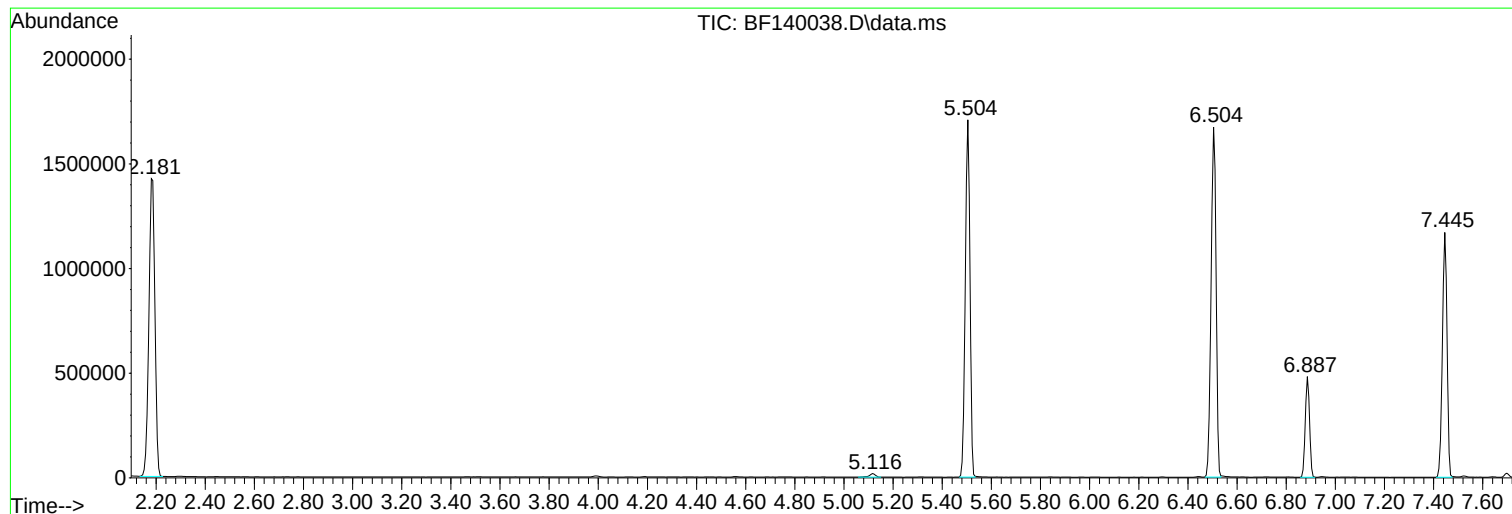
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Misc :  
ALS Vial : 14 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
TP-1

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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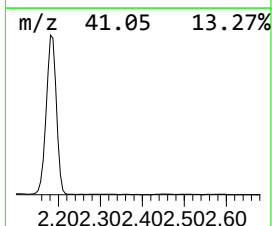
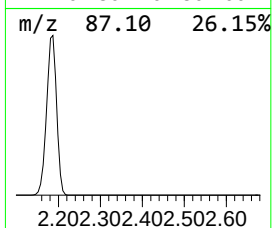
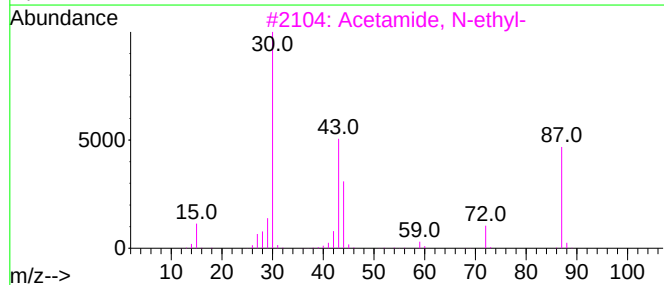
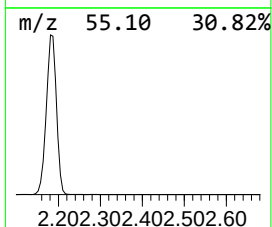
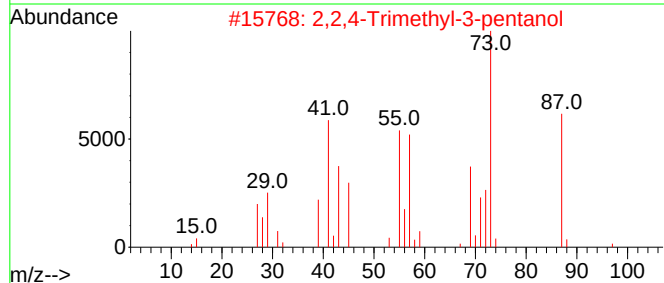
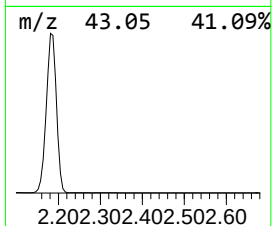
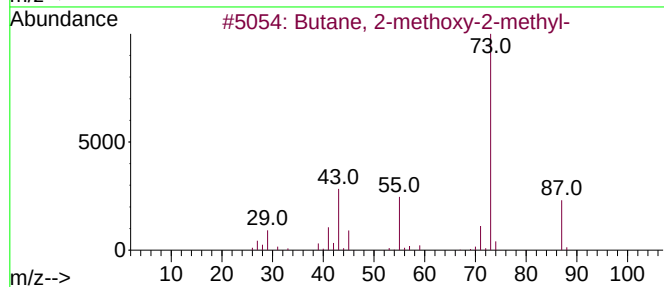
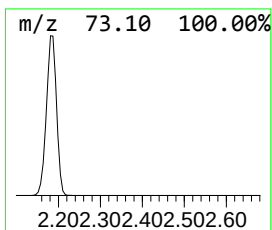
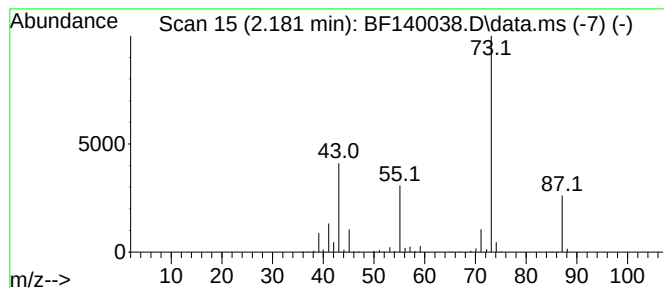
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.  |
|-------|----------|---------|------------------------|-------|
| 2.181 | 82.33 ng | 2387870 | 1,4-Dichlorobenzene-d4 | 6.887 |

| 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    |    |   | Acetamide, N-ethyl-              | 87  | C4H9NO   | 000625-50-3 | 22   |
| 4    |    |   | Octanal, 7-methoxy-3,7-dimethyl- | 186 | C11H22O2 | 003613-30-7 | 17   |
| 5    |    |   | Pentane, 3-methoxy-              | 102 | C6H14O   | 036839-67-5 | 12   |



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

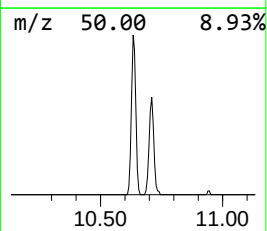
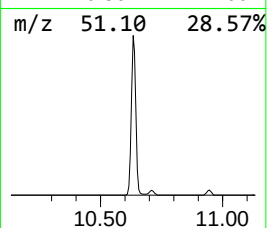
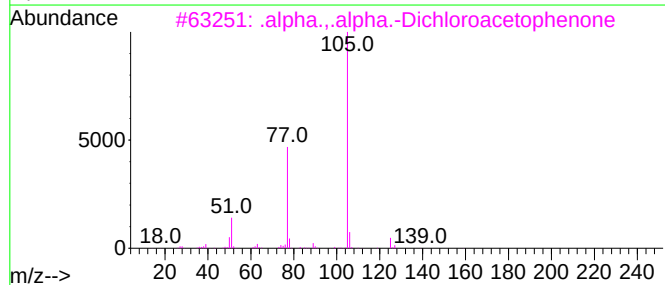
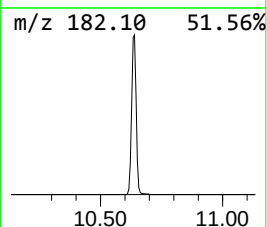
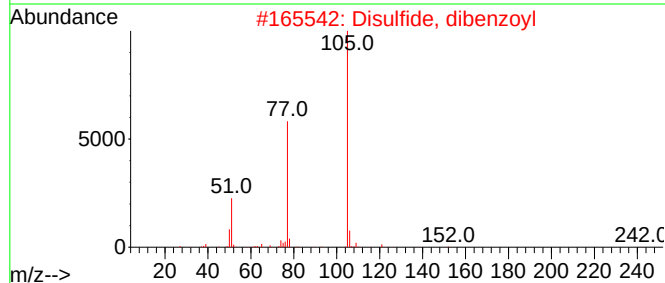
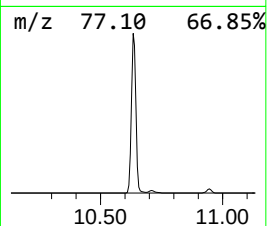
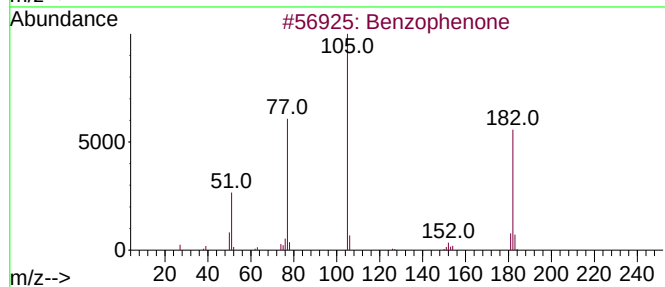
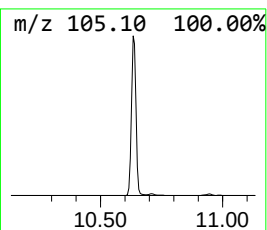
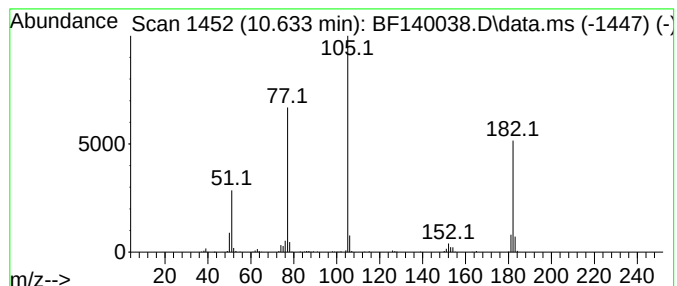
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 Benzophenone Concentration Rank 2

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.  |
|--------|---------|--------|------------------|-------|
| 10.633 | 8.78 ng | 387858 | Acenaphthene-d10 | 9.922 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|------------|--------------|------|
| 1    |    |   | Benzophenone                        | 182 | C13H10O    | 000119-61-9  | 96   |
| 2    |    |   | Disulfide, dibenzoyl                | 274 | C14H10O2S2 | 000644-32-6  | 49   |
| 3    |    |   | .alpha.,.alpha.-Dichloroacetophe... | 188 | C8H6Cl2O   | 002648-61-5  | 47   |
| 4    |    |   | 2-(2-Oxo-2-phenyl-ethyl)-malonon... | 184 | C11H8N2O   | 1000296-76-9 | 47   |
| 5    |    |   | 2-Phenyl-4-ethylidene-2-oxazolin... | 187 | C11H9NO2   | 037791-41-6  | 47   |



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Misc :  
ALS Vial : 14 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
TP-1

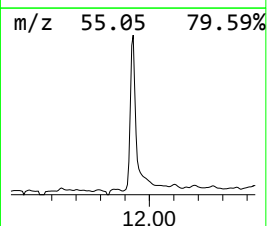
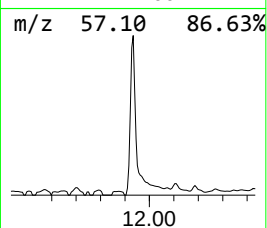
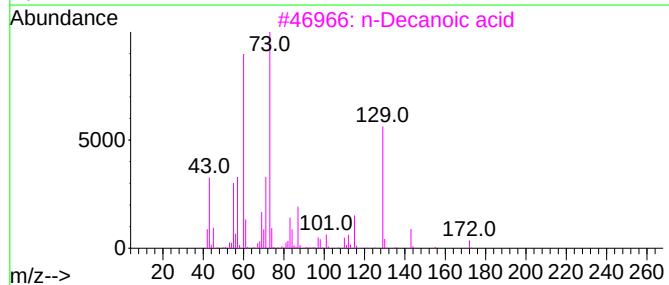
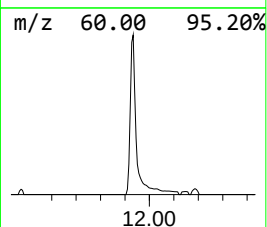
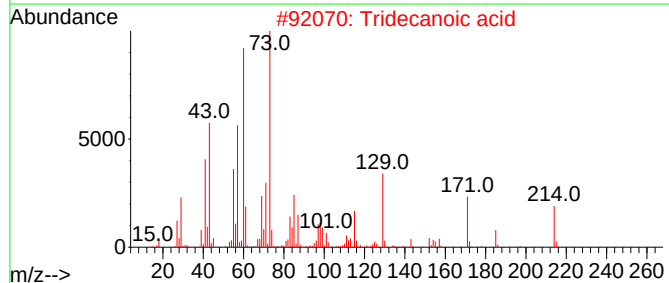
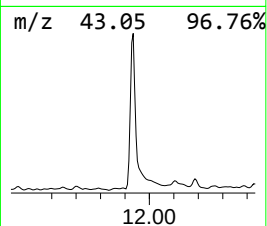
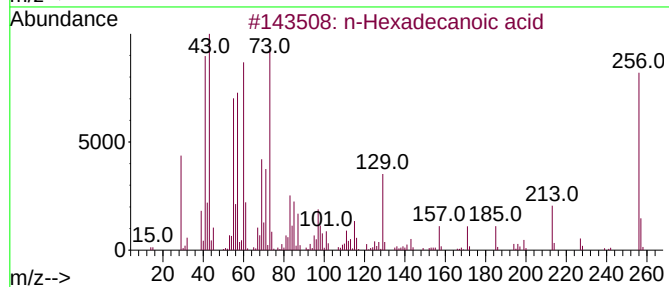
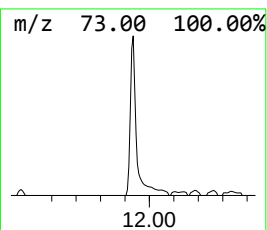
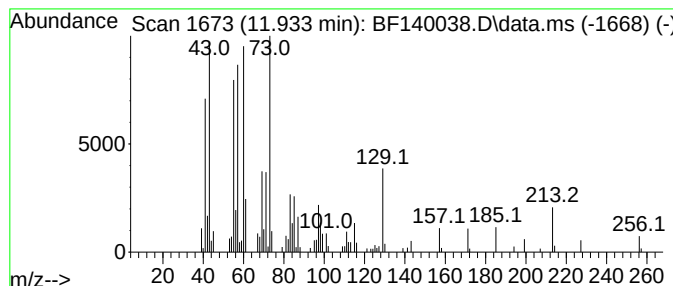
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF101824.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 11.933 | 3.98 ng | 187931 | Phenanthrene-d10 | 11.410 |

| 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 | 89   |
| 3    |    |   | n-Decanoic acid     | 172 | C10H20O2 | 000334-48-5 | 78   |
| 4    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 74   |
| 5    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 72   |



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ALS Vial : 14 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
TP-1

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

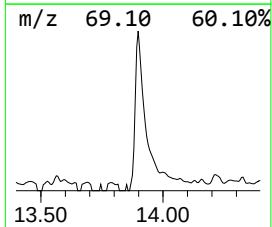
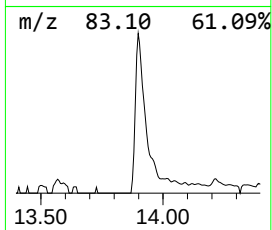
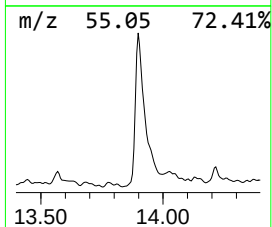
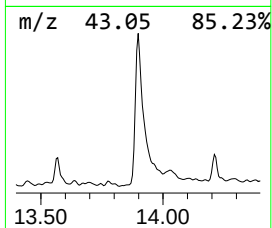
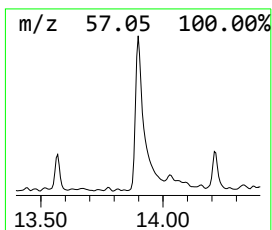
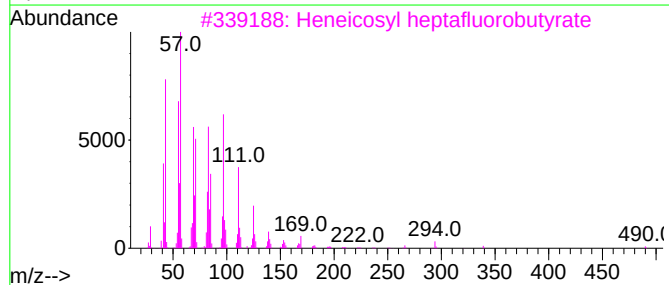
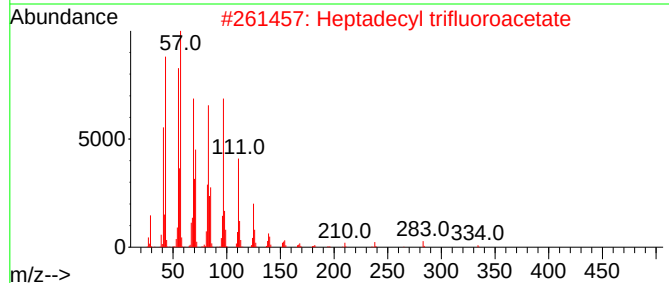
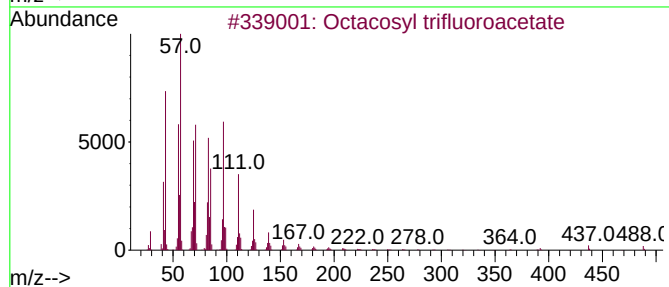
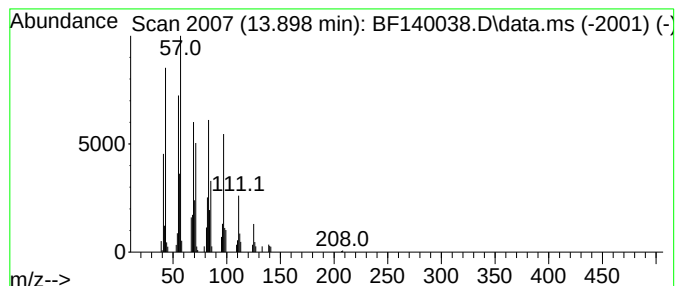
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 Octacosyl trifluoroacetate Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 13.898 | 4.91 ng | 159700 | Chrysene-d12     | 14.051 |

| Hit# | of | 5 | Tentative ID                   | MW  | MolForm    | CAS#         | Qual |
|------|----|---|--------------------------------|-----|------------|--------------|------|
| 1    |    |   | Octacosyl trifluoroacetate     | 506 | C30H57F3O2 | 1000351-74-9 | 91   |
| 2    |    |   | Heptadecyl trifluoroacetate    | 352 | C19H35F3O2 | 1010351-87-0 | 91   |
| 3    |    |   | Heneicosyl heptafluorobutyrate | 508 | C25H43F7O2 | 1000351-83-8 | 91   |
| 4    |    |   | 17-Pentatriacontene            | 491 | C35H70     | 006971-40-0  | 91   |
| 5    |    |   | Docosyl pentafluoropropionate  | 472 | C25H45F5O2 | 1000351-80-9 | 91   |



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

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| Butane, 2-metho... | 2.181  | 82.3    | ng    | 2387870  | 1                     | 6.887  | 580101 | 20.0 |
| Benzophenone       | 10.633 | 8.8     | ng    | 387858   | 3                     | 9.922  | 883622 | 20.0 |
| n-Hexadecanoic ... | 11.933 | 4.0     | ng    | 187931   | 4                     | 11.410 | 945298 | 20.0 |
| Octacosyl trifl... | 13.898 | 4.9     | ng    | 159700   | 5                     | 14.051 | 651102 | 20.0 |