

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122719\  
 Data File : BF118353.D  
 Acq On : 27 Dec 2019 22:27  
 Operator : JU  
 Sample : K6443-03 2X  
 Misc :  
 ALS Vial : 21 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 PH-3

Integration Parameters: rteint.p  
 Integrator: RTE  
 Smoothing : ON  
 Sampling : 1  
 Start Thrs: 0.2  
 Stop Thrs : 0  
 Filtering: 5  
 Min Area: 3 % of largest Peak  
 Max Peaks: 100  
 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-BF122419.M  
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

| 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         | 4.428       | 394           | 398         | 405          | rBV      | 45227          | 62390         | 3.83%           | 0.347%        |
| 2         | 5.051       | 500           | 504         | 518          | rVB      | 233965         | 279868        | 17.16%          | 1.557%        |
| 3         | 5.469       | 571           | 575         | 584          | rBV      | 1143939        | 1165492       | 71.48%          | 6.485%        |
| 4         | 6.487       | 744           | 748         | 762          | rBV      | 1225431        | 1287490       | 78.96%          | 7.164%        |
| 5         | 6.622       | 767           | 771         | 778          | rVV      | 1710363        | 1408489       | 86.38%          | 7.837%        |
| 6         | 6.675       | 778           | 780         | 787          | rVB2     | 15804          | 22026         | 1.35%           | 0.123%        |
| 7         | 6.851       | 807           | 810         | 817          | rBV      | 948653         | 789252        | 48.40%          | 4.391%        |
| 8         | 7.010       | 833           | 837         | 850          | rBV      | 1234516        | 1110377       | 68.10%          | 6.178%        |
| 9         | 7.416       | 902           | 906         | 918          | rBV      | 816641         | 774100        | 47.47%          | 4.307%        |
| 10        | 8.139       | 1025          | 1029        | 1041         | rVB      | 1119073        | 999872        | 61.32%          | 5.563%        |
| 11        | 8.857       | 1148          | 1151        | 1158         | rBV      | 27777          | 27215         | 1.67%           | 0.151%        |
| 12        | 8.957       | 1163          | 1168        | 1175         | rBV      | 22153          | 22323         | 1.37%           | 0.124%        |
| 13        | 9.216       | 1208          | 1212        | 1223         | rBV      | 1965255        | 1630583       | 100.00%         | 9.073%        |
| 14        | 9.610       | 1277          | 1279        | 1288         | rVB      | 85141          | 95534         | 5.86%           | 0.532%        |
| 15        | 9.763       | 1301          | 1305        | 1310         | rBV      | 37263          | 34034         | 2.09%           | 0.189%        |
| 16        | 9.827       | 1310          | 1316        | 1322         | rBV2     | 17711          | 21818         | 1.34%           | 0.121%        |
| 17        | 9.898       | 1325          | 1328        | 1337         | rVB      | 1153495        | 1091955       | 66.97%          | 6.076%        |
| 18        | 10.327      | 1394          | 1401        | 1403         | rBV3     | 21186          | 27516         | 1.69%           | 0.153%        |
| 19        | 10.692      | 1460          | 1463        | 1475         | rBV      | 904152         | 904499        | 55.47%          | 5.033%        |
| 20        | 10.816      | 1478          | 1484        | 1489         | rVB5     | 26273          | 42391         | 2.60%           | 0.236%        |
| 21        | 11.398      | 1579          | 1583        | 1585         | rBV      | 1037870        | 1006665       | 61.74%          | 5.601%        |
| 22        | 11.416      | 1585          | 1586        | 1590         | rVB      | 82551          | 63835         | 3.91%           | 0.355%        |
| 23        | 11.674      | 1626          | 1630        | 1635         | rVB6     | 18440          | 24430         | 1.50%           | 0.136%        |
| 24        | 11.916      | 1666          | 1671        | 1679         | rBV3     | 127264         | 209282        | 12.83%          | 1.164%        |
| 25        | 12.010      | 1684          | 1687        | 1690         | rVV2     | 44253          | 54886         | 3.37%           | 0.305%        |
| 26        | 12.033      | 1690          | 1691        | 1694         | rVV2     | 29393          | 21648         | 1.33%           | 0.120%        |
| 27        | 12.086      | 1697          | 1700        | 1705         | rBV5     | 20134          | 25095         | 1.54%           | 0.140%        |
| 28        | 12.451      | 1759          | 1762        | 1764         | rBV      | 46064          | 39456         | 2.42%           | 0.220%        |
| 29        | 12.480      | 1764          | 1767        | 1770         | rVV3     | 27992          | 38040         | 2.33%           | 0.212%        |
| 30        | 12.539      | 1774          | 1777        | 1786         | rVB10    | 18129          | 33551         | 2.06%           | 0.187%        |
| 31        | 12.616      | 1786          | 1790        | 1794         | rBV      | 125553         | 120063        | 7.36%           | 0.668%        |
| 32        | 12.710      | 1803          | 1806        | 1811         | rBV2     | 38428          | 39634         | 2.43%           | 0.221%        |
| 33        | 12.845      | 1823          | 1829        | 1835         | rBV      | 162132         | 189832        | 11.64%          | 1.056%        |
| 34        | 12.898      | 1835          | 1838        | 1842         | rVB2     | 25427          | 32552         | 2.00%           | 0.181%        |

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Misc :  
ALS Vial : 21 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PH-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-BF122419.M  
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

|    |        |      |      |      |      |         |         |        |        |
|----|--------|------|------|------|------|---------|---------|--------|--------|
| 35 | 12.980 | 1849 | 1852 | 1856 | rBV  | 1732047 | 1589389 | 97.47% | 8.843% |
| 36 | 13.057 | 1863 | 1865 | 1867 | rBV2 | 22221   | 24651   | 1.51%  | 0.137% |
| 37 | 13.174 | 1879 | 1885 | 1887 | rBV  | 40057   | 54773   | 3.36%  | 0.305% |
| 38 | 13.280 | 1900 | 1903 | 1907 | rBV2 | 33855   | 29445   | 1.81%  | 0.164% |
| 39 | 13.404 | 1921 | 1924 | 1926 | rBV  | 33818   | 26752   | 1.64%  | 0.149% |
| 40 | 13.551 | 1947 | 1949 | 1952 | rBV3 | 23266   | 21775   | 1.34%  | 0.121% |
| 41 | 13.874 | 2001 | 2004 | 2012 | rBV3 | 160739  | 246449  | 15.11% | 1.371% |
| 42 | 14.051 | 2029 | 2034 | 2037 | rBV  | 1143197 | 1116948 | 68.50% | 6.215% |
| 43 | 14.074 | 2037 | 2038 | 2042 | rVB  | 87295   | 54677   | 3.35%  | 0.304% |
| 44 | 14.504 | 2109 | 2111 | 2114 | rBV3 | 72994   | 67282   | 4.13%  | 0.374% |
| 45 | 14.892 | 2174 | 2177 | 2180 | rVB  | 70824   | 64571   | 3.96%  | 0.359% |
| 46 | 15.545 | 2283 | 2288 | 2296 | rBV  | 715828  | 979662  | 60.08% | 5.451% |

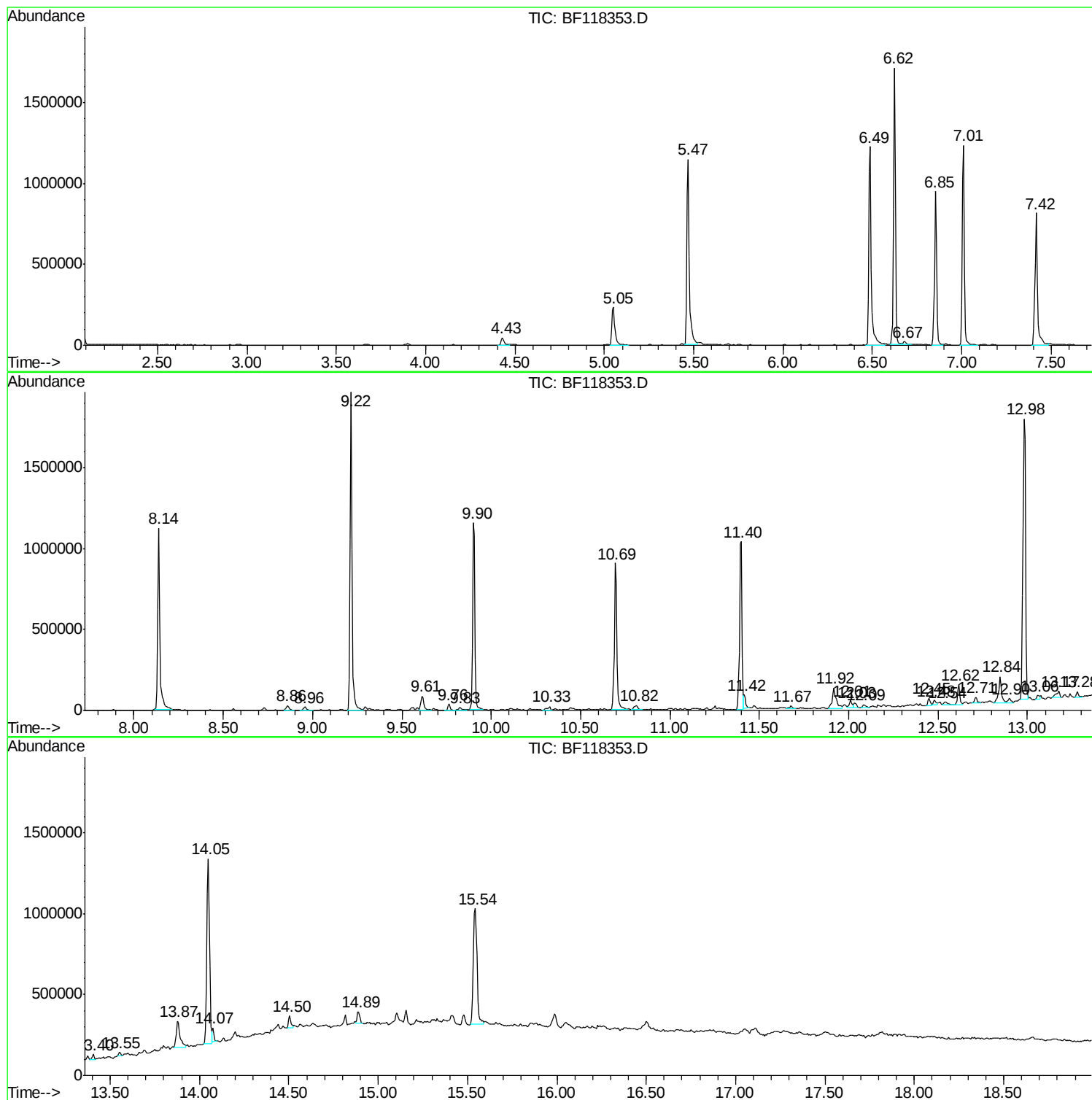
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BNA\_F  
ClientSampled :  
PH-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF122419.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P



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ALS Vial : 21 Sample Multiplier: 1

Instrument :  
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ClientSampleId :  
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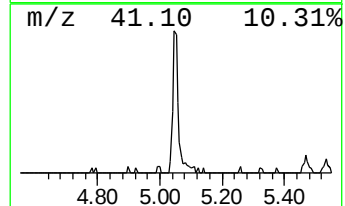
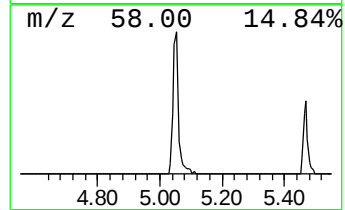
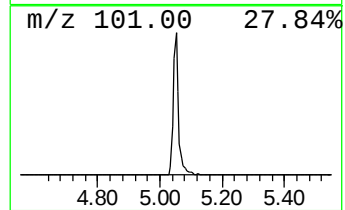
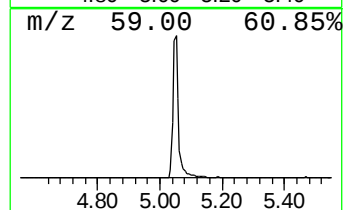
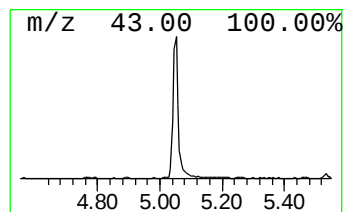
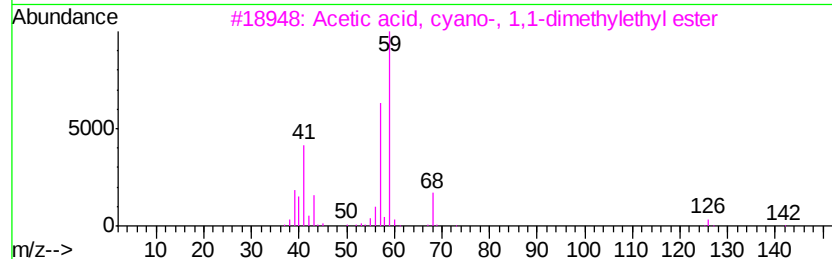
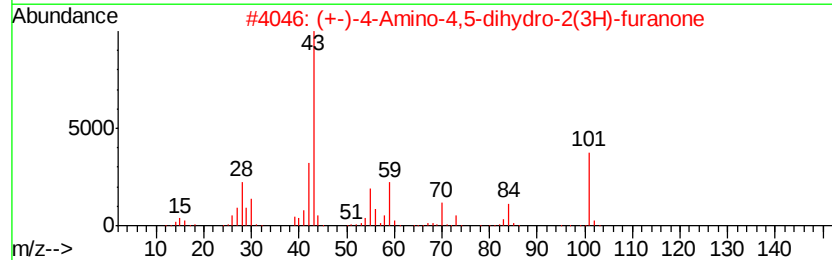
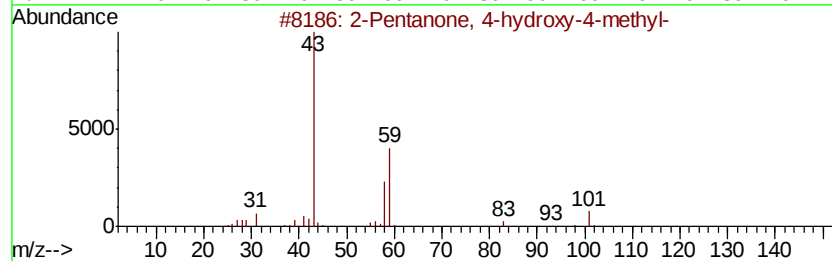
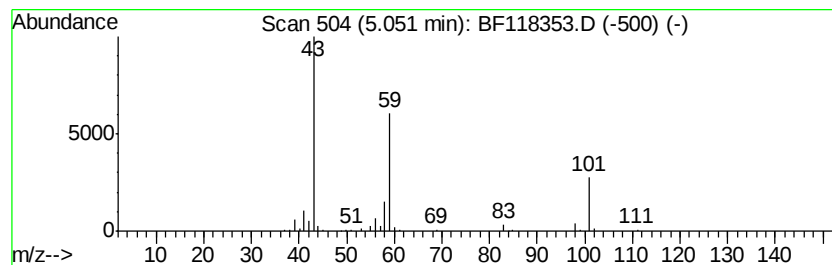
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T. | EstConc | Area   | Relative to ISTD       | R.T. |
|------|---------|--------|------------------------|------|
| 5.05 | 7.09 ng | 279868 | 1,4-Dichlorobenzene-d4 | 6.85 |

| Hit# | of | Tentative ID                           | MW  | MolForm  | CAS#        | Qual |
|------|----|----------------------------------------|-----|----------|-------------|------|
| 1    | 5  | 2-Pentanone, 4-hydroxy-4-methyl-       | 116 | C6H12O2  | 000123-42-2 | 50   |
| 2    |    | (+)-4-Amino-4,5-dihydro-2(3H)-furanone | 101 | C4H7NO2  | 016504-58-8 | 28   |
| 3    |    | Acetic acid, cyano-, 1,1-dimethyl-     | 141 | C7H11NO2 | 001116-98-9 | 25   |
| 4    |    | 2-Hexanol, 2-methyl-                   | 116 | C7H16O   | 000625-23-0 | 25   |
| 5    |    | 2,3-Butanedione, monooxime             | 101 | C4H7NO2  | 000057-71-6 | 17   |



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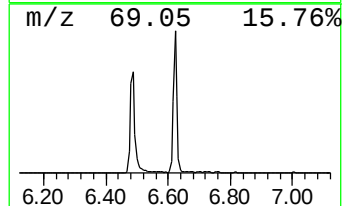
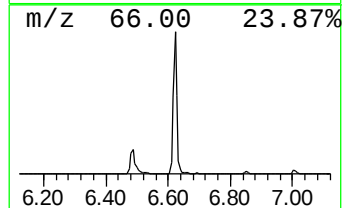
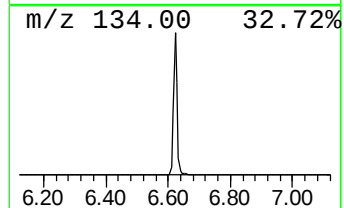
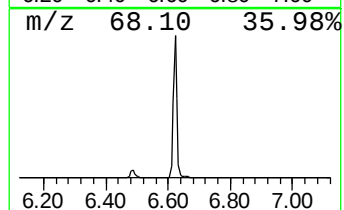
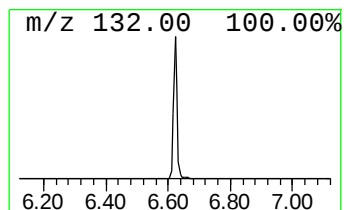
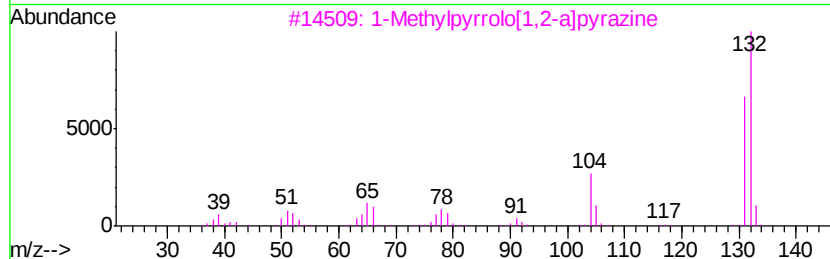
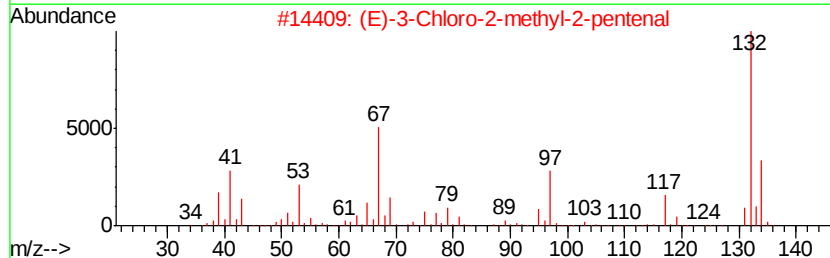
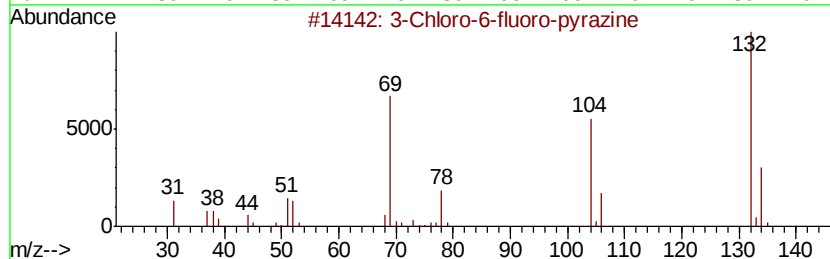
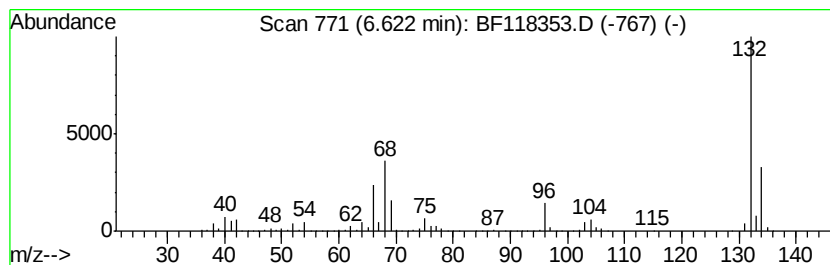
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 2 unknown6.62 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.62 | 35.69 ng | 1408490 | 1,4-Dichlorobenzene-d4 | 6.85 |

| Hit# | of | Tentative ID                     | MW  | MolForm   | CAS#         | Qual |
|------|----|----------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 3-Chloro-6-fluoro-pyrazine       | 132 | C4H2ClFN2 | 1000146-10-7 | 35   |
| 2    |    | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO   | 031357-76-3  | 25   |
| 3    |    | 1-Methylpyrrolo[1,2-a]pyrazine   | 132 | C8H8N2    | 064608-59-9  | 9    |
| 4    |    | Cyclopropanamine, 1-phenyl-      | 133 | C9H11N    | 1000351-26-2 | 9    |
| 5    |    | 5-Fluoro-2-chloropyrimidine      | 132 | C4H2ClFN2 | 062802-42-0  | 9    |



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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF122419.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

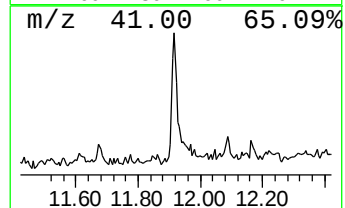
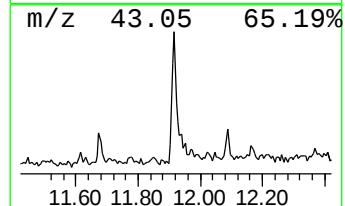
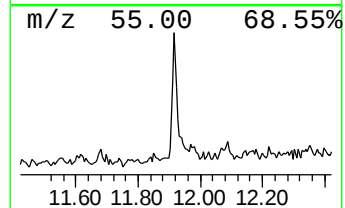
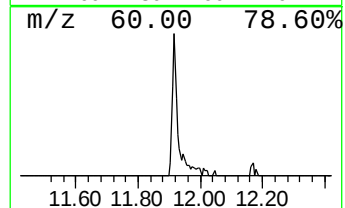
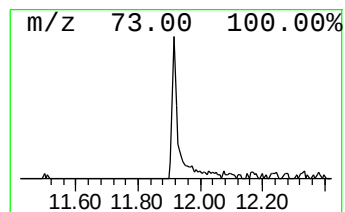
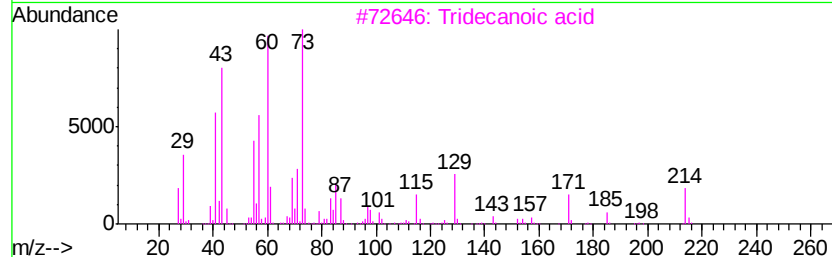
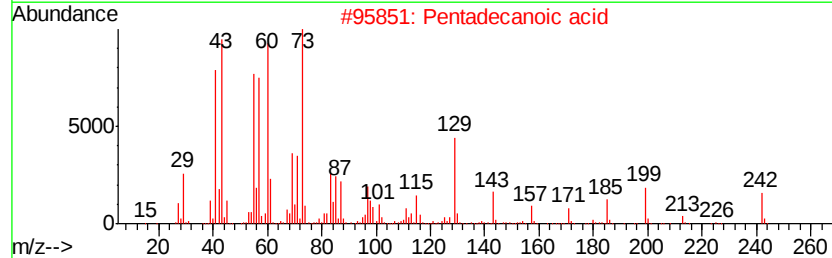
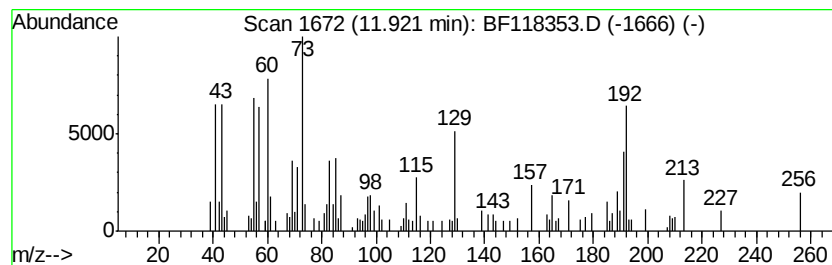
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 11.92 | 4.16 ng | 209282 | Phenanthrene-d10 | 11.40 |

| Hit# of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|---------|---|---------------------|-----|----------|-------------|------|
| 1       |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 98   |
| 2       |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 81   |
| 3       |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 81   |
| 4       |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 72   |
| 5       |   | Dodecanoic acid     | 200 | C12H24O2 | 000143-07-7 | 59   |



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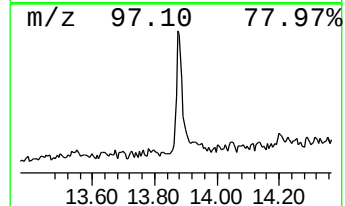
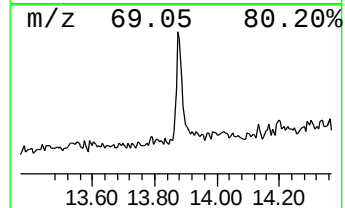
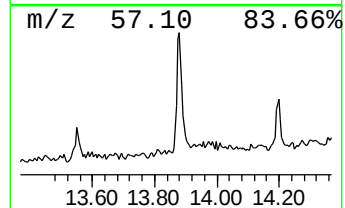
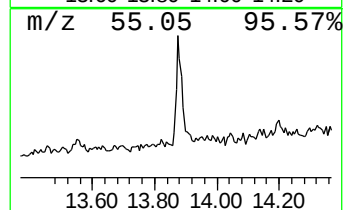
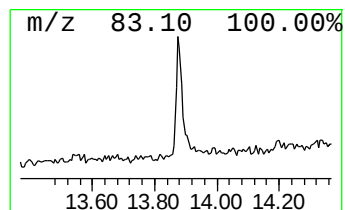
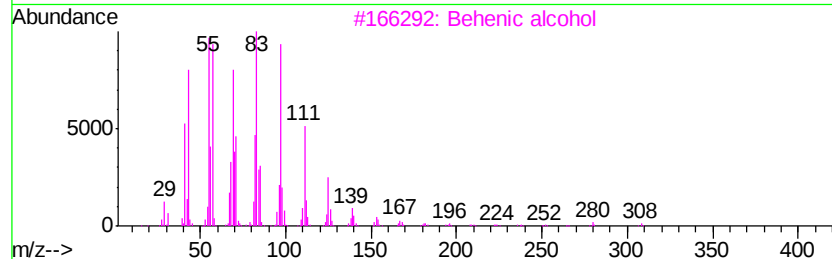
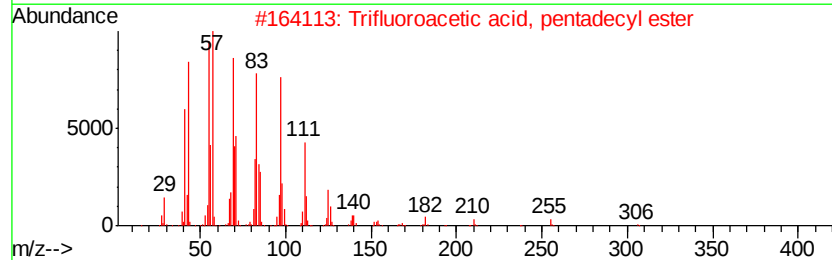
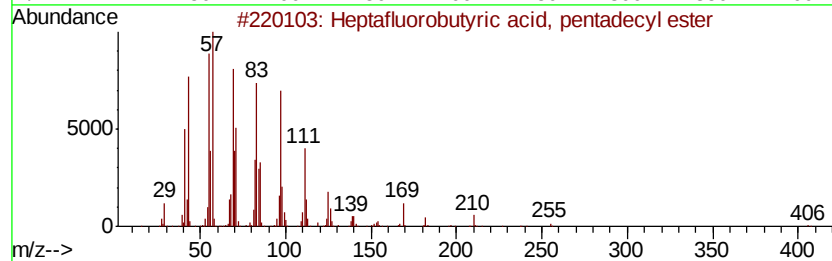
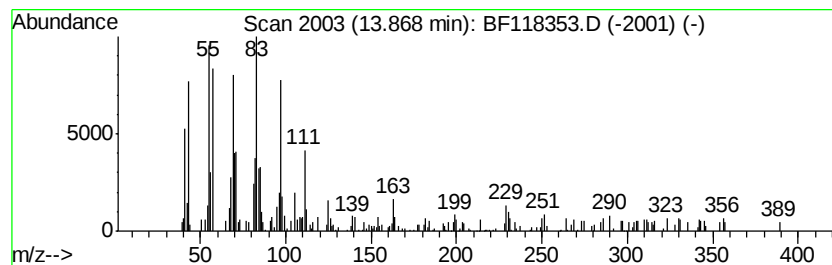
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 7 Heptafluorobutyric acid, pe... Concentration Rank 4

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 13.87 | 4.41 ng | 246449 | Chrysene-d12     | 14.05 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|------------|-------------|------|
| 1    |    |   | Heptafluorobutyric acid, pentade... | 424 | C19H31F7O2 | 959261-23-5 | 94   |
| 2    |    |   | Trifluoroacetic acid, pentadecyl... | 324 | C17H31F3O2 | 959010-23-2 | 91   |
| 3    |    |   | Behenic alcohol                     | 326 | C22H46O    | 000661-19-8 | 90   |
| 4    |    |   | 1-Docosene                          | 308 | C22H44     | 001599-67-3 | 90   |
| 5    |    |   | 1-Heneicosanol                      | 312 | C21H44O    | 015594-90-8 | 90   |



Data Path : Z:\SVOASRV\HPCHEM1\BNA\_F\DATA\BF122719\  
Data File : BF118353.D  
Acq On : 27 Dec 2019 22:27  
Operator : JU  
Sample : K6443-03 2X  
Misc :  
ALS Vial : 21 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PH-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF122419.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |         |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|---------|------|
|                      |       |         |       |          | #                     | RT    | Resp    | Conc |
| 2-Pentanone, 4-hy... | 5.05  | 7.1 ng  |       | 279868   | 1                     | 6.85  | 789252  | 20.0 |
| unknown6.62          | 6.62  | 35.7 ng |       | 1408490  | 1                     | 6.85  | 789252  | 20.0 |
| n-Hexadecanoic acid  | 11.92 | 4.2 ng  |       | 209282   | 4                     | 11.40 | 1006670 | 20.0 |
| Heptafluorobutyri... | 13.87 | 4.4 ng  |       | 246449   | 5                     | 14.05 | 1116950 | 20.0 |