

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF111924\  
 Data File : BF140468.D  
 Acq On : 19 Nov 2024 12:54  
 Operator : RC/JU  
 Sample : P4852-01  
 Misc :  
 ALS Vial : 7 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 COMP-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-BF111324.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140468.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         | 2.187       | 8             | 16          | 26           | rVB      | 770530         | 1223974       | 38.31%          | 4.921%        |
| 2         | 5.098       | 502           | 511         | 520          | rBV      | 60328          | 96769         | 3.03%           | 0.389%        |
| 3         | 5.504       | 574           | 580         | 594          | rBV      | 1875706        | 2451810       | 76.74%          | 9.857%        |
| 4         | 6.510       | 744           | 751         | 779          | rBV      | 1838427        | 2609352       | 81.67%          | 10.491%       |
| 5         | 6.869       | 807           | 812         | 820          | rBV      | 720758         | 893605        | 27.97%          | 3.593%        |
| 6         | 7.434       | 901           | 908         | 918          | rBV      | 1230131        | 1707160       | 53.43%          | 6.864%        |
| 7         | 7.687       | 946           | 951         | 962          | rBV      | 24052          | 40190         | 1.26%           | 0.162%        |
| 8         | 8.151       | 1024          | 1030        | 1049         | rBV      | 903914         | 1177259       | 36.85%          | 4.733%        |
| 9         | 9.222       | 1206          | 1212        | 1224         | rBV      | 2387457        | 3195034       | 100.00%         | 12.846%       |
| 10        | 9.904       | 1322          | 1328        | 1344         | rBV      | 1013788        | 1360976       | 42.60%          | 5.472%        |
| 11        | 10.622      | 1444          | 1450        | 1457         | rBV      | 241514         | 321549        | 10.06%          | 1.293%        |
| 12        | 10.698      | 1457          | 1463        | 1478         | rBV      | 1371084        | 1849841       | 57.90%          | 7.437%        |
| 13        | 11.392      | 1576          | 1581        | 1590         | rBV2     | 1040943        | 1595554       | 49.94%          | 6.415%        |
| 14        | 11.469      | 1590          | 1594        | 1606         | rVB2     | 39598          | 64385         | 2.02%           | 0.259%        |
| 15        | 11.922      | 1662          | 1671        | 1678         | rBV3     | 138450         | 275841        | 8.63%           | 1.109%        |
| 16        | 12.010      | 1683          | 1686        | 1695         | rVB2     | 36895          | 77985         | 2.44%           | 0.314%        |
| 17        | 12.610      | 1783          | 1788        | 1792         | rBV      | 249554         | 320765        | 10.04%          | 1.290%        |
| 18        | 12.798      | 1816          | 1820        | 1822         | rBV      | 60780          | 78387         | 2.45%           | 0.315%        |
| 19        | 12.839      | 1822          | 1827        | 1831         | rVV      | 199428         | 296118        | 9.27%           | 1.191%        |
| 20        | 12.869      | 1831          | 1832        | 1843         | rVB3     | 32955          | 45199         | 1.41%           | 0.182%        |
| 21        | 12.980      | 1845          | 1851        | 1859         | rVB      | 2153299        | 2741701       | 85.81%          | 11.023%       |
| 22        | 13.057      | 1859          | 1864        | 1875         | rVB5     | 17014          | 34741         | 1.09%           | 0.140%        |
| 23        | 13.169      | 1875          | 1883        | 1886         | rVB2     | 17463          | 37897         | 1.19%           | 0.152%        |
| 24        | 13.504      | 1936          | 1940        | 1944         | rVB      | 36174          | 41821         | 1.31%           | 0.168%        |
| 25        | 13.892      | 2002          | 2006        | 2013         | rVB3     | 26991          | 44652         | 1.40%           | 0.180%        |
| 26        | 14.051      | 2026          | 2033        | 2045         | rVB2     | 723899         | 1117941       | 34.99%          | 4.495%        |
| 27        | 14.845      | 2164          | 2168        | 2175         | rVB3     | 19151          | 36528         | 1.14%           | 0.147%        |
| 28        | 15.127      | 2211          | 2216        | 2224         | rBV      | 68555          | 158983        | 4.98%           | 0.639%        |
| 29        | 15.433      | 2264          | 2268        | 2274         | rVB      | 32930          | 51558         | 1.61%           | 0.207%        |
| 30        | 15.498      | 2275          | 2279        | 2285         | rVV      | 48118          | 76880         | 2.41%           | 0.309%        |
| 31        | 15.568      | 2285          | 2291        | 2303         | rVB      | 467801         | 798674        | 25.00%          | 3.211%        |
| 32        | 17.074      | 2541          | 2547        | 2555         | rVB3     | 20793          | 49548         | 1.55%           | 0.199%        |

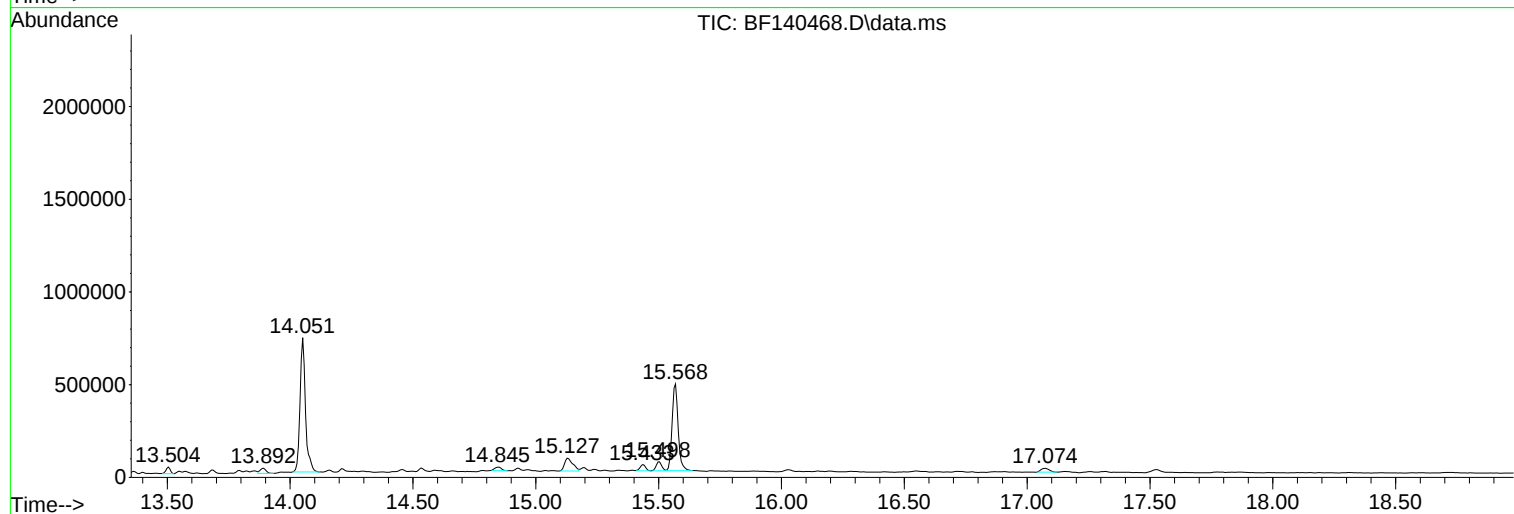
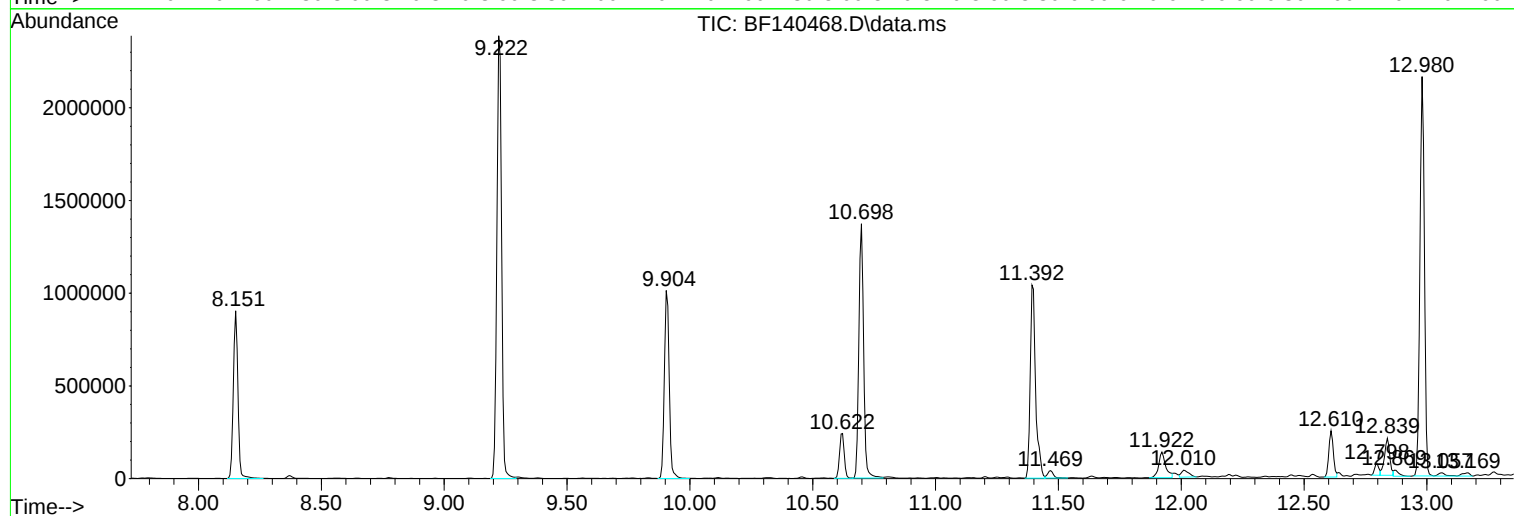
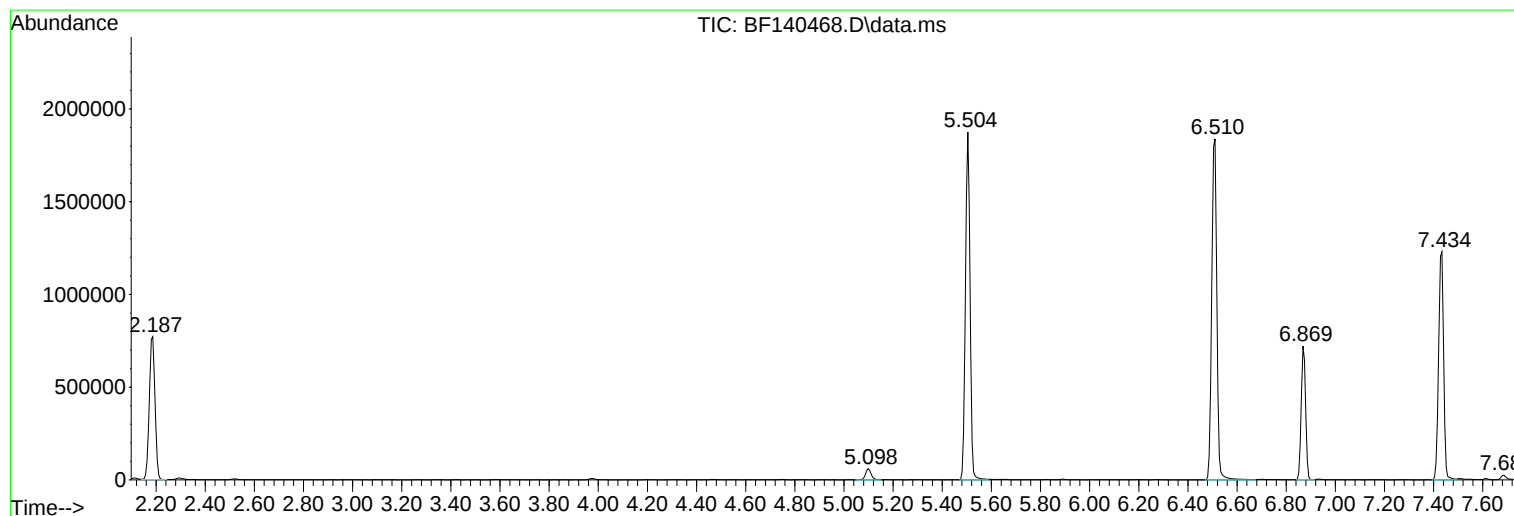
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Sample : P4852-01  
Misc :  
ALS Vial : 7 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
COMP-1

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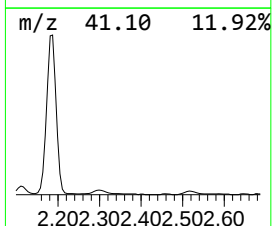
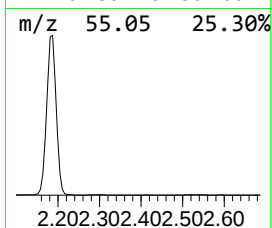
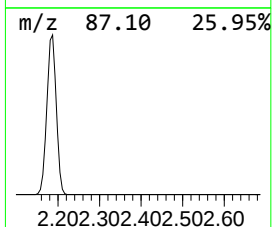
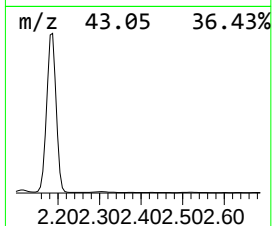
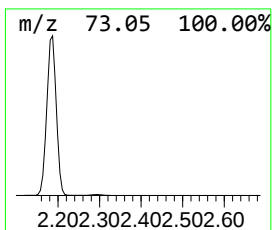
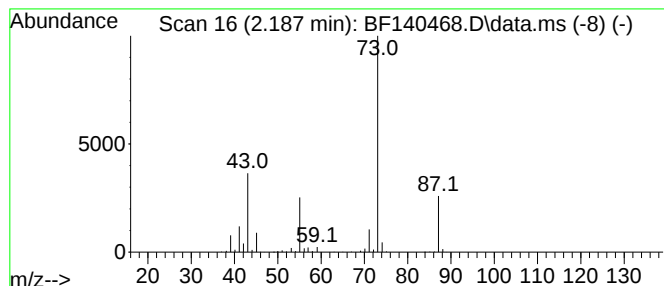
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF111324.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.  |
|-------|----------|---------|------------------------|-------|
| 2.187 | 27.39 ng | 1223970 | 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 | 78   |
| 2    |    |   | 2,2,4-Trimethyl-3-pentanol  | 130 | C8H18O  | 005162-48-1 | 39   |
| 3    |    |   | 1,3-Dioxolane, 2-methyl-    | 88  | C4H8O2  | 000497-26-7 | 37   |
| 4    |    |   | Pentane, 3-methoxy-         | 102 | C6H14O  | 036839-67-5 | 23   |
| 5    |    |   | Silane, tetramethyl-        | 88  | C4H12Si | 000075-76-3 | 17   |



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Misc :  
ALS Vial : 7 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
COMP-1

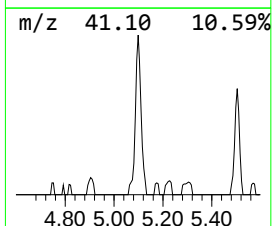
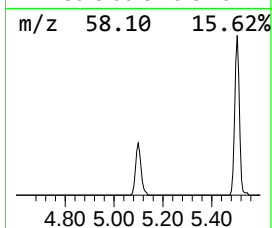
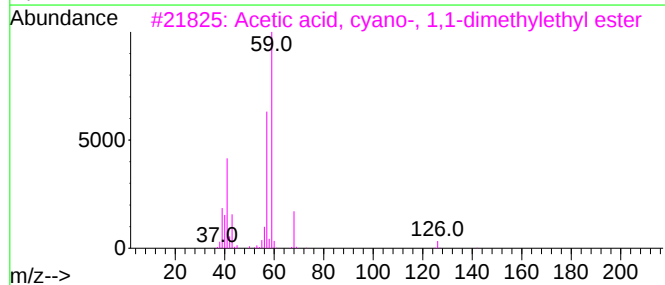
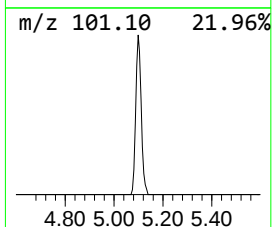
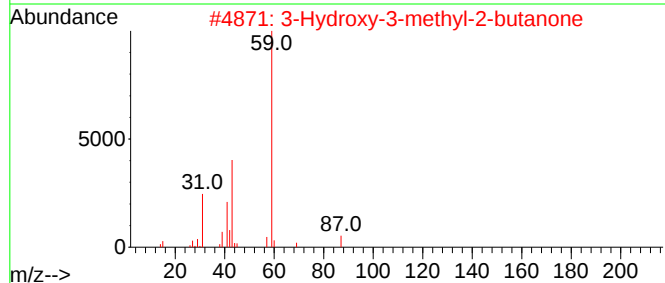
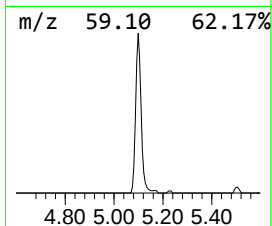
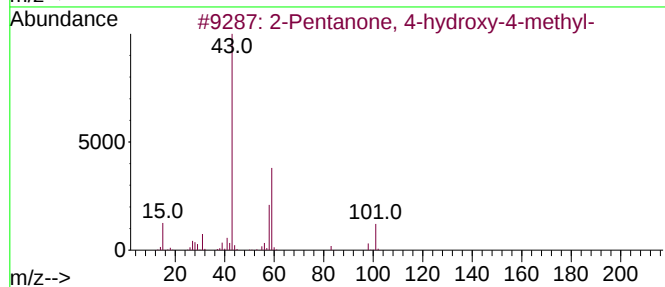
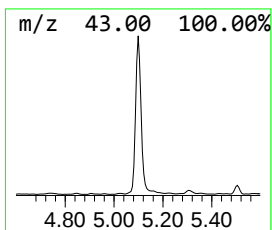
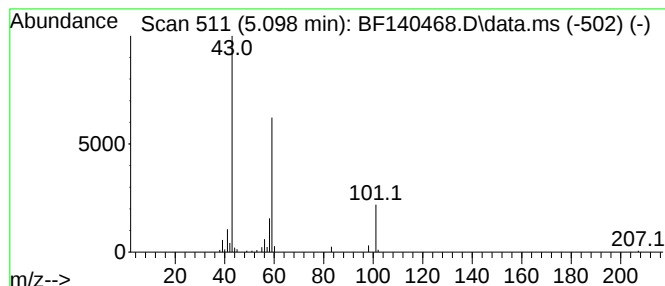
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF111324.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

| R.T.  | EstConc | Area  | Relative to ISTD       | R.T.  |
|-------|---------|-------|------------------------|-------|
| 5.098 | 2.17 ng | 96769 | 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    | 3-Hydroxy-3-methyl-2-butanone       | 102 | C5H10O2      | 000115-22-0 | 25      |      |      |
| 3    | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2     | 001116-98-9 | 17      |      |      |
| 4    | 1-Propen-2-ol, acetate              | 100 | C5H8O2       | 000108-22-5 | 10      |      |      |
| 5    | Morpholine, 4-methyl-               | 101 | C5H11NO      | 000109-02-4 | 9       |      |      |



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Misc :  
ALS Vial : 7 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
COMP-1

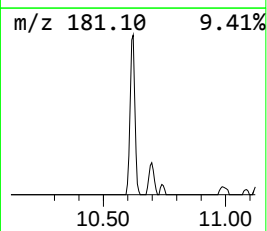
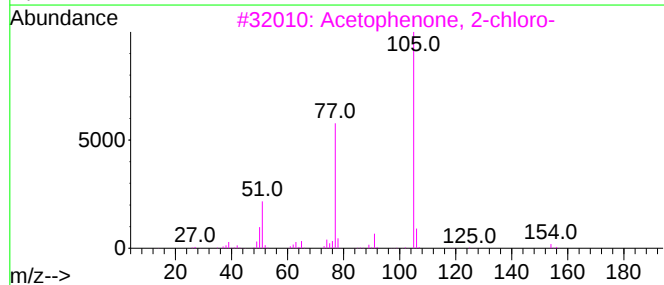
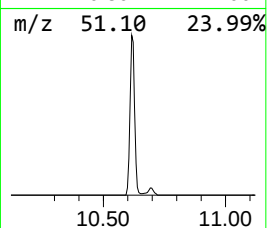
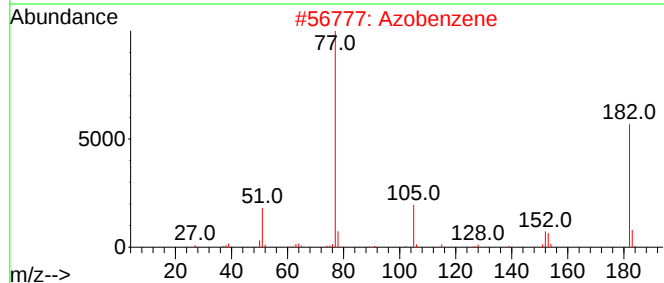
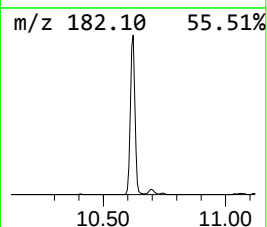
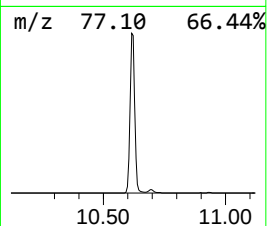
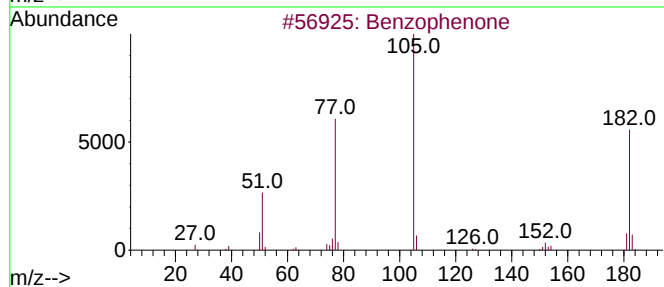
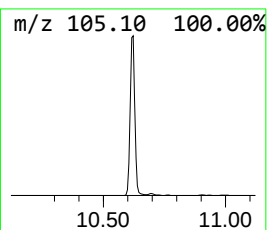
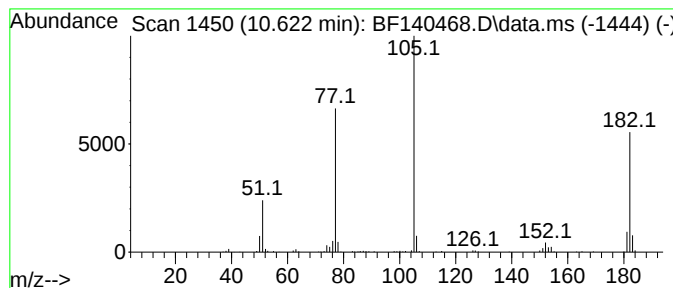
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF111324.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 3 Benzophenone Concentration Rank 2

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.  |
|--------|---------|--------|------------------|-------|
| 10.622 | 4.73 ng | 321549 | Acenaphthene-d10 | 9.904 |

| Hit# | of | 5 | Tentative ID                   | MW  | MolForm  | CAS#        | Qual |
|------|----|---|--------------------------------|-----|----------|-------------|------|
| 1    |    |   | Benzophenone                   | 182 | C13H10O  | 000119-61-9 | 96   |
| 2    |    |   | Azobenzene                     | 182 | C12H10N2 | 000103-33-3 | 64   |
| 3    |    |   | Acetophenone, 2-chloro-        | 154 | C8H7ClO  | 000532-27-4 | 49   |
| 4    |    |   | 1-Propanone, 2-bromo-1-phenyl- | 212 | C9H9BrO  | 002114-00-3 | 47   |
| 5    |    |   | N-Methoxy-N-methylbenzamide    | 165 | C9H11NO2 | 006919-61-5 | 47   |



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BNA\_F  
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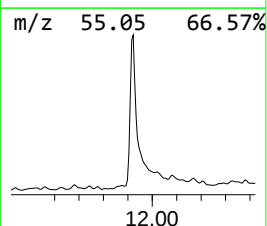
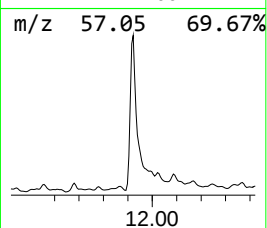
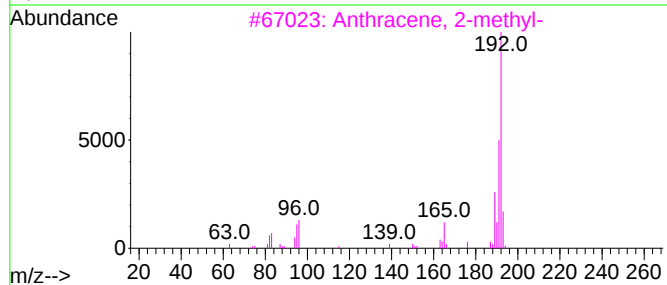
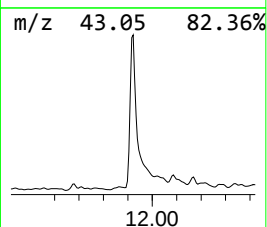
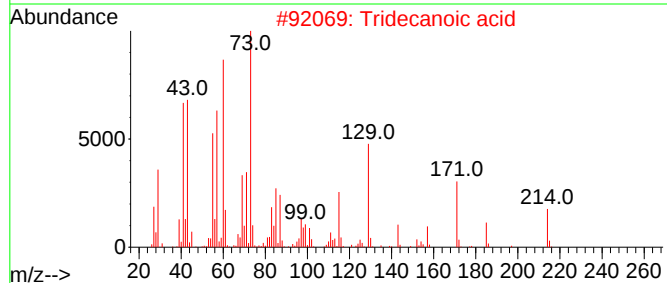
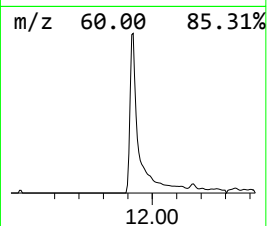
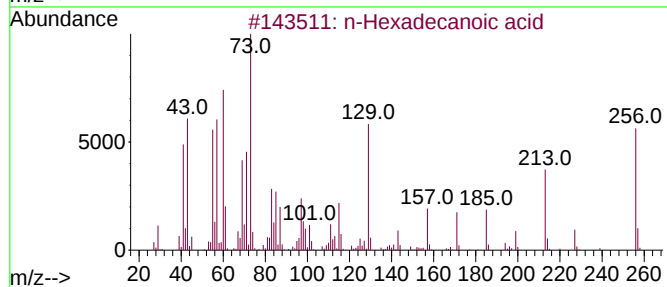
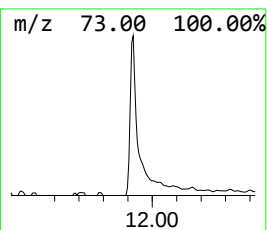
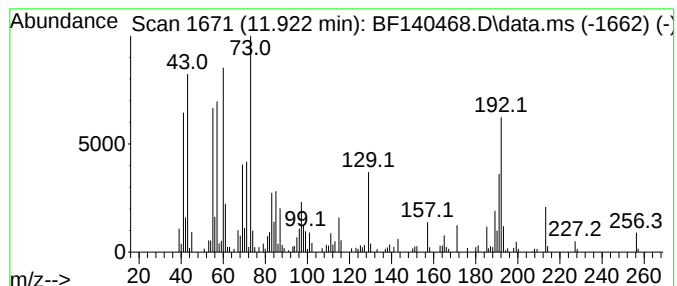
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TIC Library : C:\Database\NIST20.L  
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 11.922 | 3.46 ng | 275841 | 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 | 91   |
| 3    |    |   | Anthracene, 2-methyl- | 192 | C15H12   | 000613-12-7 | 91   |
| 4    |    |   | Anthracene, 9-methyl- | 192 | C15H12   | 000779-02-2 | 90   |
| 5    |    |   | Tetradecanoic acid    | 228 | C14H28O2 | 000544-63-8 | 70   |



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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... | 2.187  | 27.4    | ng    | 1223970  | 1                     | 6.869  | 893605  | 20.0 |
| 2-Pentanone, 4-... | 5.098  | 2.2     | ng    | 96769    | 1                     | 6.869  | 893605  | 20.0 |
| Benzophenone       | 10.622 | 4.7     | ng    | 321549   | 3                     | 9.904  | 1360980 | 20.0 |
| n-Hexadecanoic ... | 11.922 | 3.5     | ng    | 275841   | 4                     | 11.392 | 1595550 | 20.0 |