

Data Path : Z:\HPCHEM1\BNA F\DATA\BF032918\  
 Data File : BF104047.D  
 Acq On : 29 Mar 2018 13:37  
 Operator : JU/SJ  
 Sample : J1754-15 5X  
 Misc :  
 ALS Vial : 5 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 CL-02-032718-C

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:\HPCHEM1\BNA\_F\METHODS\8270-BF032818.M  
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|--------|----------|------------|----------|-----------|-------|-------------|------------|--------------|------------|
| 1      | 2.246    | 24         | 27       | 38        | rVB   | 21741       | 36877      | 3.73%        | 0.321%     |
| 2      | 5.187    | 524        | 527      | 535       | rVB   | 11218       | 13709      | 1.39%        | 0.119%     |
| 3      | 5.598    | 593        | 597      | 613       | rBV   | 73632       | 257339     | 26.06%       | 2.240%     |
| 4      | 6.598    | 764        | 767      | 787       | rBV   | 110701      | 423281     | 42.86%       | 3.685%     |
| 5      | 6.733    | 787        | 790      | 812       | rVB   | 250362      | 495024     | 50.13%       | 4.310%     |
| 6      | 6.963    | 826        | 829      | 852       | rBV   | 347068      | 608981     | 61.67%       | 5.302%     |
| 7      | 7.116    | 852        | 855      | 870       | rVV   | 292593      | 417912     | 42.32%       | 3.638%     |
| 8      | 7.216    | 870        | 872      | 880       | rVB5  | 11003       | 18602      | 1.88%        | 0.162%     |
| 9      | 7.533    | 922        | 926      | 941       | rBV2  | 92455       | 269850     | 27.33%       | 2.349%     |
| 10     | 8.245    | 1043       | 1047     | 1071      | rBV   | 590435      | 891730     | 90.30%       | 7.764%     |
| 11     | 8.816    | 1139       | 1144     | 1148      | rBV5  | 10457       | 15043      | 1.52%        | 0.131%     |
| 12     | 9.063    | 1182       | 1186     | 1190      | rVB3  | 8814        | 11907      | 1.21%        | 0.104%     |
| 13     | 9.245    | 1215       | 1217     | 1222      | rVB3  | 11695       | 10172      | 1.03%        | 0.089%     |
| 14     | 9.316    | 1225       | 1229     | 1238      | rBV   | 522614      | 668319     | 67.68%       | 5.819%     |
| 15     | 9.380    | 1238       | 1240     | 1244      | rVB2  | 25080       | 30323      | 3.07%        | 0.264%     |
| 16     | 9.704    | 1290       | 1295     | 1303      | rBV2  | 32572       | 57652      | 5.84%        | 0.502%     |
| 17     | 9.857    | 1318       | 1321     | 1326      | rBV5  | 10330       | 20578      | 2.08%        | 0.179%     |
| 18     | 9.910    | 1327       | 1330     | 1334      | rVB   | 39943       | 36435      | 3.69%        | 0.317%     |
| 19     | 10.004   | 1342       | 1346     | 1359      | rBV   | 889704      | 987488     | 100.00%      | 8.597%     |
| 20     | 10.233   | 1382       | 1385     | 1389      | rBV3  | 10430       | 14349      | 1.45%        | 0.125%     |
| 21     | 10.410   | 1410       | 1415     | 1418      | rBV2  | 93880       | 110378     | 11.18%       | 0.961%     |
| 22     | 10.533   | 1432       | 1436     | 1439      | rBV6  | 12824       | 22409      | 2.27%        | 0.195%     |
| 23     | 10.569   | 1439       | 1442     | 1445      | rVB5  | 8718        | 11525      | 1.17%        | 0.100%     |
| 24     | 10.627   | 1449       | 1452     | 1456      | rBV   | 28273       | 34892      | 3.53%        | 0.304%     |
| 25     | 10.798   | 1477       | 1481     | 1493      | rBV   | 250884      | 376476     | 38.12%       | 3.278%     |
| 26     | 10.886   | 1493       | 1496     | 1501      | rVB2  | 45211       | 69342      | 7.02%        | 0.604%     |
| 27     | 11.110   | 1531       | 1534     | 1536      | rVB3  | 13330       | 14182      | 1.44%        | 0.123%     |
| 28     | 11.133   | 1536       | 1538     | 1541      | rBV4  | 10159       | 14020      | 1.42%        | 0.122%     |
| 29     | 11.333   | 1570       | 1572     | 1574      | rBV   | 34944       | 27102      | 2.74%        | 0.236%     |
| 30     | 11.363   | 1574       | 1577     | 1580      | rVB   | 31996       | 27648      | 2.80%        | 0.241%     |
| 31     | 11.498   | 1596       | 1600     | 1612      | rBV   | 734140      | 974968     | 98.73%       | 8.488%     |
| 32     | 11.580   | 1612       | 1614     | 1617      | rVB4  | 10435       | 12183      | 1.23%        | 0.106%     |
| 33     | 11.763   | 1643       | 1645     | 1648      | rVB   | 30721       | 25036      | 2.54%        | 0.218%     |
| 34     | 11.833   | 1654       | 1657     | 1659      | rBV4  | 16120       | 15378      | 1.56%        | 0.134%     |

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ALS Vial : 5 Sample Multiplier: 1

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BNA\_F  
ClientSampleId :  
CL-02-032718-C

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:\HPCHEM1\BNA\_F\METHODS\8270-BF032818.M  
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

|    |        |      |      |      |      |        |        |        |        |
|----|--------|------|------|------|------|--------|--------|--------|--------|
| 35 | 11.863 | 1659 | 1662 | 1668 | rVB  | 232946 | 197082 | 19.96% | 1.716% |
| 36 | 12.004 | 1683 | 1686 | 1688 | rBV3 | 26034  | 32568  | 3.30%  | 0.284% |
| 37 | 12.115 | 1702 | 1705 | 1707 | rBV4 | 11771  | 12946  | 1.31%  | 0.113% |
| 38 | 12.168 | 1712 | 1714 | 1717 | rBV  | 24821  | 22093  | 2.24%  | 0.192% |
| 39 | 12.327 | 1738 | 1741 | 1747 | rVB8 | 18543  | 30693  | 3.11%  | 0.267% |
| 40 | 12.557 | 1776 | 1780 | 1781 | rBV  | 827024 | 778286 | 78.81% | 6.776% |
| 41 | 12.574 | 1781 | 1783 | 1791 | rVV2 | 559459 | 558853 | 56.59% | 4.866% |
| 42 | 12.657 | 1794 | 1797 | 1802 | rVB  | 104231 | 102605 | 10.39% | 0.893% |
| 43 | 12.715 | 1804 | 1807 | 1815 | rVV  | 92749  | 121128 | 12.27% | 1.055% |
| 44 | 12.880 | 1832 | 1835 | 1839 | rVB2 | 74724  | 77866  | 7.89%  | 0.678% |
| 45 | 12.951 | 1844 | 1847 | 1852 | rVB  | 98402  | 126764 | 12.84% | 1.104% |
| 46 | 13.080 | 1865 | 1869 | 1880 | rVB  | 562194 | 579235 | 58.66% | 5.043% |
| 47 | 13.286 | 1902 | 1904 | 1907 | rVB  | 42339  | 33118  | 3.35%  | 0.288% |
| 48 | 13.586 | 1953 | 1955 | 1958 | rVB2 | 55547  | 48625  | 4.92%  | 0.423% |
| 49 | 13.627 | 1960 | 1962 | 1965 | rBV  | 58594  | 60728  | 6.15%  | 0.529% |
| 50 | 13.957 | 2016 | 2018 | 2022 | rBV2 | 75774  | 73365  | 7.43%  | 0.639% |
| 51 | 14.151 | 2047 | 2051 | 2061 | rBV  | 589735 | 812406 | 82.27% | 7.073% |
| 52 | 14.280 | 2071 | 2073 | 2076 | rVB  | 68006  | 50200  | 5.08%  | 0.437% |
| 53 | 14.592 | 2123 | 2126 | 2130 | rVB  | 68241  | 73764  | 7.47%  | 0.642% |
| 54 | 15.698 | 2310 | 2314 | 2327 | rVB  | 385422 | 672590 | 68.11% | 5.856% |

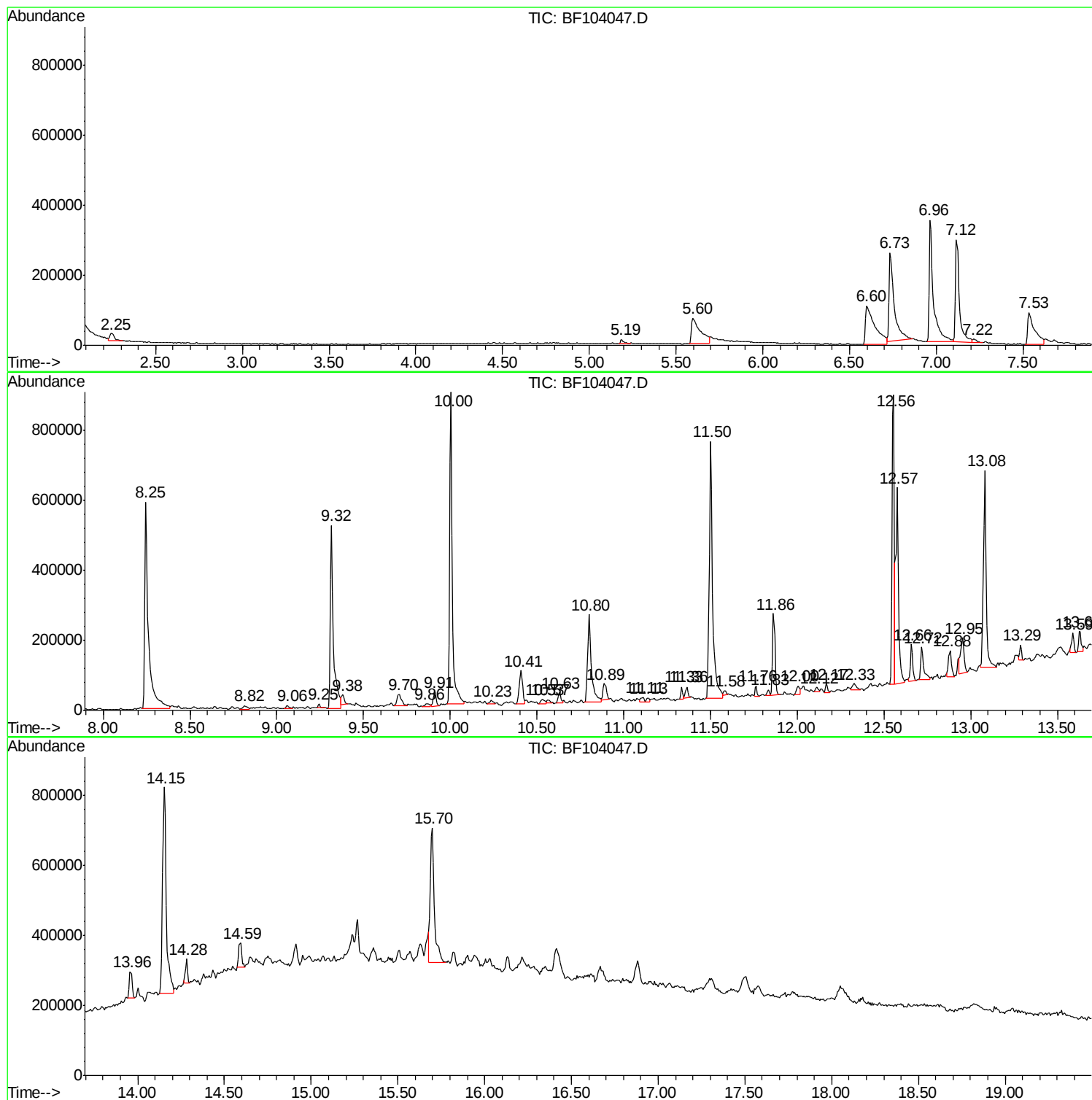
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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF032818.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF032918\  
Data File : BF104047.D  
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Operator : JU/SJ  
Sample : J1754-15 5X  
Misc :  
ALS Vial : 5 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
CL-02-032718-C

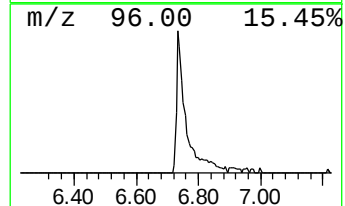
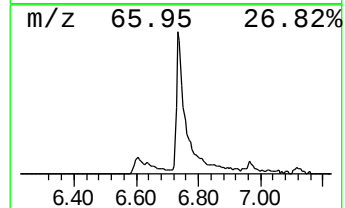
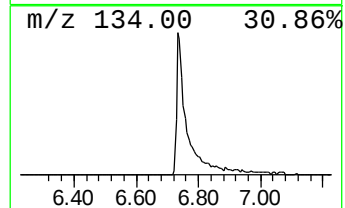
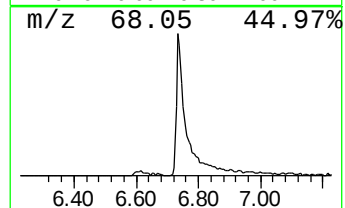
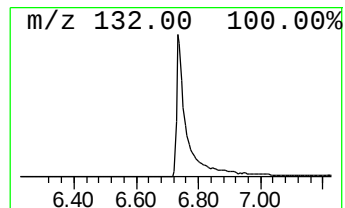
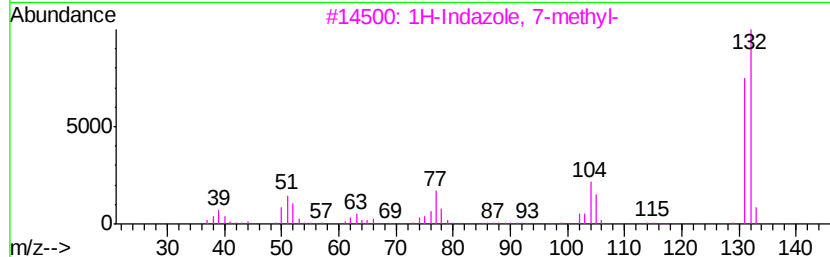
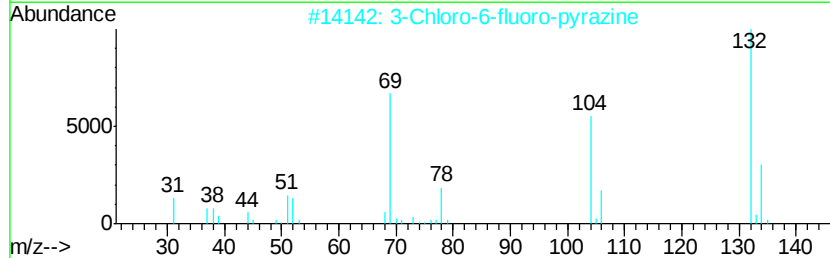
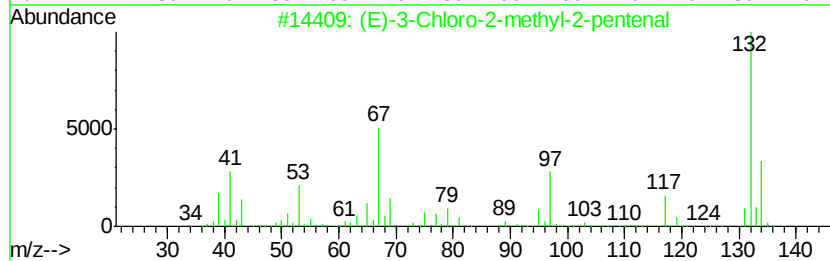
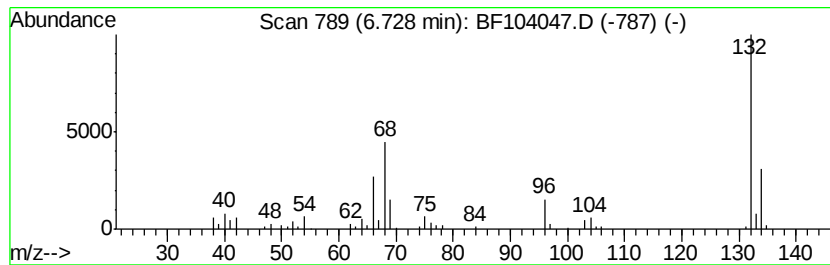
Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF032818.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 unknown6.73 Concentration Rank 1

| R.T. | EstConc  | Area   | Relative to ISTD       | R.T. |
|------|----------|--------|------------------------|------|
| 6.73 | 16.26 ng | 495024 | 1,4-Dichlorobenzene-d4 | 6.96 |

| Hit# | of | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|-------------------------------------|-----|-----------|--------------|------|
| 1    | 5  | (E)-3-Chloro-2-methyl-2-pentenal    | 132 | C6H9ClO   | 031357-76-3  | 35   |
| 2    |    | 3-Chloro-6-fluoro-pyrazine          | 132 | C4H2ClFN2 | 1000146-10-7 | 25   |
| 3    |    | 1H-Indazole, 7-methyl-              | 132 | C8H8N2    | 1000316-00-7 | 10   |
| 4    |    | 1-Methylpyrrolo[1,2-a]pyrazine      | 132 | C8H8N2    | 064608-59-9  | 9    |
| 5    |    | 2H-Cyclopenta[d]pyridazine, 2-me... | 132 | C8H8N2    | 022291-85-6  | 9    |



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CL-02-032718-C

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF032818.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

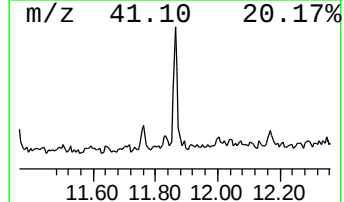
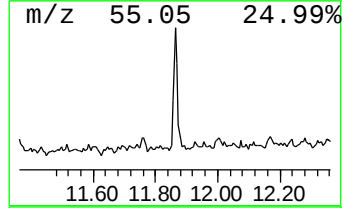
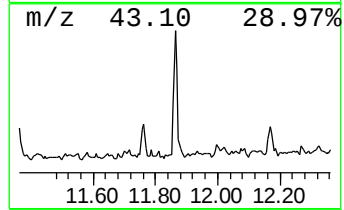
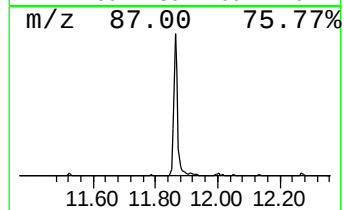
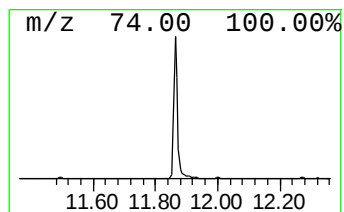
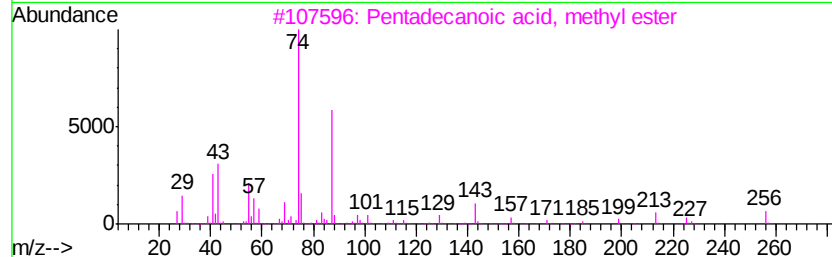
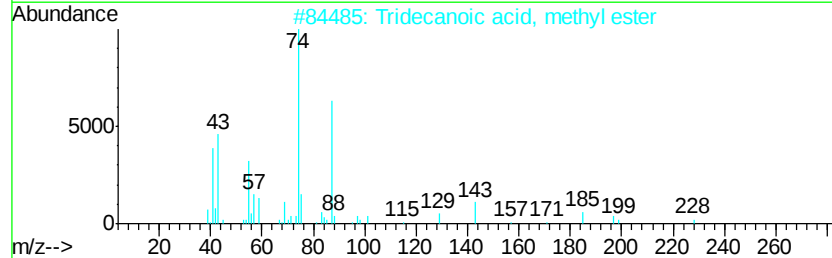
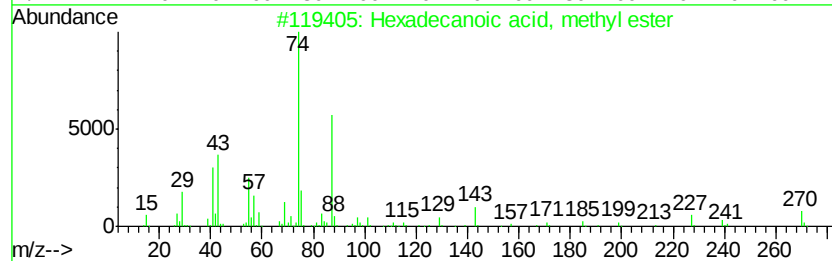
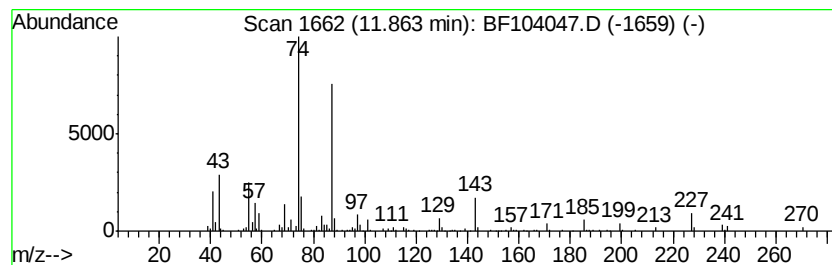
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 3 Hexadecanoic acid, methyl e... Concentration Rank 5

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 11.86 | 4.04 ng | 197082 | Phenanthrene-d10 | 11.50 |

| Hit# | of | Tentative ID                     | MW  | MolForm  | CAS#        | Qual |
|------|----|----------------------------------|-----|----------|-------------|------|
| 1    | 5  | Hexadecanoic acid, methyl ester  | 270 | C17H34O2 | 000112-39-0 | 96   |
| 2    |    | Tridecanoic acid, methyl ester   | 228 | C14H28O2 | 001731-88-0 | 91   |
| 3    |    | Pentadecanoic acid, methyl ester | 256 | C16H32O2 | 007132-64-1 | 86   |
| 4    |    | Decanoic acid, methyl ester      | 186 | C11H22O2 | 000110-42-9 | 83   |
| 5    |    | Methyl tetradecanoate            | 242 | C15H30O2 | 000124-10-7 | 80   |



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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032818.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

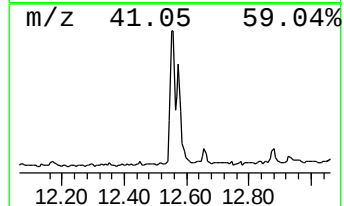
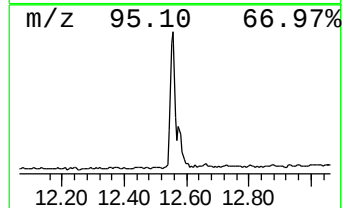
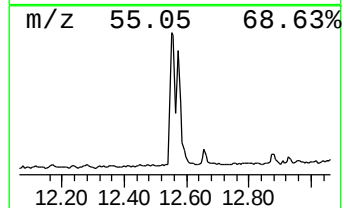
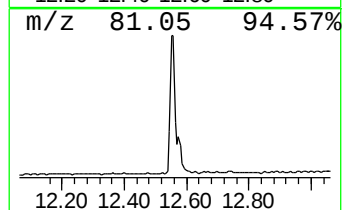
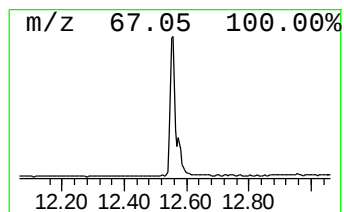
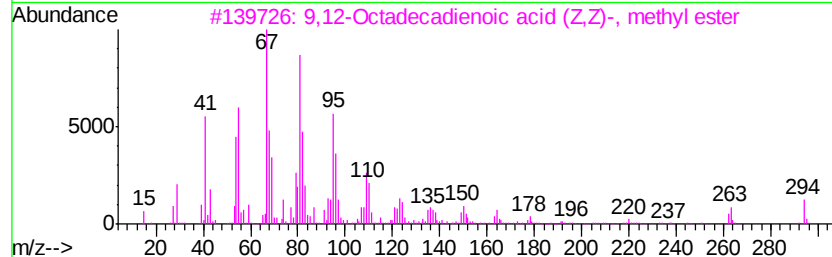
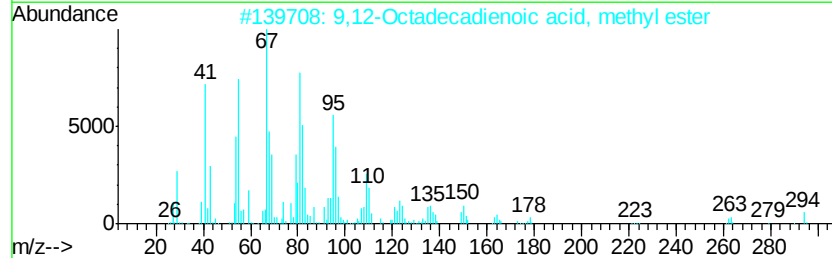
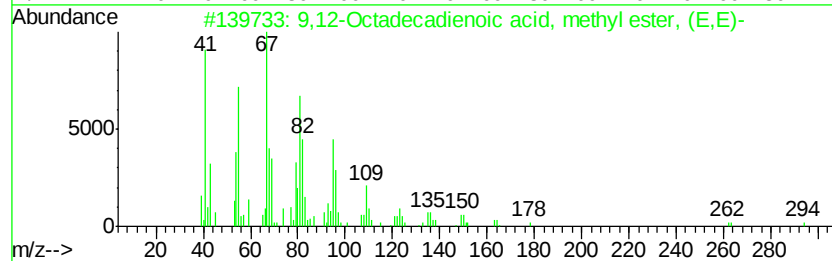
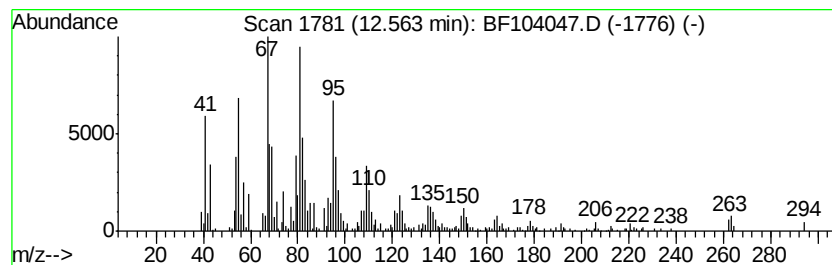
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 9,12-Octadecadienoic acid, ... Concentration Rank 2

| R.T.  | EstConc  | Area   | Relative to ISTD | R.T.  |
|-------|----------|--------|------------------|-------|
| 12.56 | 15.97 ng | 778286 | Phenanthrene-d10 | 11.50 |

| Hit# | of | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|------|----|-------------------------------------|-----|----------|--------------|------|
| 1    | 5  | 9,12-Octadecadienoic acid, methy... | 294 | C19H34O2 | 002566-97-4  | 99   |
| 2    |    | 9,12-Octadecadienoic acid, methy... | 294 | C19H34O2 | 002462-85-3  | 99   |
| 3    |    | 9,12-Octadecadienoic acid (Z,Z)-... | 294 | C19H34O2 | 000112-63-0  | 99   |
| 4    |    | 11,14-Octadecadienoic acid, meth... | 294 | C19H34O2 | 056554-61-1  | 98   |
| 5    |    | Methyl 10-trans,12-cis-octadecad... | 294 | C19H34O2 | 1000336-44-2 | 98   |



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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

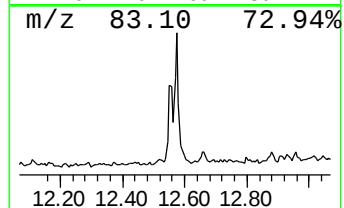
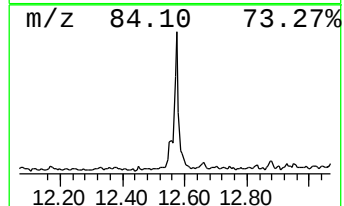
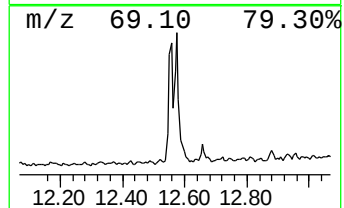
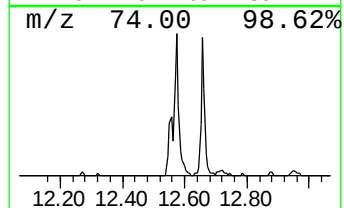
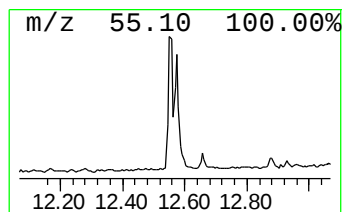
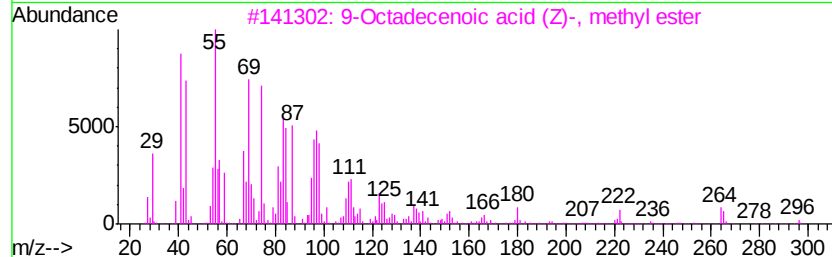
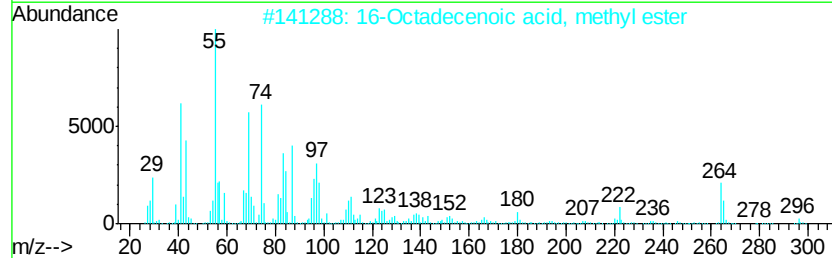
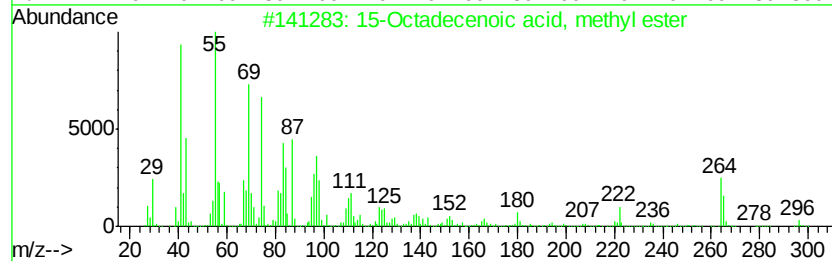
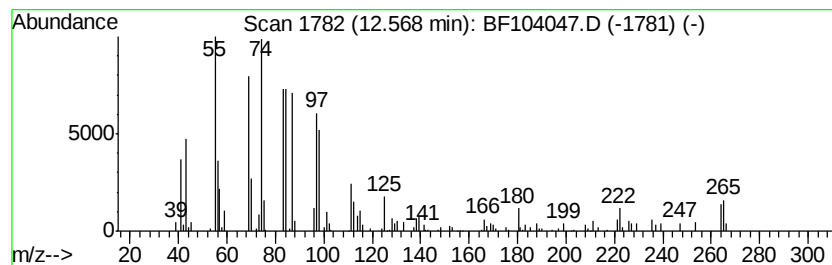
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 5 15-Octadecenoic acid, methyl ester Concentration Rank 4

| R.T.  | EstConc  | Area   | Relative to ISTD | R.T.  |
|-------|----------|--------|------------------|-------|
| 12.57 | 11.46 ng | 558853 | Phenanthrene-d10 | 11.50 |

| Hit# of | 5 | Tentative ID                           | MW  | MolForm  | CAS#        | Qual |
|---------|---|----------------------------------------|-----|----------|-------------|------|
| 1       |   | 15-Octadecenoic acid, methyl ester     | 296 | C19H36O2 | 004764-72-1 | 95   |
| 2       |   | 16-Octadecenoic acid, methyl ester     | 296 | C19H36O2 | 056554-49-5 | 95   |
| 3       |   | 9-Octadecenoic acid (Z)-, methyl ester | 296 | C19H36O2 | 000112-62-9 | 93   |
| 4       |   | 11-Octadecenoic acid, methyl ester     | 296 | C19H36O2 | 052380-33-3 | 93   |
| 5       |   | 11-Octadecenoic acid, methyl ester     | 296 | C19H36O2 | 001937-63-9 | 89   |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF032918\  
Data File : BF104047.D  
Acq On : 29 Mar 2018 13:37  
Operator : JU/SJ  
Sample : J1754-15 5X  
Misc :  
ALS Vial : 5 Sample Multiplier: 1

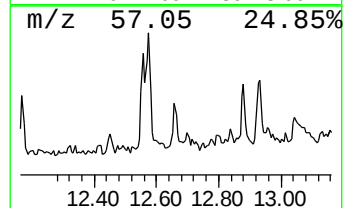
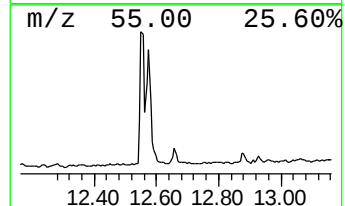
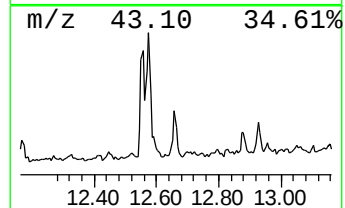
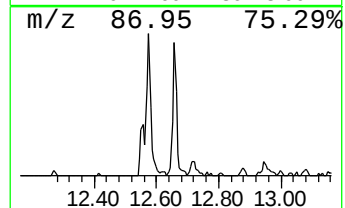
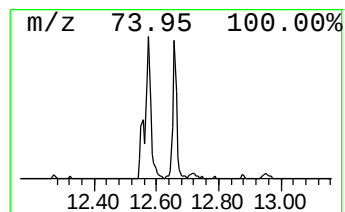
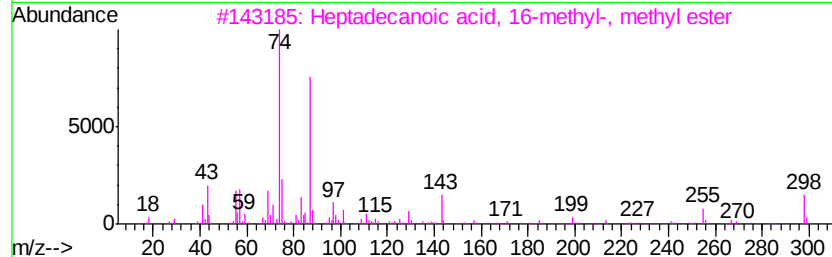
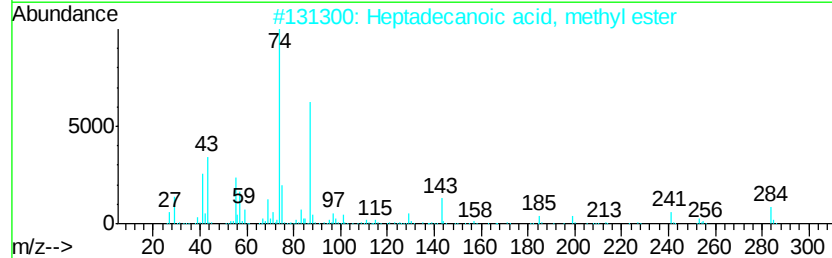
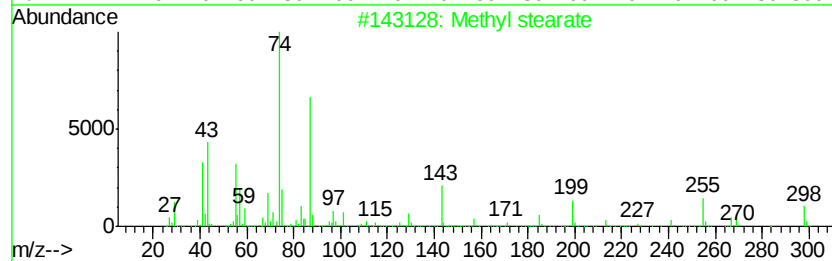
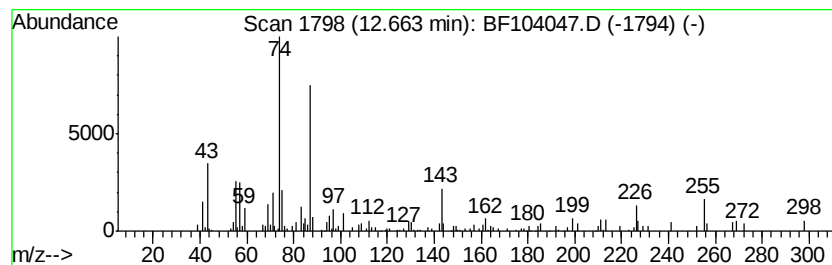
Instrument :  
BNA\_F  
ClientSampleId :  
CL-02-032718-C

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032818.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 6 Methyl stearate Concentration Rank 6

| R.T.      | EstConc                             | Area   | Relative to ISTD | R.T.        |      |
|-----------|-------------------------------------|--------|------------------|-------------|------|
| 12.66     | 2.10 ng                             | 102605 | Phenanthrene-d10 | 11.50       |      |
| Hit# of 5 | Tentative ID                        | MW     | MolForm          | CAS#        | Qual |
| 1         | Methyl stearate                     | 298    | C19H38O2         | 000112-61-8 | 94   |
| 2         | Heptadecanoic acid, methyl ester    | 284    | C18H36O2         | 001731-92-6 | 87   |
| 3         | Heptadecanoic acid, 16-methyl-, ... | 298    | C19H38O2         | 005129-61-3 | 86   |
| 4         | Pentadecanoic acid, methyl ester    | 256    | C16H32O2         | 007132-64-1 | 83   |
| 5         | Nonanoic acid, methyl ester         | 172    | C10H20O2         | 001731-84-6 | 80   |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF032918\  
Data File : BF104047.D  
Acq On : 29 Mar 2018 13:37  
Operator : JU/SJ  
Sample : J1754-15 5X  
Misc :  
ALS Vial : 5 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
CL-02-032718-C

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF032818.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 |
| unknown6.73          | 6.73  | 16.3    | ng    | 495024   | 1                     | 6.96  | 608981 | 20.0 |
| Hexadecanoic acid... | 11.86 | 4.0     | ng    | 197082   | 4                     | 11.50 | 974968 | 20.0 |
| 9,12-Octadecadien... | 12.56 | 16.0    | ng    | 778286   | 4                     | 11.50 | 974968 | 20.0 |
| 15-Octadecenoic a... | 12.57 | 11.5    | ng    | 558853   | 4                     | 11.50 | 974968 | 20.0 |
| Methyl stearate      | 12.66 | 2.1     | ng    | 102605   | 4                     | 11.50 | 974968 | 20.0 |