

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF062724\  
 Data File : BF138379.D  
 Acq On : 27 Jun 2024 21:38  
 Operator : CG\JU  
 Sample : P3077-07  
 Misc :  
 ALS Vial : 19 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 1-S-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-BF061224.M  
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138379.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         | 2.169       | 8             | 14          | 21           | rVB      | 1816457        | 2207324       | 77.54%          | 7.991%        |
| 2         | 2.275       | 28            | 32          | 37           | rVB      | 28460          | 35697         | 1.25%           | 0.129%        |
| 3         | 3.393       | 214           | 222         | 230          | rBV2     | 65268          | 153822        | 5.40%           | 0.557%        |
| 4         | 5.098       | 508           | 512         | 520          | rVB      | 206091         | 236585        | 8.31%           | 0.857%        |
| 5         | 5.363       | 554           | 557         | 561          | rBV      | 49022          | 46196         | 1.62%           | 0.167%        |
| 6         | 5.475       | 572           | 576         | 578          | rBV      | 240983         | 254745        | 8.95%           | 0.922%        |
| 7         | 5.504       | 578           | 581         | 585          | rVB      | 2959163        | 2846825       | 100.00%         | 10.306%       |
| 8         | 5.728       | 616           | 619         | 623          | rBV      | 319393         | 276784        | 9.72%           | 1.002%        |
| 9         | 6.516       | 748           | 753         | 760          | rBV      | 3052882        | 2798060       | 98.29%          | 10.130%       |
| 10        | 6.704       | 782           | 785         | 789          | rBV2     | 62679          | 57471         | 2.02%           | 0.208%        |
| 11        | 6.881       | 811           | 815         | 818          | rBV      | 1622794        | 1233329       | 43.32%          | 4.465%        |
| 12        | 7.016       | 835           | 838         | 843          | rBV      | 86727          | 73114         | 2.57%           | 0.265%        |
| 13        | 7.439       | 906           | 910         | 913          | rBV      | 2081921        | 1787333       | 62.78%          | 6.471%        |
| 14        | 7.692       | 949           | 953         | 960          | rVB      | 110949         | 86781         | 3.05%           | 0.314%        |
| 15        | 8.157       | 1029          | 1032        | 1035         | rBV      | 1644743        | 1465714       | 51.49%          | 5.306%        |
| 16        | 8.469       | 1081          | 1085        | 1089         | rBV      | 161862         | 138834        | 4.88%           | 0.503%        |
| 17        | 8.869       | 1150          | 1153        | 1157         | rVB      | 107647         | 80297         | 2.82%           | 0.291%        |
| 18        | 8.969       | 1167          | 1170        | 1174         | rVB      | 62421          | 46692         | 1.64%           | 0.169%        |
| 19        | 9.233       | 1211          | 1215        | 1218         | rBV      | 3506345        | 2733687       | 96.03%          | 9.897%        |
| 20        | 9.910       | 1327          | 1330        | 1334         | rBV      | 1657054        | 1320491       | 46.38%          | 4.781%        |
| 21        | 10.010      | 1342          | 1347        | 1349         | rBV      | 70251          | 89160         | 3.13%           | 0.323%        |
| 22        | 10.639      | 1452          | 1454        | 1458         | rVB      | 147203         | 118629        | 4.17%           | 0.429%        |
| 23        | 10.698      | 1460          | 1464        | 1477         | rVV      | 1947560        | 1612468       | 56.64%          | 5.838%        |
| 24        | 11.398      | 1579          | 1583        | 1585         | rBV      | 1502333        | 1188843       | 41.76%          | 4.304%        |
| 25        | 11.422      | 1585          | 1587        | 1590         | rVV      | 203314         | 160929        | 5.65%           | 0.583%        |
| 26        | 11.469      | 1590          | 1595        | 1598         | rVB      | 55979          | 57074         | 2.00%           | 0.207%        |
| 27        | 11.922      | 1669          | 1672        | 1678         | rVB2     | 137570         | 139210        | 4.89%           | 0.504%        |
| 28        | 12.010      | 1684          | 1687        | 1689         | rBV      | 51469          | 50221         | 1.76%           | 0.182%        |
| 29        | 12.445      | 1758          | 1761        | 1764         | rBV      | 34396          | 35900         | 1.26%           | 0.130%        |
| 30        | 12.610      | 1785          | 1789        | 1792         | rBV      | 380915         | 326342        | 11.46%          | 1.181%        |
| 31        | 12.704      | 1802          | 1805        | 1809         | rBV4     | 46751          | 53998         | 1.90%           | 0.195%        |
| 32        | 12.839      | 1822          | 1828        | 1833         | rBV      | 344112         | 366262        | 12.87%          | 1.326%        |
| 33        | 12.980      | 1848          | 1852        | 1855         | rBV      | 3239406        | 2570109       | 90.28%          | 9.305%        |
| 34        | 13.163      | 1877          | 1883        | 1886         | rBV      | 57346          | 72758         | 2.56%           | 0.263%        |
| 35        | 13.268      | 1898          | 1901        | 1904         | rBV2     | 45593          | 42495         | 1.49%           | 0.154%        |
| 36        | 13.874      | 2001          | 2004        | 2014         | rVB      | 163896         | 202370        | 7.11%           | 0.733%        |

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ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
1-S-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-BF061224.M  
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

|    |        |      |      |      |     |         |         |        |        |
|----|--------|------|------|------|-----|---------|---------|--------|--------|
| 37 | 14.033 | 2026 | 2031 | 2034 | rBV | 1461690 | 1391677 | 48.89% | 5.038% |
| 38 | 14.057 | 2034 | 2035 | 2040 | rVB | 163360  | 116653  | 4.10%  | 0.422% |
| 39 | 15.074 | 2204 | 2208 | 2211 | rBV | 118433  | 181617  | 6.38%  | 0.658% |
| 40 | 15.439 | 2267 | 2270 | 2276 | rVB | 87364   | 108669  | 3.82%  | 0.393% |
| 41 | 15.504 | 2277 | 2281 | 2285 | rBV | 740531  | 856902  | 30.10% | 3.102% |

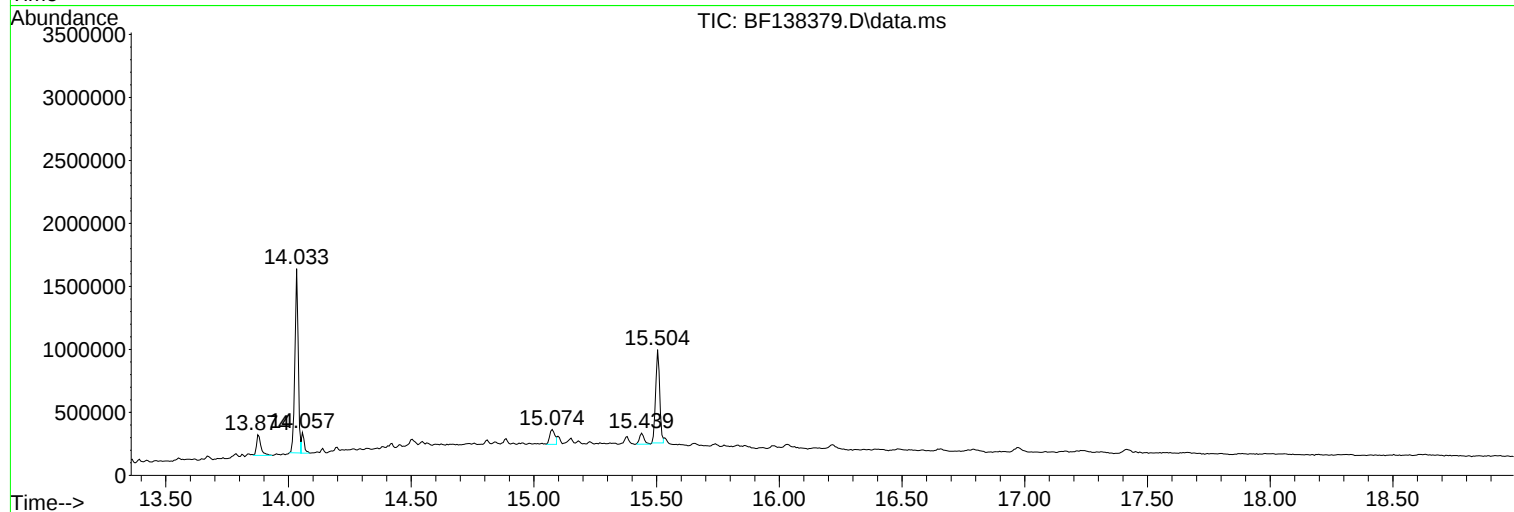
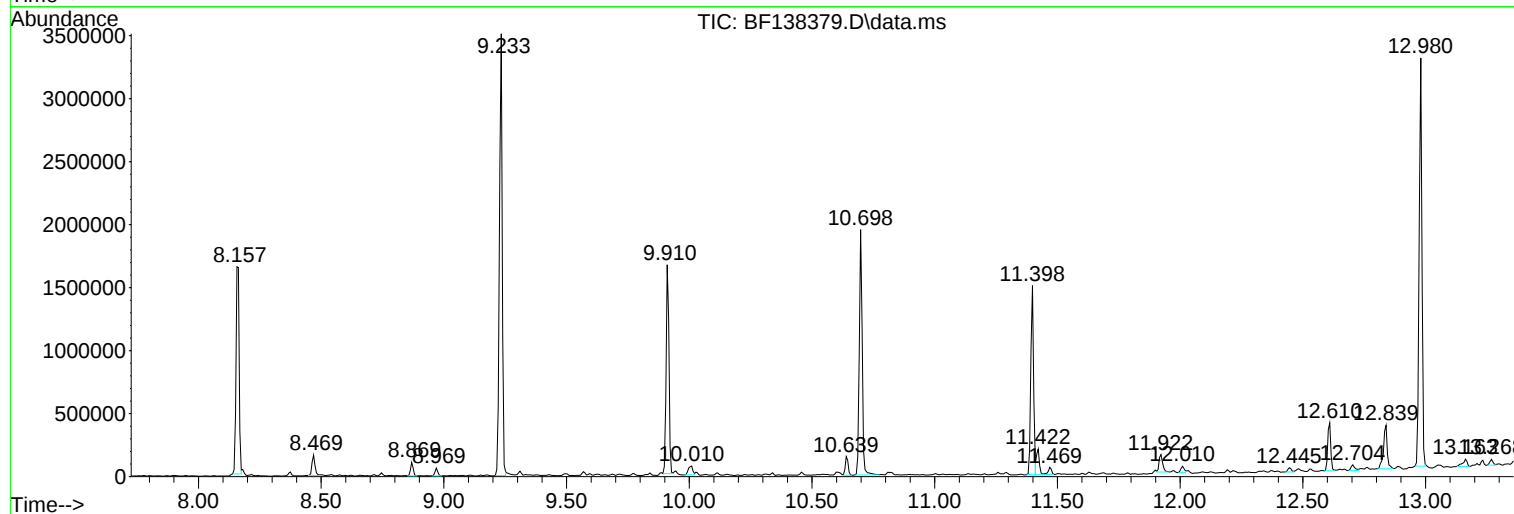
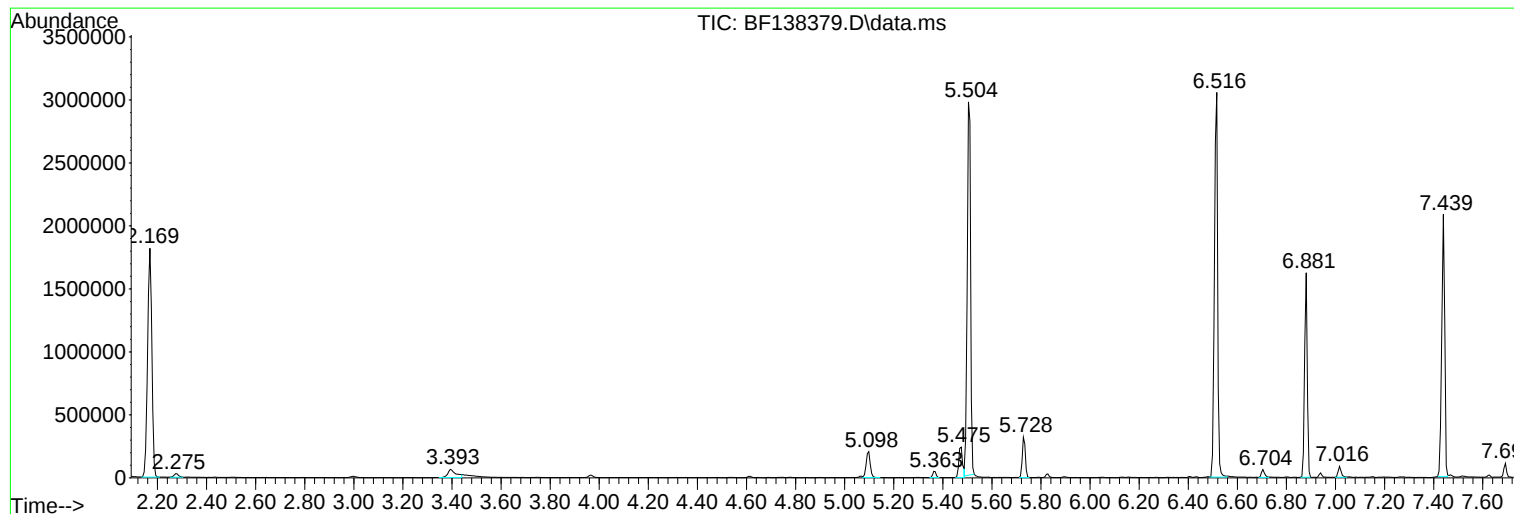
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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF061224.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Sample : P3077-07  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
1-S-1

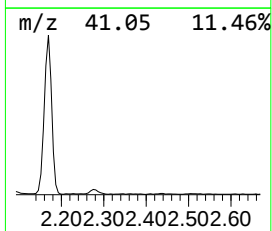
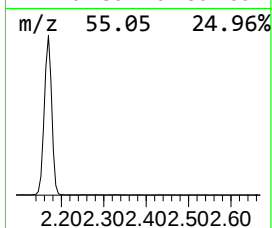
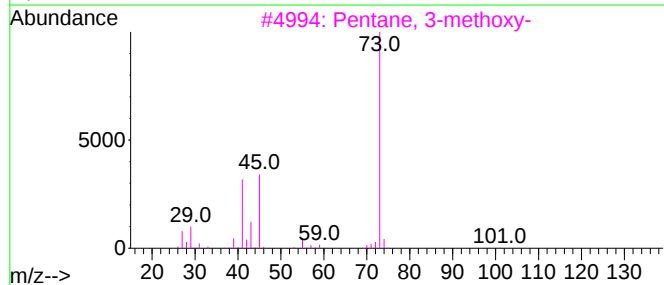
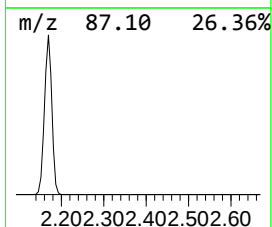
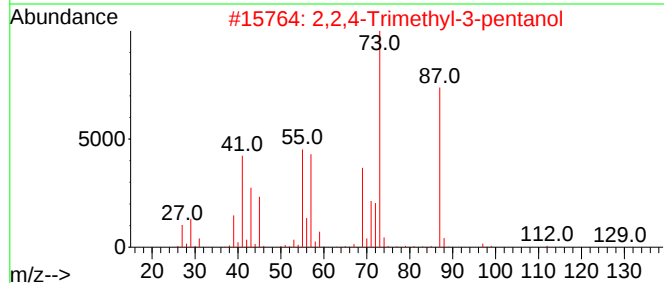
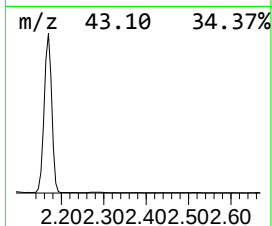
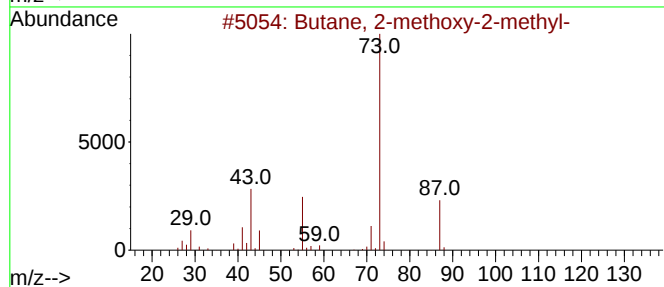
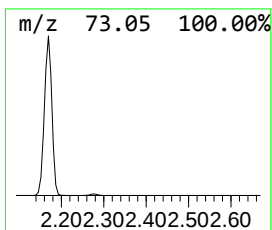
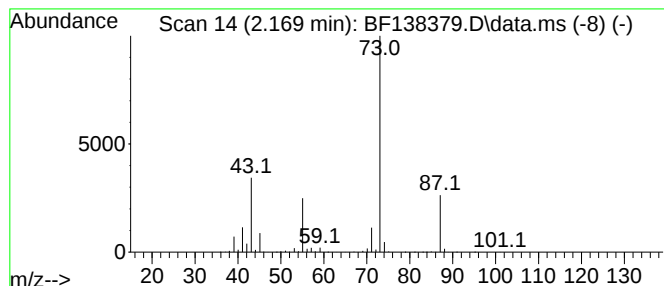
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.  |
|-------|----------|---------|------------------------|-------|
| 2.169 | 35.79 ng | 2207320 | 1,4-Dichlorobenzene-d4 | 6.881 |

| 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    |    |   | Pentane, 3-methoxy-         | 102 | C6H14O  | 036839-67-5 | 23   |
| 4    |    |   | Borane, dimethoxy-          | 74  | C2H7BO2 | 004542-61-4 | 9    |
| 5    |    |   | Silane, tetramethyl-        | 88  | C4H12Si | 000075-76-3 | 9    |



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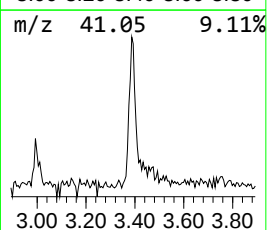
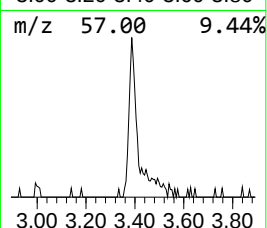
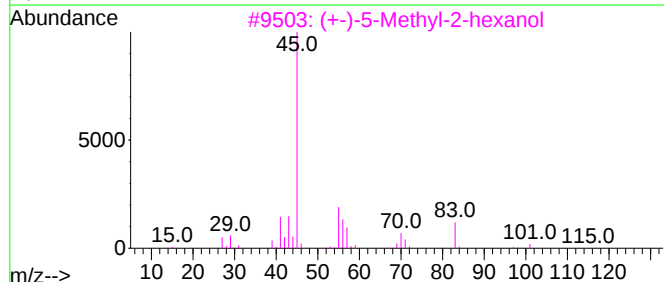
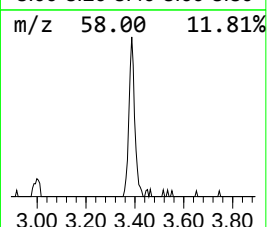
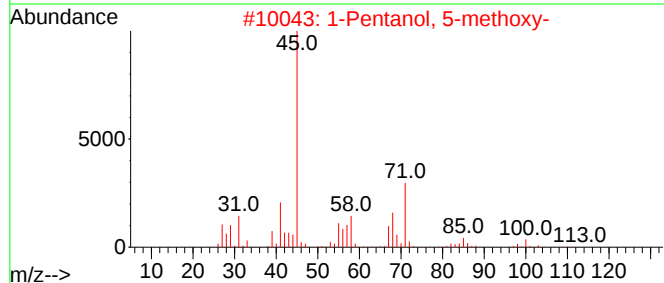
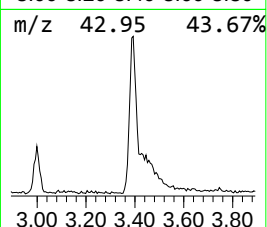
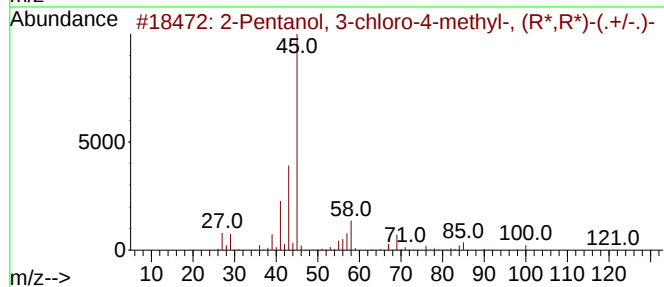
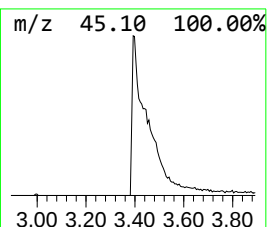
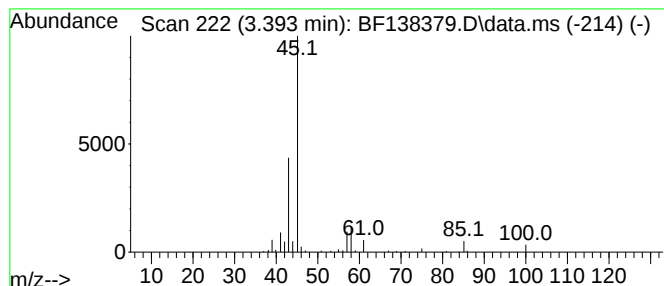
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 unknown3.393 Concentration Rank 5

| R.T.  | EstConc | Area   | Relative to ISTD       | R.T.  |
|-------|---------|--------|------------------------|-------|
| 3.393 | 2.49 ng | 153822 | 1,4-Dichlorobenzene-d4 | 6.881 |

| Hit# | of 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|------|-------------------------------------|-----|----------|-------------|------|
| 1    |      | 2-Pentanol, 3-chloro-4-methyl-, ... | 136 | C6H13ClO | 074685-47-5 | 43   |
| 2    |      | 1-Pentanol, 5-methoxy-              | 118 | C6H14O2  | 004799-62-6 | 39   |
| 3    |      | (+)-5-Methyl-2-hexanol              | 116 | C7H16O   | 111768-09-3 | 36   |
| 4    |      | Propane, 2-ethoxy-                  | 88  | C5H12O   | 000625-54-7 | 36   |
| 5    |      | 2-Pentanol, 3-chloro-4-methyl-, ... | 136 | C6H13ClO | 074685-48-6 | 28   |



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Instrument :  
BNA\_F  
ClientSampleId :  
1-S-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF061224.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

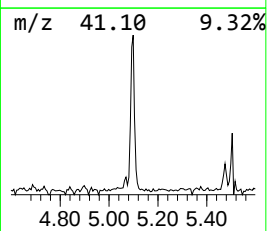
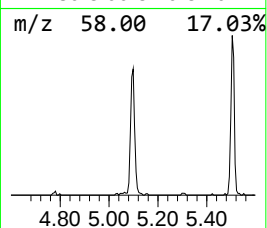
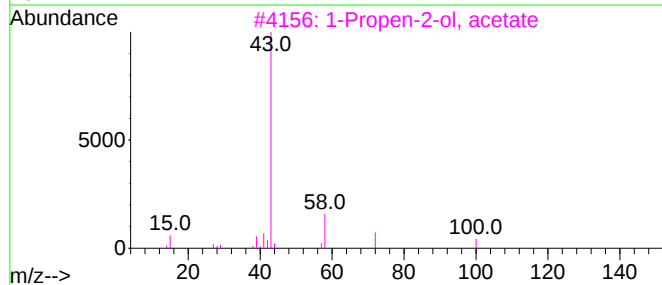
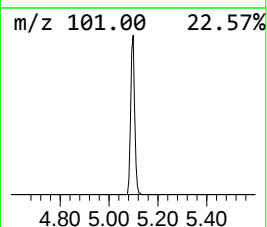
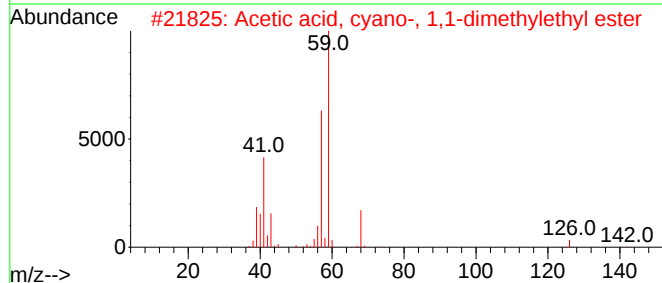
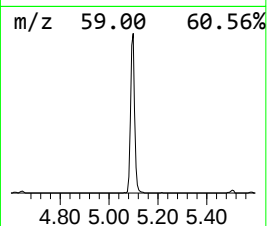
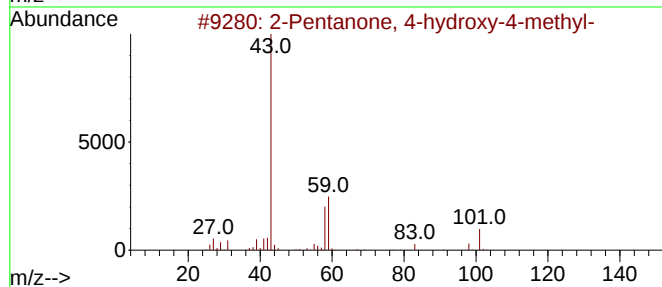
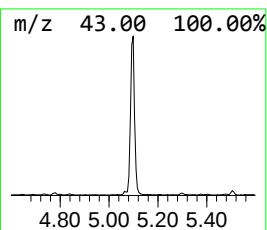
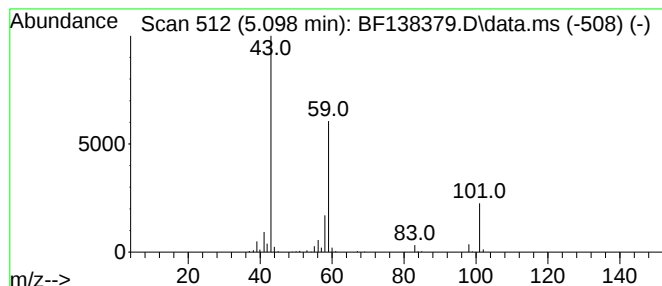
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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

| R.T.  | EstConc | Area   | Relative to ISTD       | R.T.  |
|-------|---------|--------|------------------------|-------|
| 5.098 | 3.84 ng | 236585 | 1,4-Dichlorobenzene-d4 | 6.881 |

| 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 | 17   |
| 3    |      | 1-Propen-2-ol, acetate              | 100 | C5H8O2   | 000108-22-5 | 10   |
| 4    |      | Butane                              | 58  | C4H10    | 000106-97-8 | 9    |
| 5    |      | Morpholine, 4-methyl-               | 101 | C5H11NO  | 000109-02-4 | 9    |



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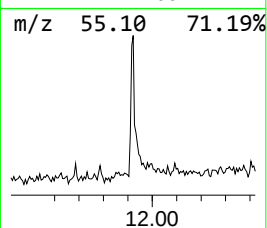
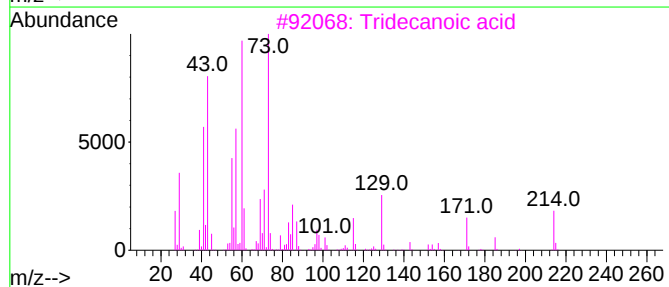
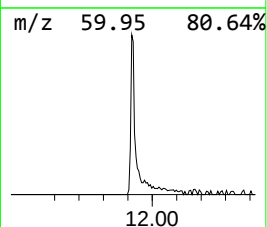
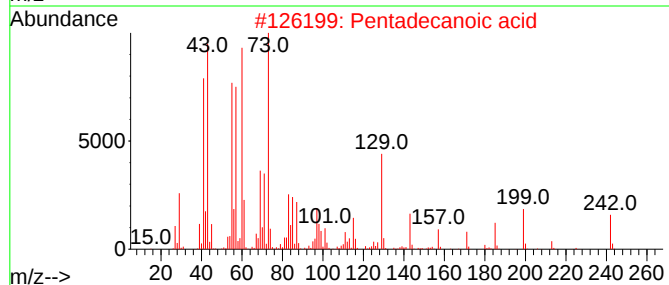
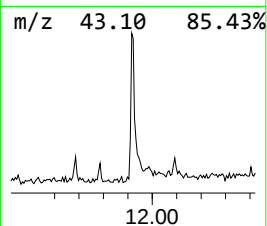
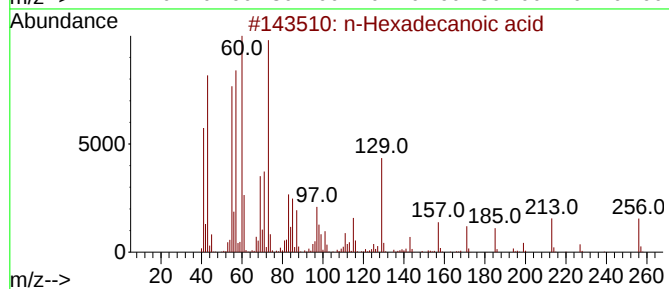
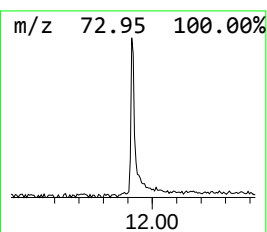
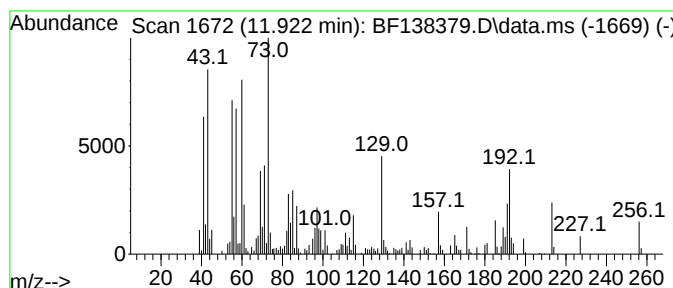
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF061224.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 11.922 | 2.34 ng | 139210 | Phenanthrene-d10 | 11.398 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 99   |
| 2    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 64   |
| 3    |    |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 60   |
| 4    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 58   |
| 5    |    |   | n-Decanoic acid     | 172 | C10H20O2 | 000334-48-5 | 55   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF062724\  
Data File : BF138379.D  
Acq On : 27 Jun 2024 21:38  
Operator : CG\JU  
Sample : P3077-07  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
1-S-1

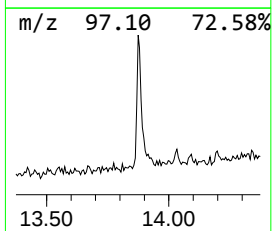
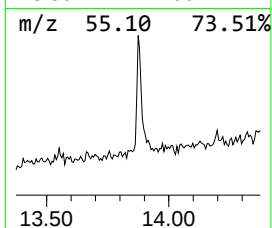
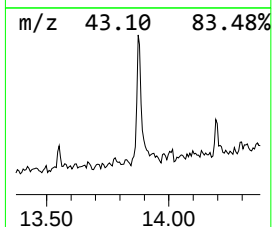
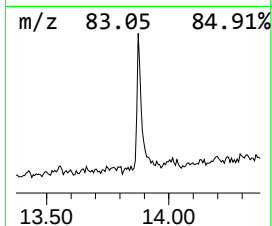
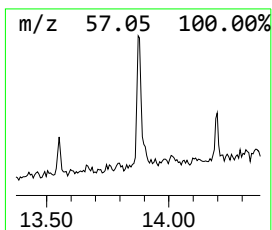
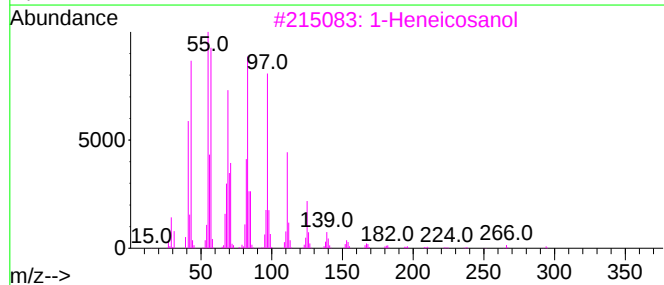
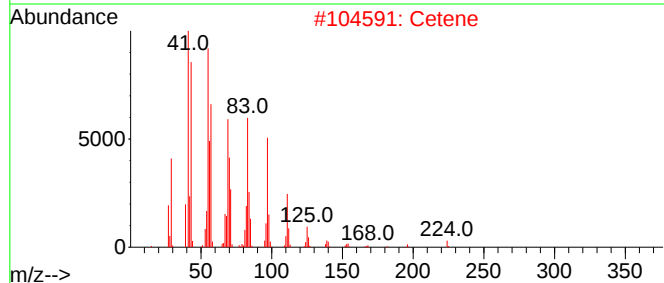
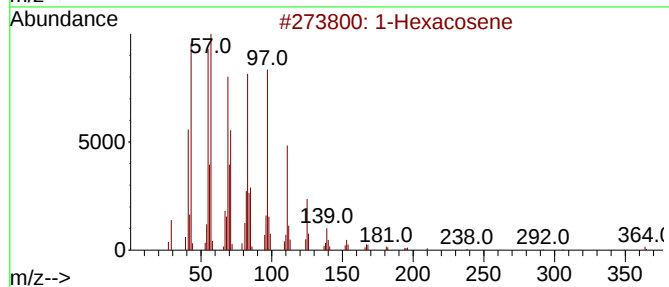
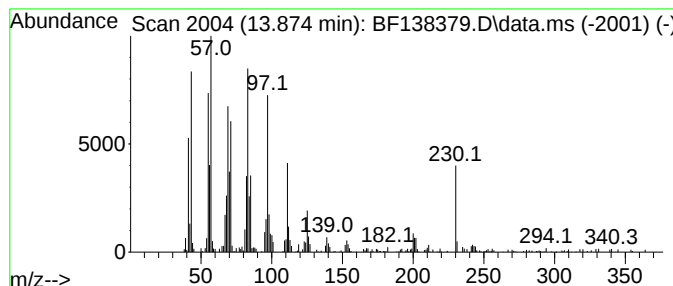
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 6 1-Hexacosene Concentration Rank 4

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 13.874 | 2.91 ng | 202370 | Chrysene-d12     | 14.033 |

| Hit# | of                          | 5 | Tentative ID | MW  | MolForm    | CAS#         | Qual |
|------|-----------------------------|---|--------------|-----|------------|--------------|------|
| 1    | 1-Hexacosene                |   |              | 364 | C26H52     | 018835-33-1  | 99   |
| 2    | Cetene                      |   |              | 224 | C16H32     | 000629-73-2  | 95   |
| 3    | 1-Heneicosanol              |   |              | 312 | C21H44O    | 015594-90-8  | 93   |
| 4    | n-Heptadecanol-1            |   |              | 256 | C17H36O    | 001454-85-9  | 93   |
| 5    | Heptadecyl trifluoroacetate |   |              | 352 | C19H35F3O2 | 1010351-87-0 | 91   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF062724\  
Data File : BF138379.D  
Acq On : 27 Jun 2024 21:38  
Operator : CG\JU  
Sample : P3077-07  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
1-S-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF061224.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... | 2.169  | 35.8    | ng    | 2207320  | 1                     | 6.881  | 1233330 | 20.0 |
| unknown3.393       | 3.393  | 2.5     | ng    | 153822   | 1                     | 6.881  | 1233330 | 20.0 |
| 2-Pentanone, 4-... | 5.098  | 3.8     | ng    | 236585   | 1                     | 6.881  | 1233330 | 20.0 |
| n-Hexadecanoic ... | 11.922 | 2.3     | ng    | 139210   | 4                     | 11.398 | 1188840 | 20.0 |
| 1-Hexacosene       | 13.874 | 2.9     | ng    | 202370   | 5                     | 14.033 | 1391680 | 20.0 |