

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF111424\  
 Data File : BF140363.D  
 Acq On : 14 Nov 2024 15:39  
 Operator : RC/JU  
 Sample : P4718-04  
 Misc :  
 ALS Vial : 14 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 WB-307-SW

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-BF111324.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140363.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         | 2.163       | 3             | 12          | 18           | rBV      | 5236869        | 9048173       | 100.00%         | 29.872%       |
| 2         | 4.740       | 444           | 450         | 457          | rBV      | 88229          | 120895        | 1.34%           | 0.399%        |
| 3         | 5.087       | 500           | 509         | 524          | rVB      | 255818         | 384092        | 4.24%           | 1.268%        |
| 4         | 5.492       | 571           | 578         | 589          | rBV      | 1528568        | 2030789       | 22.44%          | 6.704%        |
| 5         | 6.492       | 740           | 748         | 766          | rBV      | 1369975        | 1893398       | 20.93%          | 6.251%        |
| 6         | 6.869       | 807           | 812         | 820          | rBV      | 650115         | 813239        | 8.99%           | 2.685%        |
| 7         | 7.433       | 901           | 908         | 913          | rBV      | 1453141        | 1996894       | 22.07%          | 6.593%        |
| 8         | 8.151       | 1024          | 1030        | 1043         | rVB      | 824229         | 1051528       | 11.62%          | 3.472%        |
| 9         | 9.227       | 1206          | 1213        | 1223         | rBV      | 2764542        | 3689213       | 40.77%          | 12.180%       |
| 10        | 9.904       | 1323          | 1328        | 1338         | rBV      | 944831         | 1188638       | 13.14%          | 3.924%        |
| 11        | 10.621      | 1444          | 1450        | 1457         | rBV      | 220028         | 288895        | 3.19%           | 0.954%        |
| 12        | 10.698      | 1457          | 1463        | 1477         | rBV      | 1554445        | 2153215       | 23.80%          | 7.109%        |
| 13        | 11.392      | 1576          | 1581        | 1588         | rBV      | 921943         | 1162704       | 12.85%          | 3.839%        |
| 14        | 11.916      | 1665          | 1670        | 1685         | rBV3     | 77066          | 174248        | 1.93%           | 0.575%        |
| 15        | 12.980      | 1845          | 1851        | 1856         | rBV      | 2292241        | 2908373       | 32.14%          | 9.602%        |
| 16        | 14.045      | 2025          | 2032        | 2043         | rVB      | 491224         | 677917        | 7.49%           | 2.238%        |
| 17        | 15.562      | 2284          | 2290        | 2303         | rBV      | 436909         | 708047        | 7.83%           | 2.338%        |

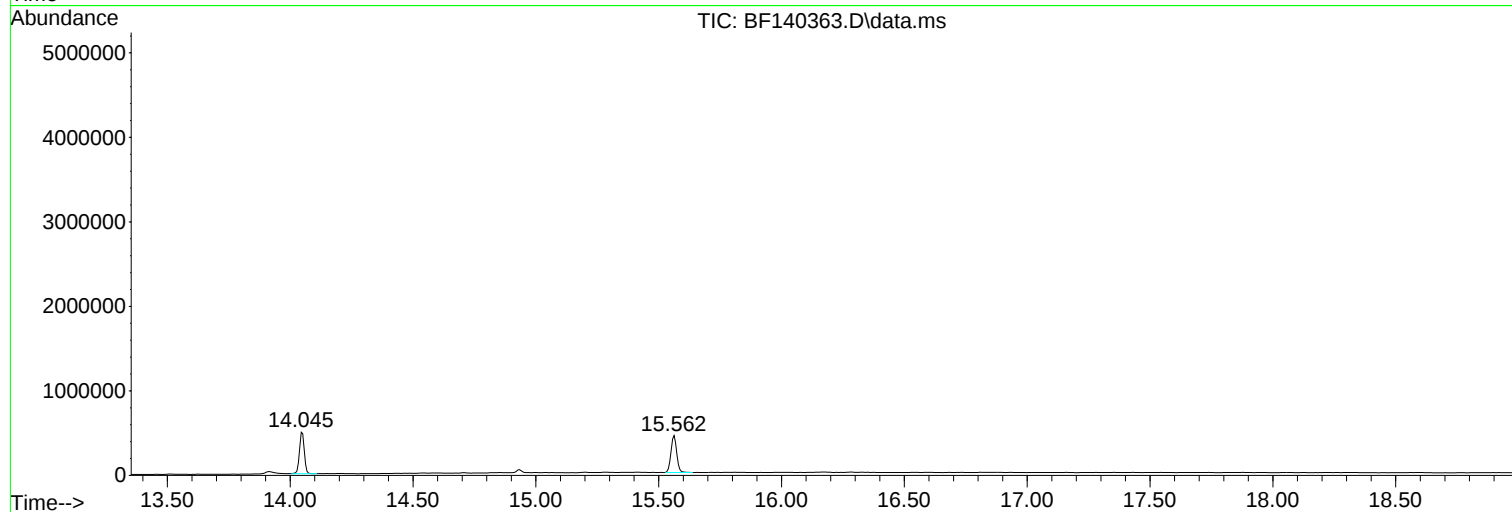
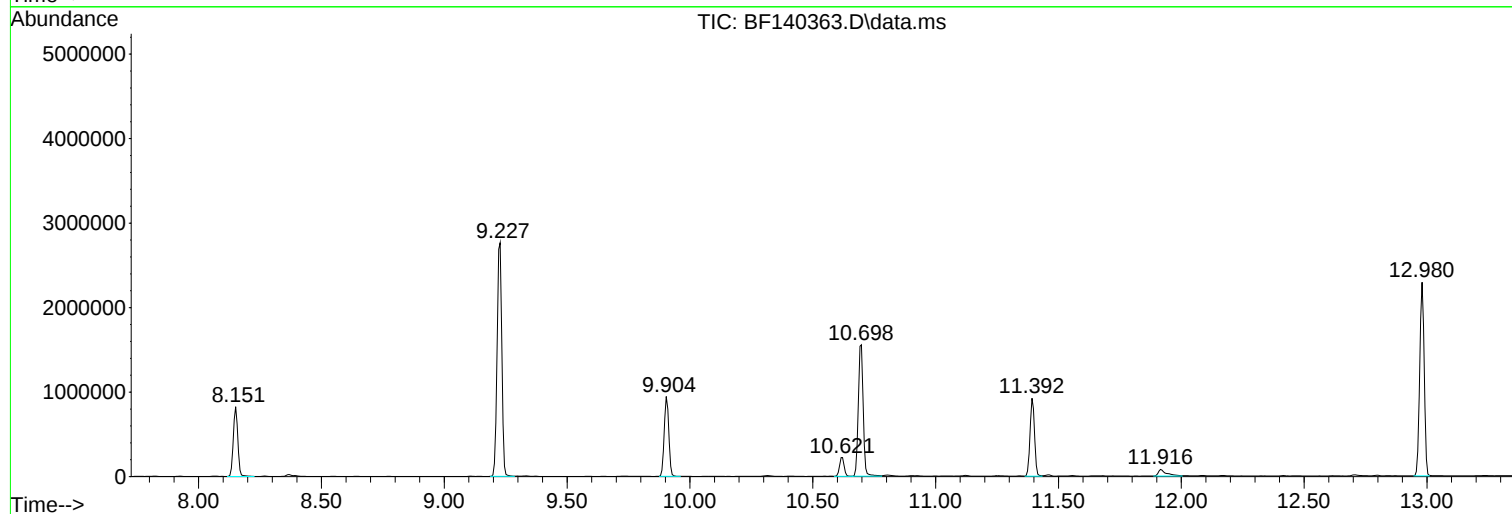
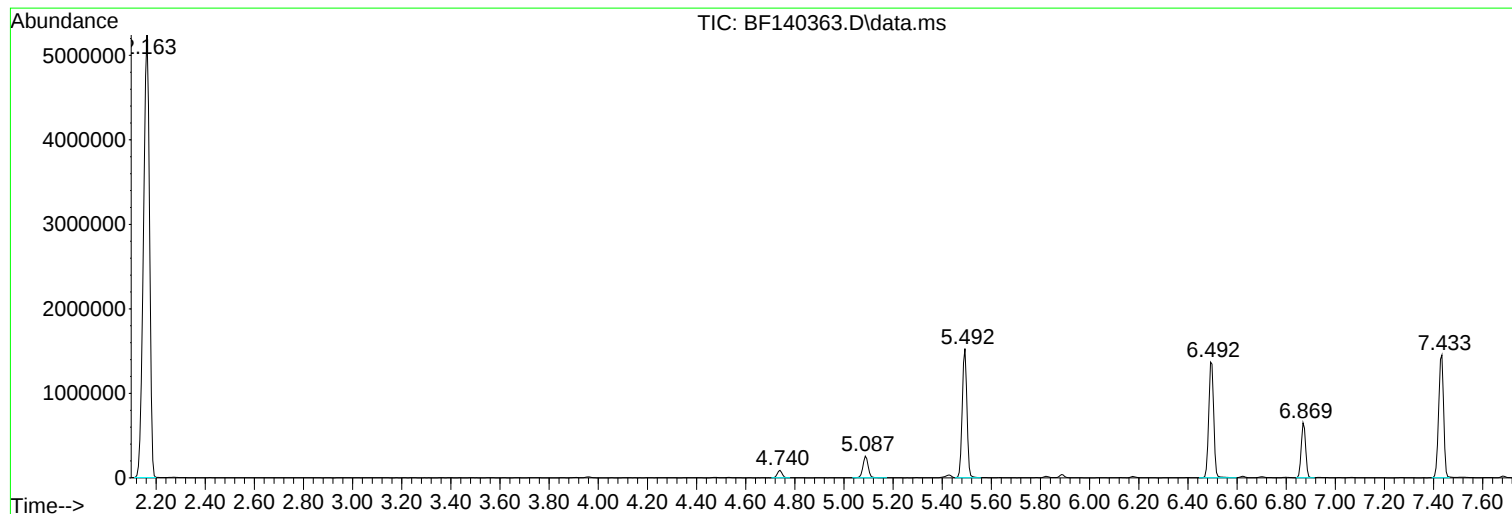
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BNA\_F  
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WB-307-SW

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF111324.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\BF111424\  
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ALS Vial : 14 Sample Multiplier: 1

Instrument :  
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ClientSampleId :  
WB-307-SW

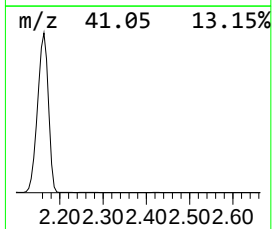
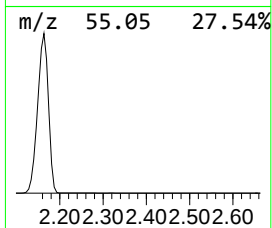
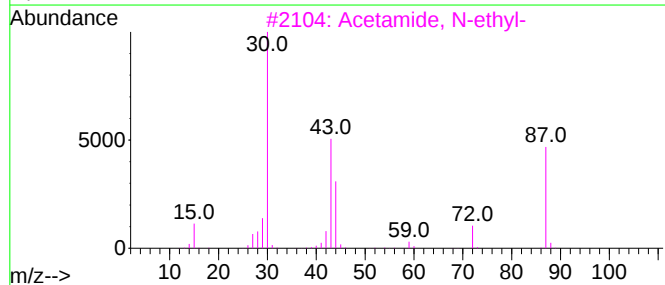
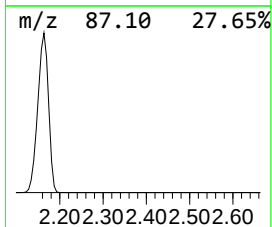
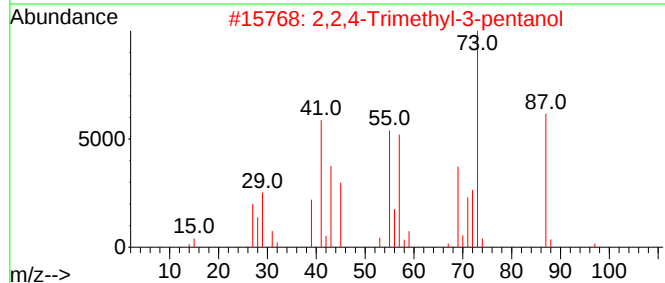
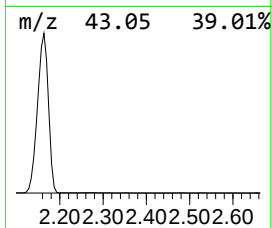
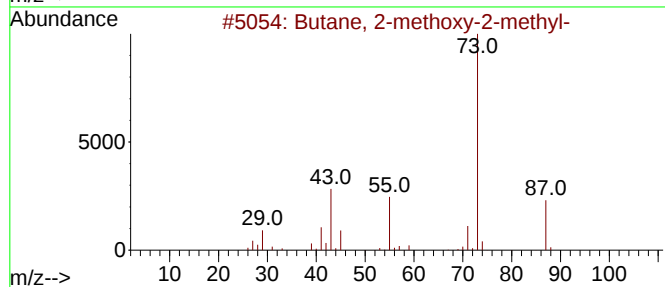
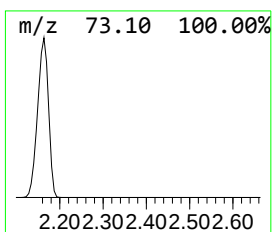
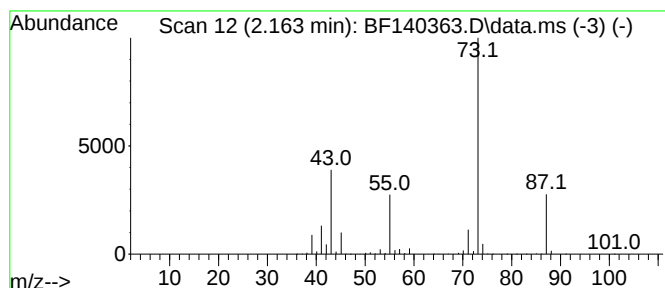
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF111324.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.  |
|-------|-----------|---------|------------------------|-------|
| 2.163 | 222.52 ng | 9048170 | 1,4-Dichlorobenzene-d4 | 6.869 |

| 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    |    |   | Acetamide, N-ethyl-              | 87  | C4H9NO   | 000625-50-3 | 27   |
| 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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ClientSampleId :  
WB-307-SW

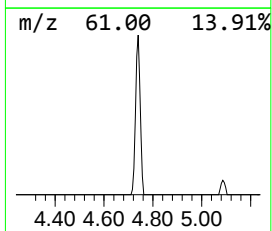
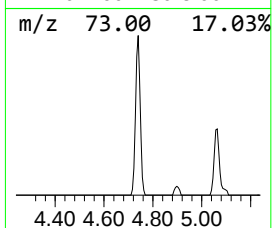
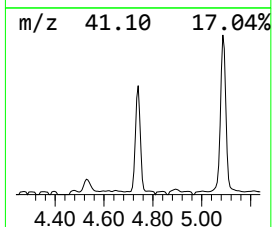
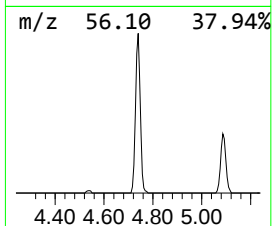
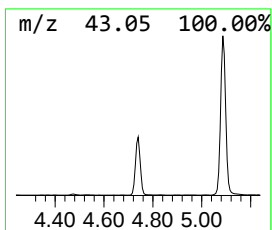
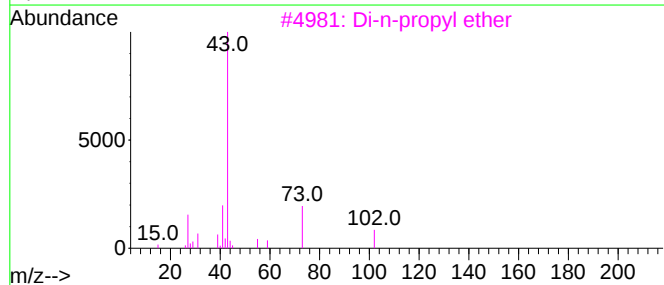
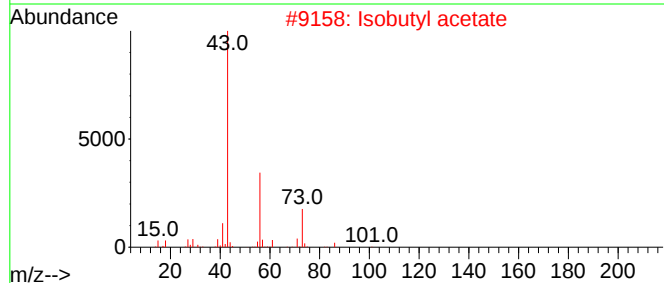
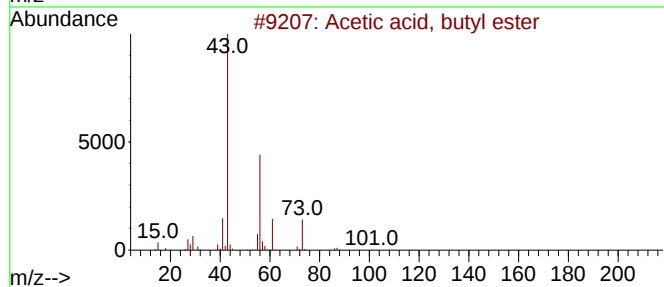
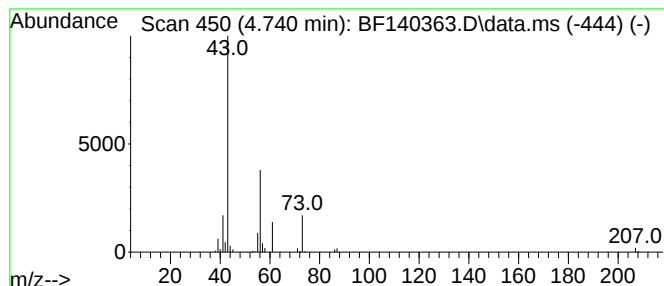
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF111324.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 2 Acetic acid, butyl ester Concentration Rank 5

| R.T.  | EstConc | Area   | Relative to ISTD       | R.T.  |
|-------|---------|--------|------------------------|-------|
| 4.740 | 2.97 ng | 120895 | 1,4-Dichlorobenzene-d4 | 6.869 |

| Hit# | of 5 | Tentative ID             | MW  | MolForm | CAS#        | Qual |
|------|------|--------------------------|-----|---------|-------------|------|
| 1    |      | Acetic acid, butyl ester | 116 | C6H12O2 | 000123-86-4 | 78   |
| 2    |      | Isobutyl acetate         | 116 | C6H12O2 | 000110-19-0 | 39   |
| 3    |      | Di-n-propyl ether        | 102 | C6H14O  | 000111-43-3 | 16   |
| 4    |      | Isobutylamine            | 73  | C4H11N  | 000078-81-9 | 9    |
| 5    |      | Acetic acid, hexyl ester | 144 | C8H16O2 | 000142-92-7 | 9    |



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Sample : P4718-04  
Misc :  
ALS Vial : 14 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
WB-307-SW

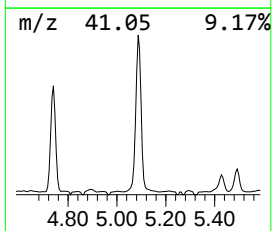
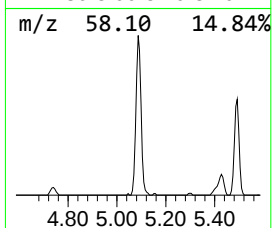
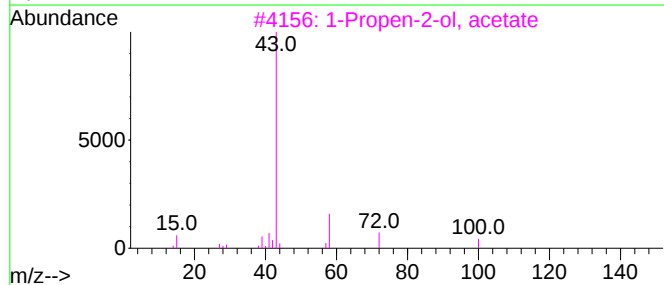
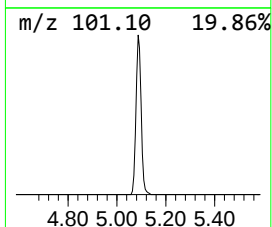
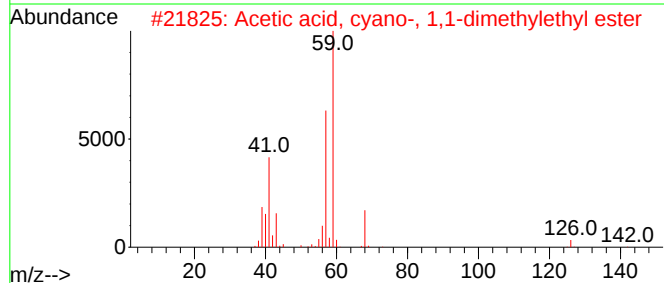
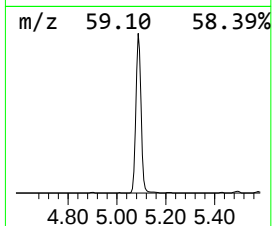
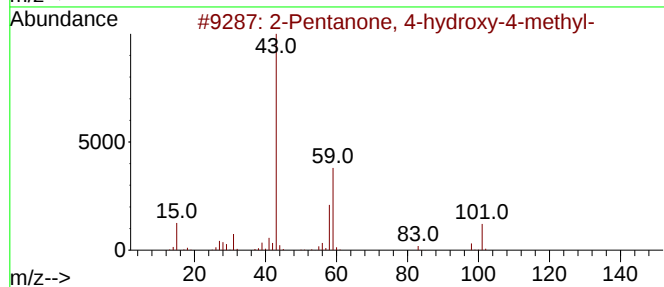
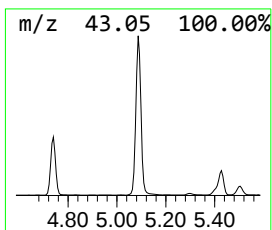
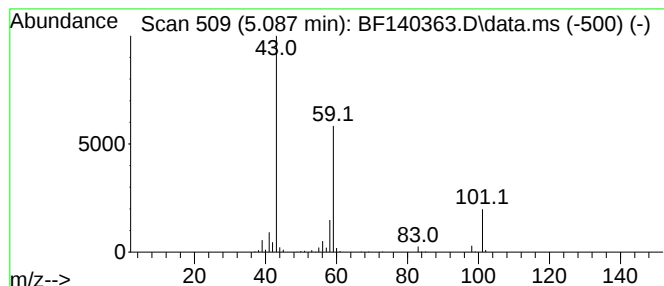
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF111324.M  
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TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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

| R.T.      | EstConc                             | Area   | Relative to ISTD       | R.T.        |      |
|-----------|-------------------------------------|--------|------------------------|-------------|------|
| 5.087     | 9.45 ng                             | 384092 | 1,4-Dichlorobenzene-d4 | 6.869       |      |
| Hit# of 5 | Tentative ID                        | MW     | MolForm                | CAS#        | Qual |
| 1         | 2-Pentanone, 4-hydroxy-4-methyl-    | 116    | C6H12O2                | 000123-42-2 | 56   |
| 2         | Acetic acid, cyano-, 1,1-dimethy... | 141    | C7H11NO2               | 001116-98-9 | 23   |
| 3         | 1-Propen-2-ol, acetate              | 100    | C5H8O2                 | 000108-22-5 | 10   |
| 4         | 2,3-Butanedione, monooxime          | 101    | C4H7NO2                | 000057-71-6 | 9    |
| 5         | 3-Hexanol, 4-ethyl-                 | 130    | C8H18O                 | 019780-44-0 | 9    |



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ALS Vial : 14 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
WB-307-SW

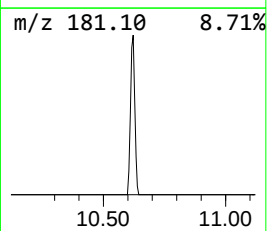
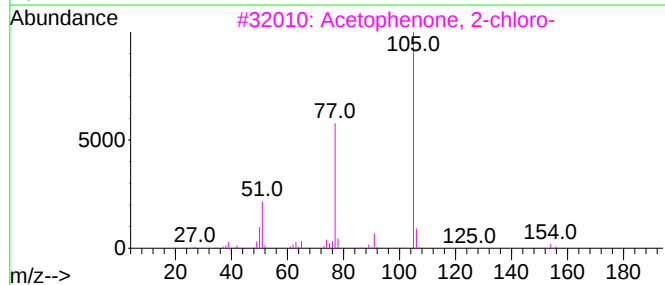
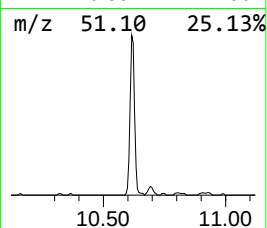
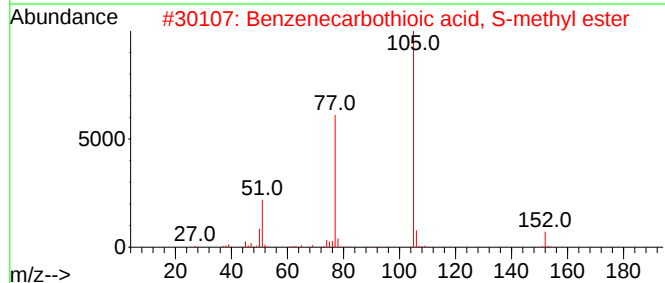
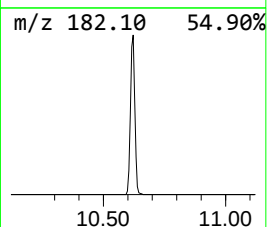
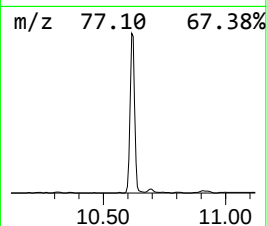
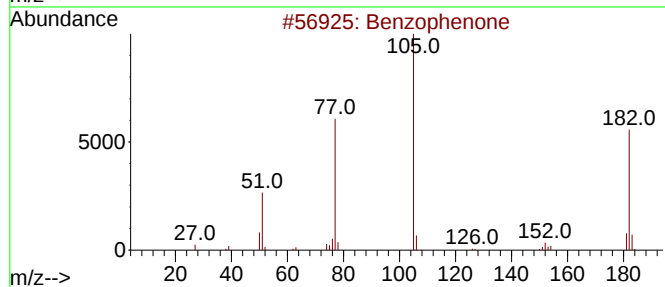
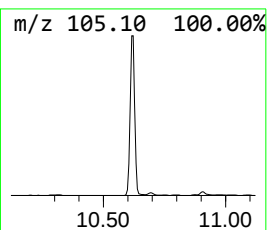
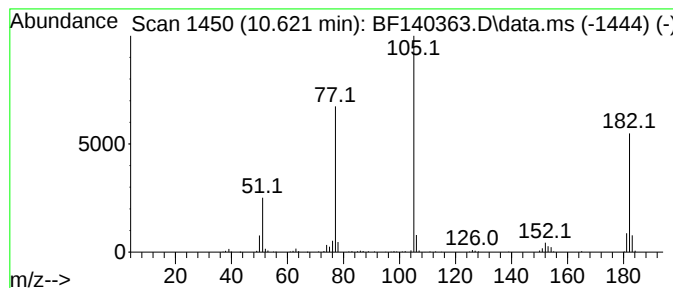
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Peak Number 4 Benzophenone Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.  |
|--------|---------|--------|------------------|-------|
| 10.621 | 4.86 ng | 288895 | Acenaphthene-d10 | 9.904 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | Benzophenone                        | 182 | C13H10O  | 000119-61-9 | 96   |
| 2    |    |   | Benzenecarbothioic acid, S-methy... | 152 | C8H8OS   | 005925-68-8 | 58   |
| 3    |    |   | Acetophenone, 2-chloro-             | 154 | C8H7ClO  | 000532-27-4 | 49   |
| 4    |    |   | 2-Chloro-1-phenyl-1-propanone       | 168 | C9H9ClO  | 006084-17-9 | 47   |
| 5    |    |   | N-Methoxy-N-methylbenzamide         | 165 | C9H11NO2 | 006919-61-5 | 47   |



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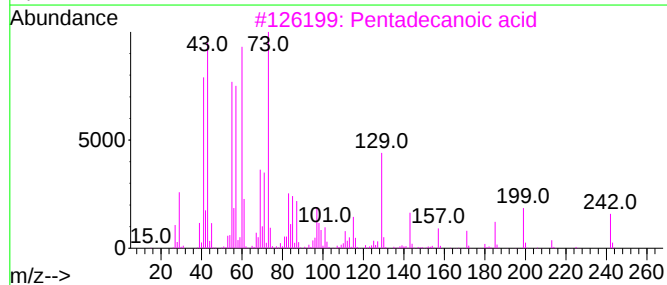
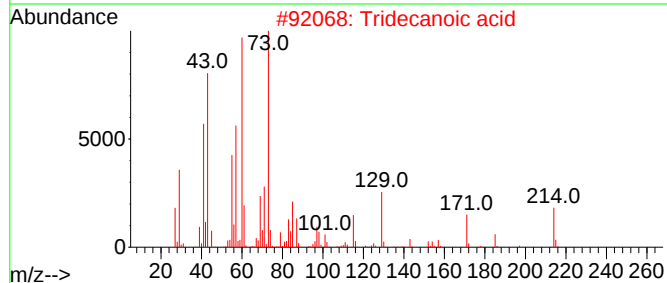
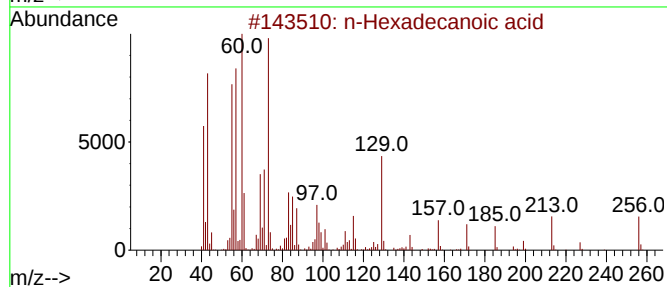
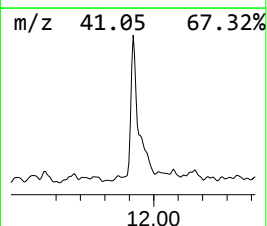
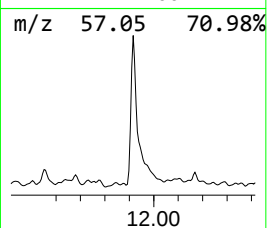
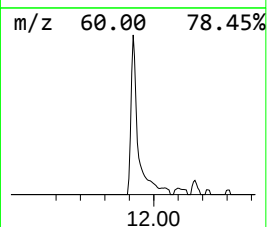
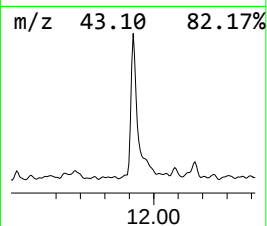
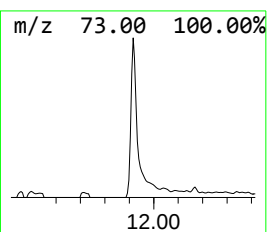
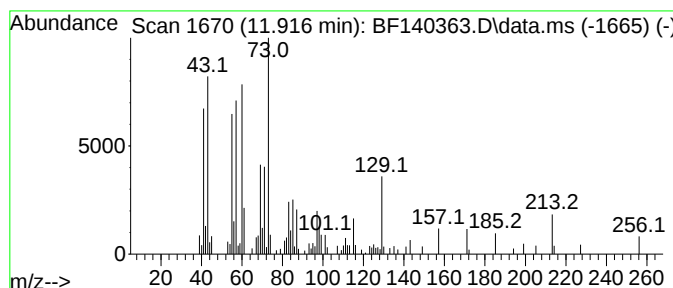
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 11.916 | 3.00 ng | 174248 | Phenanthrene-d10 | 11.392 |

| 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 | 93   |
| 3    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 91   |
| 4    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 86   |
| 5    |    |   | n-Decanoic acid     | 172 | C10H20O2 | 000334-48-5 | 46   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF111424\  
Data File : BF140363.D  
Acq On : 14 Nov 2024 15:39  
Operator : RC/JU  
Sample : P4718-04  
Misc :  
ALS Vial : 14 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
WB-307-SW

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF111324.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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... | 2.163  | 222.5   | ng    | 9048170  | 1                     | 6.869  | 813239  | 20.0 |
| Acetic acid, bu... | 4.740  | 3.0     | ng    | 120895   | 1                     | 6.869  | 813239  | 20.0 |
| 2-Pentanone, 4-... | 5.087  | 9.4     | ng    | 384092   | 1                     | 6.869  | 813239  | 20.0 |
| Benzophenone       | 10.621 | 4.9     | ng    | 288895   | 3                     | 9.904  | 1188640 | 20.0 |
| n-Hexadecanoic ... | 11.916 | 3.0     | ng    | 174248   | 4                     | 11.392 | 1162700 | 20.0 |