

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF011823\  
 Data File : BF132136.D  
 Acq On : 19 Jan 2023 00:52  
 Operator : CG\JU  
 Sample : 01190-08  
 Misc :  
 ALS Vial : 17 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 PE-7

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-BF011823.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132136.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         | 5.349       | 418           | 427         | 436          | rBV      | 1620630        | 2262198       | 40.27%          | 5.539%        |
| 2         | 5.725       | 485           | 491         | 494          | rBV      | 4132941        | 4452506       | 79.25%          | 10.902%       |
| 3         | 6.707       | 652           | 658         | 661          | rBV      | 4001258        | 4556977       | 81.11%          | 11.157%       |
| 4         | 7.095       | 720           | 724         | 727          | rBV      | 1571357        | 1214623       | 21.62%          | 2.974%        |
| 5         | 7.660       | 814           | 820         | 823          | rBV      | 3127916        | 3006593       | 53.52%          | 7.361%        |
| 6         | 8.384       | 939           | 943         | 946          | rBV      | 1774232        | 1529617       | 27.23%          | 3.745%        |
| 7         | 9.460       | 1121          | 1126        | 1129         | rBV      | 5620744        | 5128943       | 91.29%          | 12.558%       |
| 8         | 10.148      | 1239          | 1243        | 1246         | rVB      | 2010587        | 1757612       | 31.29%          | 4.303%        |
| 9         | 10.860      | 1361          | 1364        | 1368         | rVB      | 275294         | 205380        | 3.66%           | 0.503%        |
| 10        | 10.936      | 1373          | 1377        | 1381         | rBV      | 3630920        | 3748988       | 66.73%          | 9.179%        |
| 11        | 11.036      | 1391          | 1394        | 1400         | rVB      | 65389          | 83588         | 1.49%           | 0.205%        |
| 12        | 11.642      | 1493          | 1497        | 1501         | rBV      | 2115677        | 1908293       | 33.97%          | 4.672%        |
| 13        | 12.154      | 1580          | 1584        | 1589         | rBV      | 572001         | 573916        | 10.22%          | 1.405%        |
| 14        | 12.725      | 1678          | 1681        | 1685         | rBV      | 63770          | 69464         | 1.24%           | 0.170%        |
| 15        | 12.866      | 1700          | 1705        | 1707         | rBV3     | 68275          | 83728         | 1.49%           | 0.205%        |
| 16        | 12.942      | 1715          | 1718        | 1730         | rBV      | 173866         | 202396        | 3.60%           | 0.496%        |
| 17        | 13.042      | 1732          | 1735        | 1739         | rVB      | 239964         | 196589        | 3.50%           | 0.481%        |
| 18        | 13.095      | 1742          | 1744        | 1747         | rBV      | 100558         | 86485         | 1.54%           | 0.212%        |
| 19        | 13.242      | 1764          | 1769        | 1772         | rBV      | 5740616        | 5618017       | 100.00%         | 13.755%       |
| 20        | 13.430      | 1795          | 1801        | 1803         | rBV      | 60737          | 72590         | 1.29%           | 0.178%        |
| 21        | 13.454      | 1803          | 1805        | 1809         | rVB      | 111548         | 99226         | 1.77%           | 0.243%        |
| 22        | 13.801      | 1860          | 1864        | 1867         | rBV      | 130919         | 104798        | 1.87%           | 0.257%        |
| 23        | 14.130      | 1917          | 1920        | 1922         | rBV      | 103465         | 92028         | 1.64%           | 0.225%        |
| 24        | 14.177      | 1922          | 1928        | 1942         | rVV4     | 112863         | 489215        | 8.71%           | 1.198%        |
| 25        | 14.307      | 1946          | 1950        | 1959         | rVV      | 1665738        | 1536008       | 27.34%          | 3.761%        |
| 26        | 14.395      | 1959          | 1965        | 1972         | rVV      | 422005         | 478153        | 8.51%           | 1.171%        |
| 27        | 14.448      | 1972          | 1974        | 1984         | rVB      | 73199          | 80860         | 1.44%           | 0.198%        |
| 28        | 15.907      | 2215          | 2222        | 2230         | rBV      | 847910         | 1203634       | 21.42%          | 2.947%        |

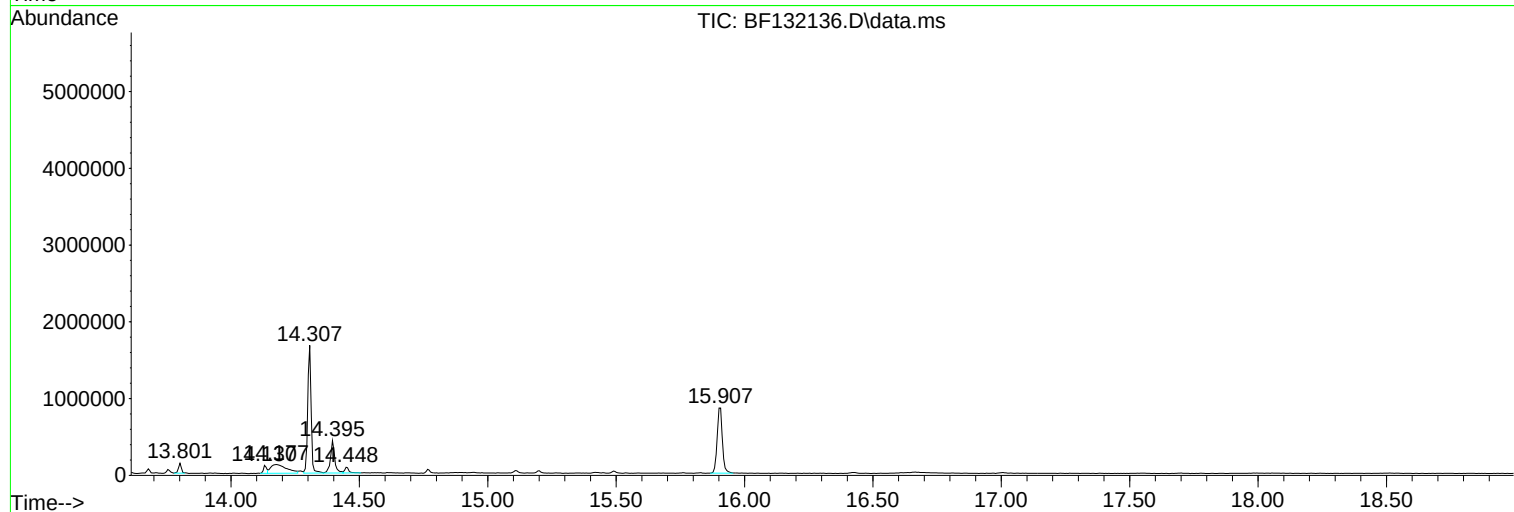
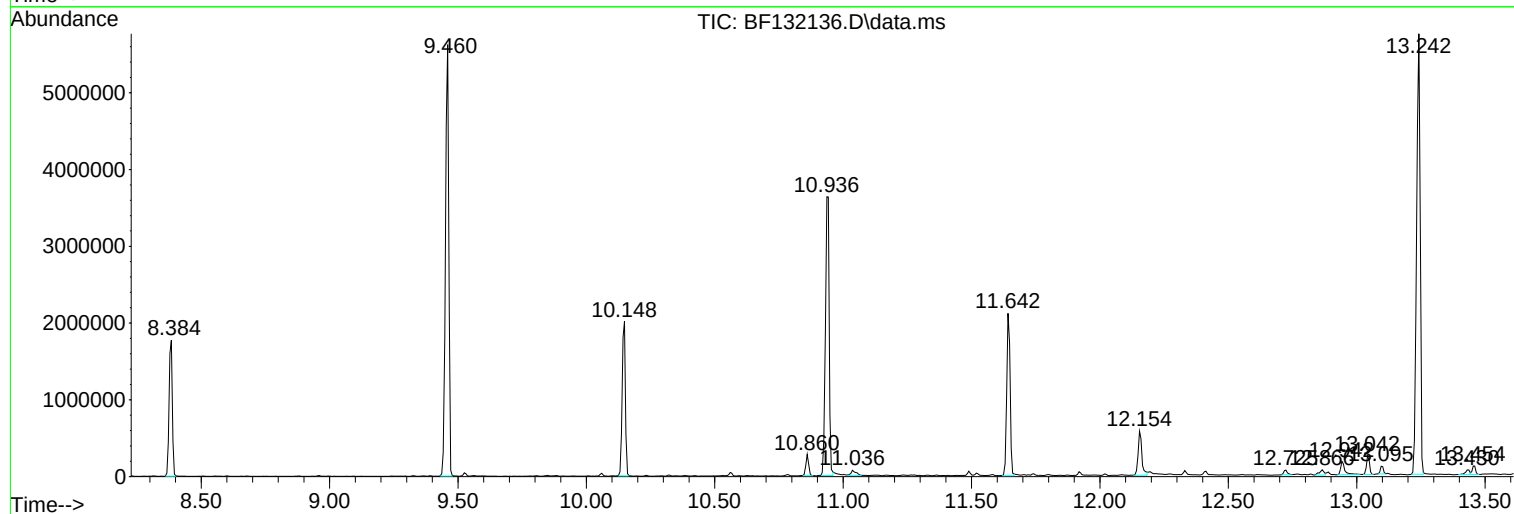
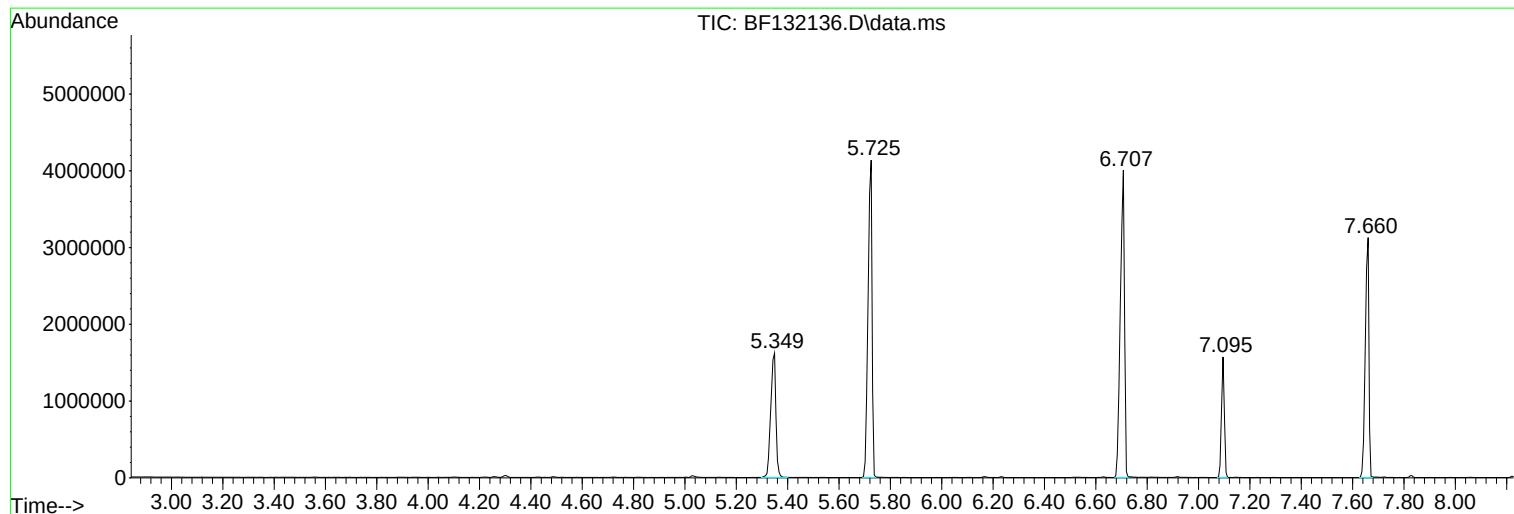
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BNA\_F  
ClientSampleId :  
PE-7

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF011823.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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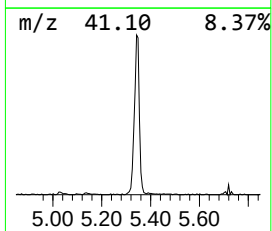
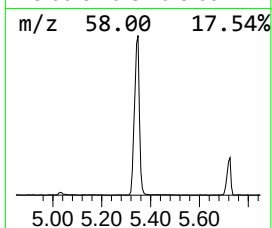
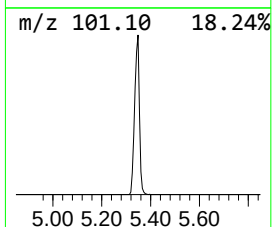
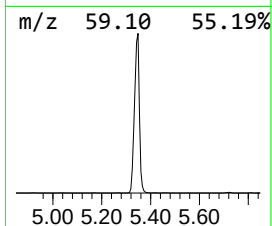
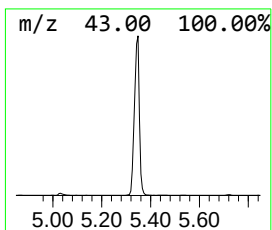
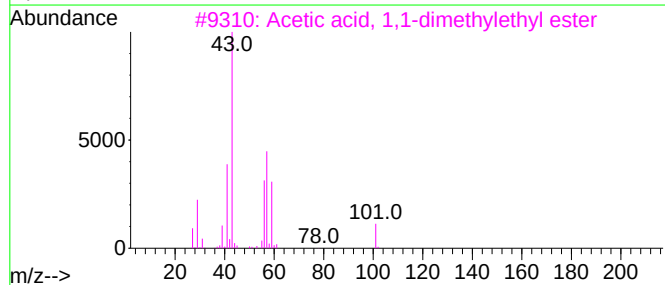
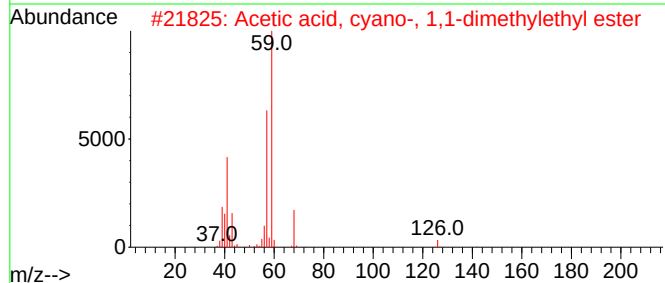
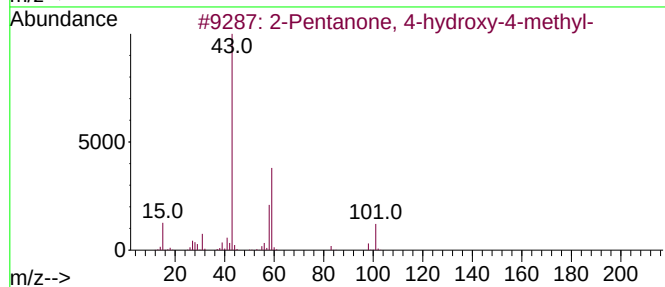
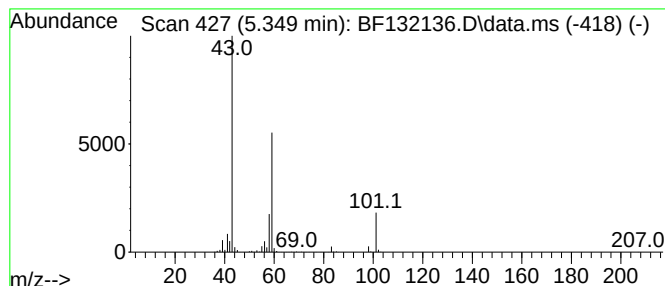
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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

| R.T.  | EstConc  | Area    | Relative to ISTD       | R.T.  |
|-------|----------|---------|------------------------|-------|
| 5.349 | 37.25 ng | 2262200 | 1,4-Dichlorobenzene-d4 | 7.095 |

| 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 | 37      |      |      |
| 3    | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2      | 000540-88-5 | 28      |      |      |
| 4    | 2,3-Butanedione, monooxime          | 101 | C4H7NO2      | 000057-71-6 | 27      |      |      |
| 5    | Acetone                             | 58  | C3H6O        | 000067-64-1 | 12      |      |      |



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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF011823.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

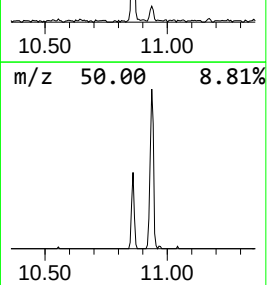
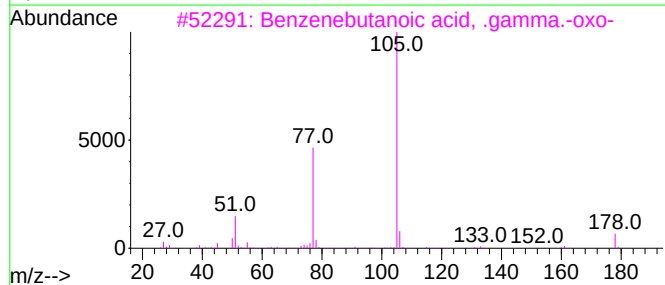
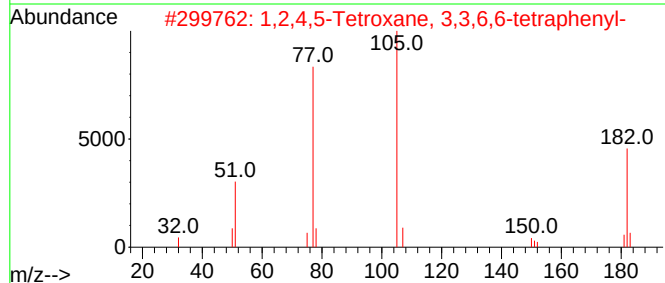
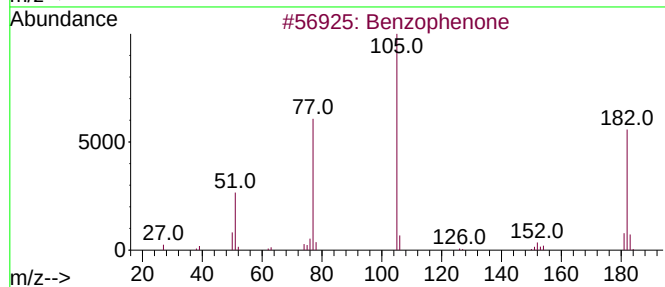
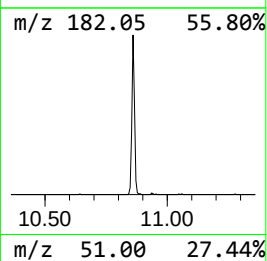
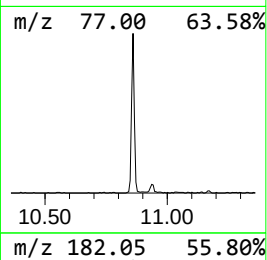
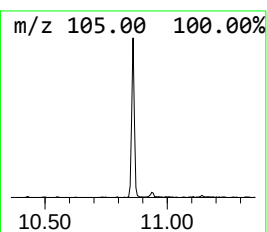
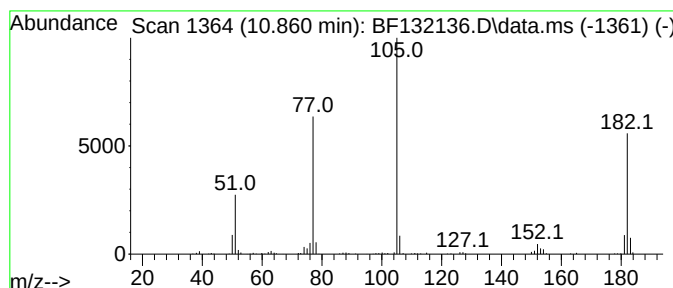
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 Benzophenone Concentration Rank 6

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 10.860 | 2.34 ng | 205380 | Acenaphthene-d10 | 10.148 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | Benzophenone                        | 182 | C13H10O  | 000119-61-9 | 96   |
| 2    |    |   | 1,2,4,5-Tetroxane, 3,3,6,6-tetra... | 396 | C26H20O4 | 016204-36-7 | 78   |
| 3    |    |   | Benzenebutanoic acid, .gamma.-oxo-  | 178 | C10H10O3 | 002051-95-8 | 47   |
| 4    |    |   | Vinyl benzoate                      | 148 | C9H8O2   | 000769-78-8 | 47   |
| 5    |    |   | N-cyanobenzamide                    | 146 | C8H6N2O  | 015150-25-1 | 47   |



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Instrument :  
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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF011823.M  
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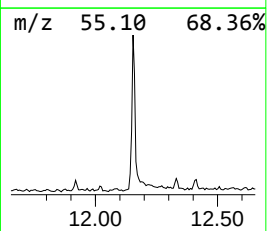
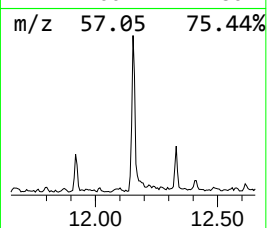
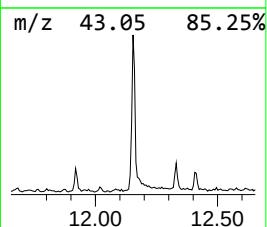
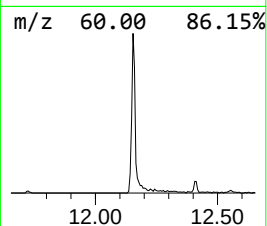
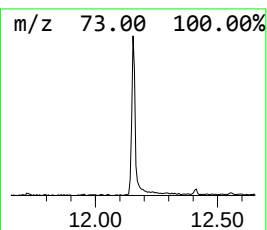
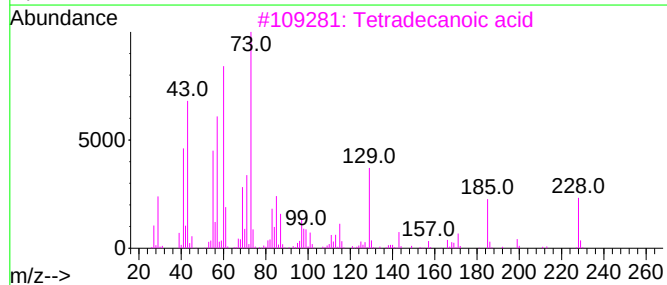
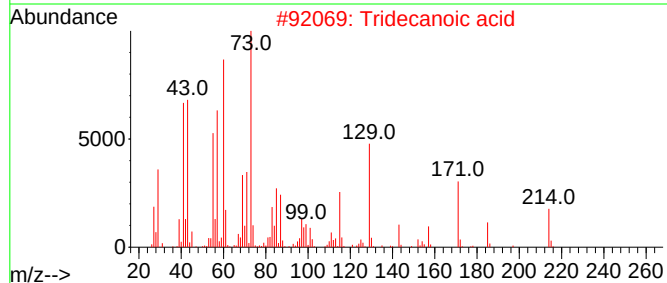
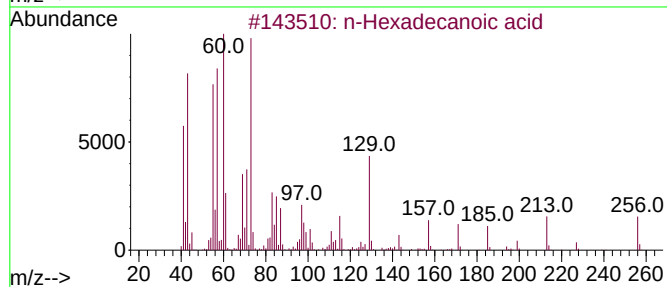
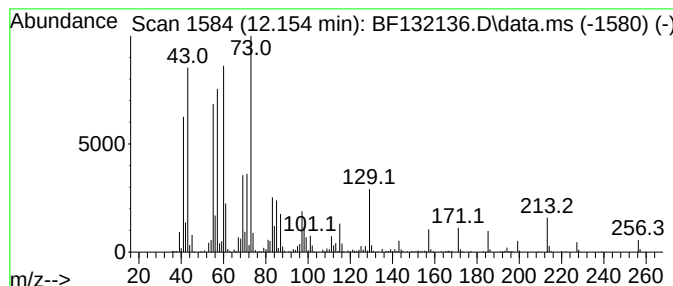
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 12.154 | 6.01 ng | 573916 | Phenanthrene-d10 | 11.642 |

| 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 | 95   |
| 3    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 95   |
| 4    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 90   |
| 5    |    |   | Isopropyl palmitate | 298 | C19H38O2 | 000142-91-6 | 64   |



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PE-7

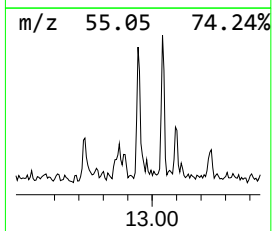
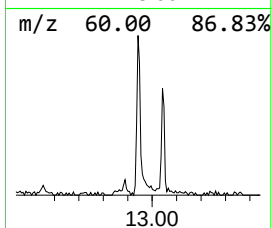
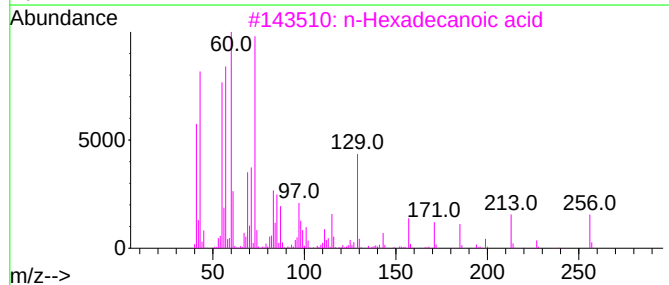
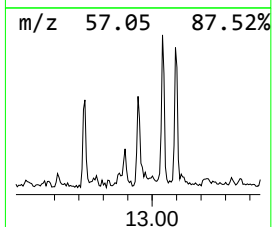
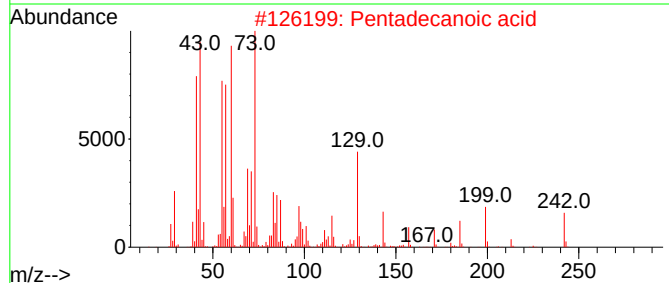
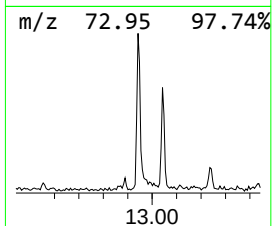
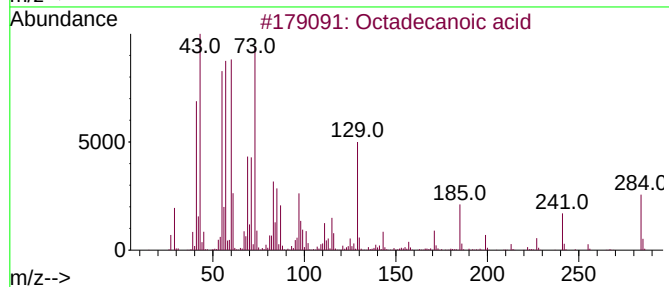
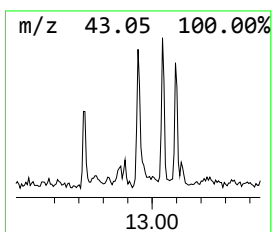
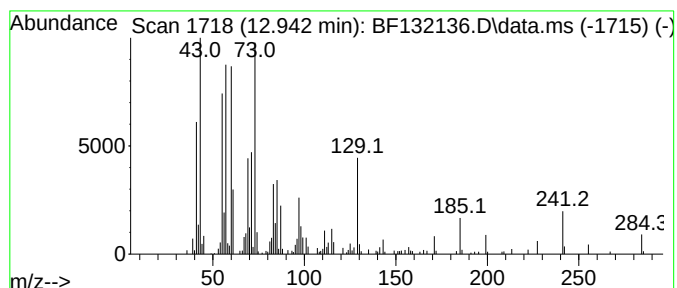
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Peak Number 4 Octadecanoic acid Concentration Rank 7

| R.T.      | EstConc               | Area   | Relative to ISTD | R.T.        |      |
|-----------|-----------------------|--------|------------------|-------------|------|
| 12.942    | 2.12 ng               | 202396 | Phenanthrene-d10 | 11.642      |      |
| Hit# of 5 | Tentative ID          | MW     | MolForm          | CAS#        | Qual |
| 1         | Octadecanoic acid     | 284    | C18H36O2         | 000057-11-4 | 99   |
| 2         | Pentadecanoic acid    | 242    | C15H30O2         | 001002-84-2 | 93   |
| 3         | n-Hexadecanoic acid   | 256    | C16H32O2         | 000057-10-3 | 87   |
| 4         | n-Decanoic acid       | 172    | C10H20O2         | 000334-48-5 | 68   |
| 5         | 8-Methylnonanoic acid | 172    | C10H20O2         | 005963-14-4 | 55   |



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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

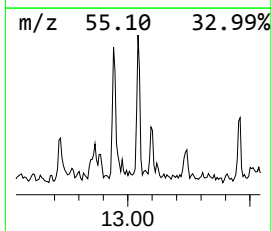
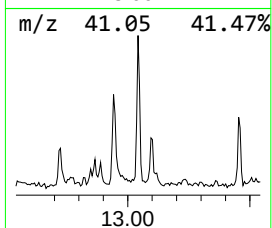
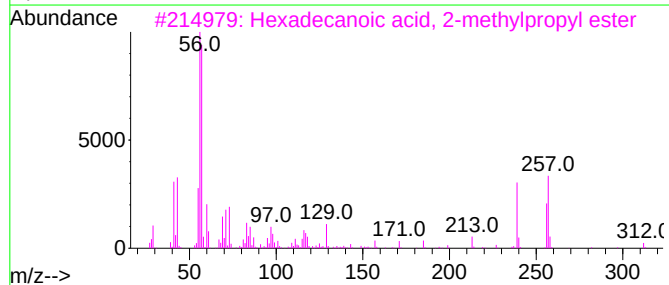
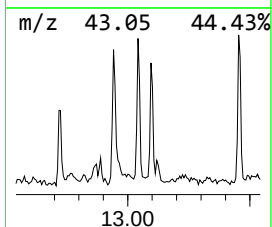
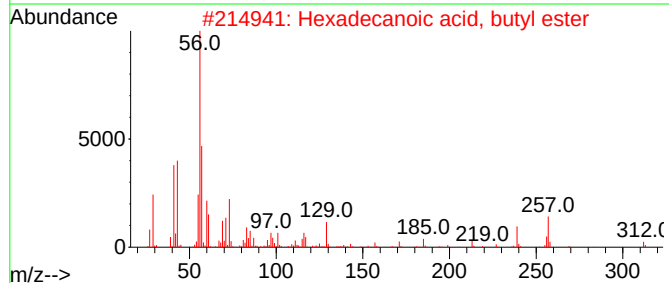
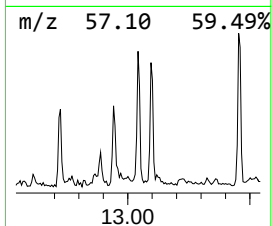
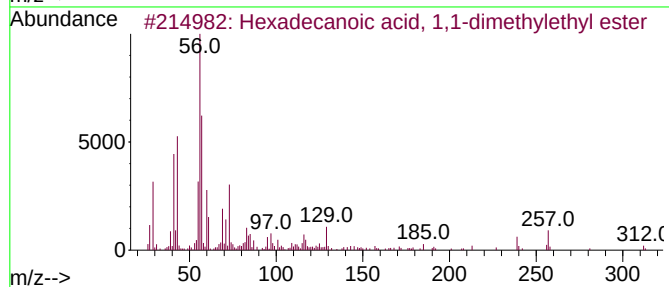
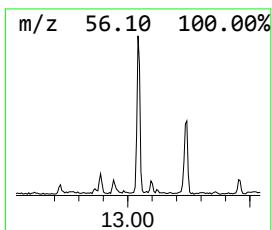
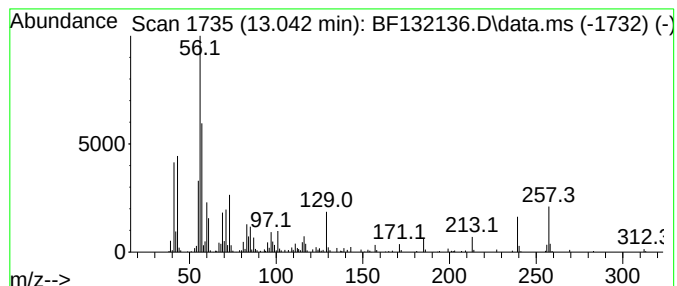
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 Hexadecanoic acid, 1,1-dime... Concentration Rank 5

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 13.042 | 2.56 ng | 196589 | Chrysene-d12     | 14.307 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | Hexadecanoic acid, 1,1-dimethyle... | 312 | C20H40O2 | 031158-91-5 | 93   |
| 2    |    |   | Hexadecanoic acid, butyl ester      | 312 | C20H40O2 | 000111-06-8 | 91   |
| 3    |    |   | Hexadecanoic acid, 2-methylpropy... | 312 | C20H40O2 | 000110-34-9 | 70   |
| 4    |    |   | 2,2-Dimethyl-1,3-butanediol         | 118 | C6H14O2  | 000076-35-7 | 38   |
| 5    |    |   | Cyclohexylamine                     | 99  | C6H13N   | 000108-91-8 | 27   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF011823\  
Data File : BF132136.D  
Acq On : 19 Jan 2023 00:52  
Operator : CG\JU  
Sample : 01190-08  
Misc :  
ALS Vial : 17 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PE-7

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF011823.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

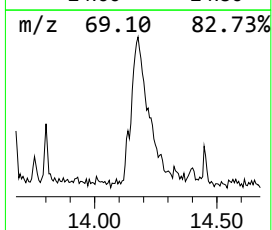
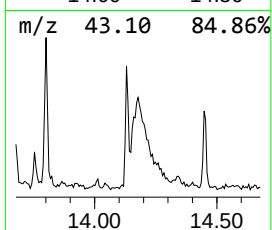
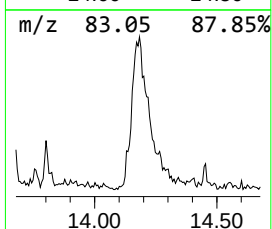
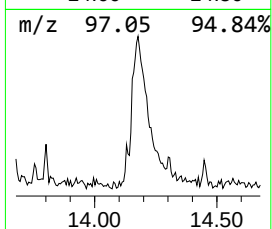
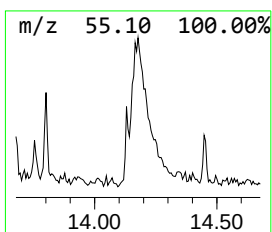
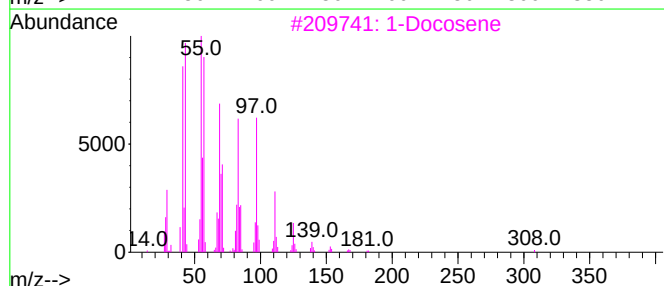
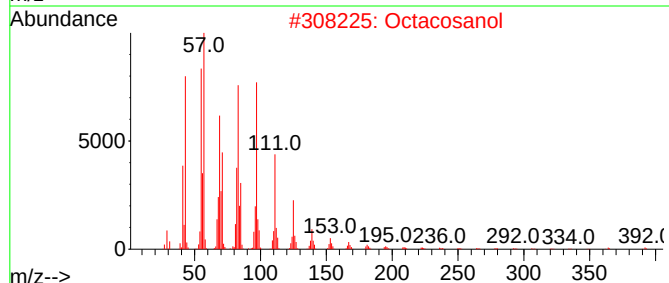
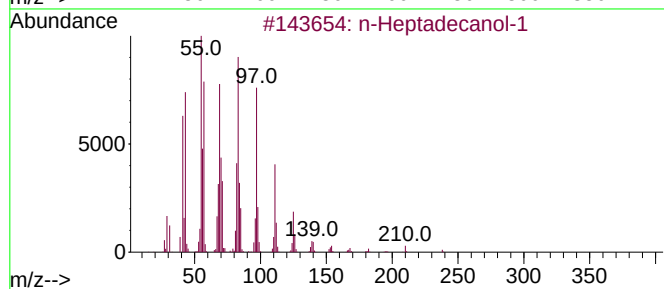
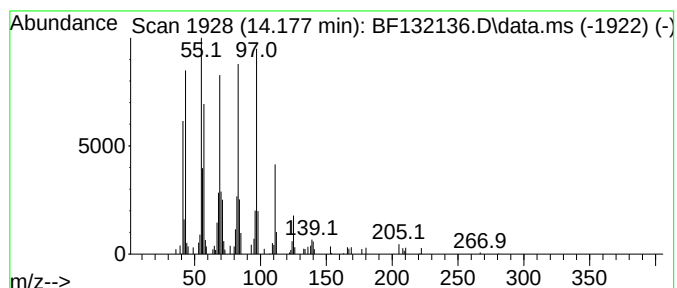
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 6 n-Heptadecanol-1 Concentration Rank 2

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 14.177 | 6.37 ng | 489215 | Chrysene-d12     | 14.307 |

| Hit# | of 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|------|-------------------------------------|-----|---------|-------------|------|
| 1    |      | n-Heptadecanol-1                    | 256 | C17H36O | 001454-85-9 | 80   |
| 2    |      | Octacosanol                         | 410 | C28H58O | 000557-61-9 | 68   |
| 3    |      | 1-Docosene                          | 308 | C22H44  | 001599-67-3 | 58   |
| 4    |      | 1-Octadecanol                       | 270 | C18H38O | 000112-92-5 | 52   |
| 5    |      | Cyclopentane, 2-isopropyl-1,3-di... | 140 | C10H20  | 032281-85-9 | 52   |





Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF011823\  
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Acq On : 19 Jan 2023 00:52  
Operator : CG\JU  
Sample : 01190-08  
Misc :  
ALS Vial : 17 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PE-7

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF011823.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

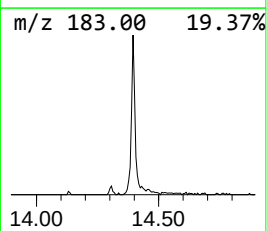
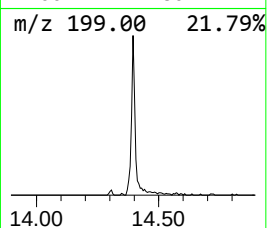
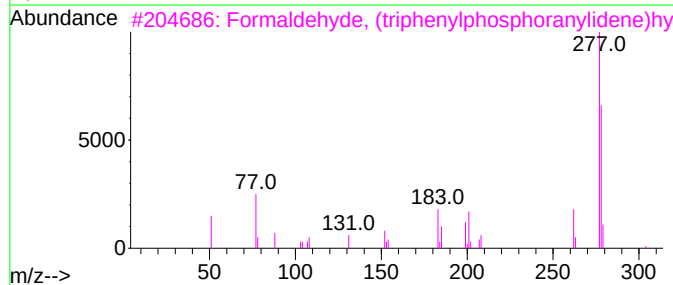
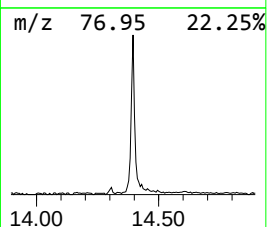
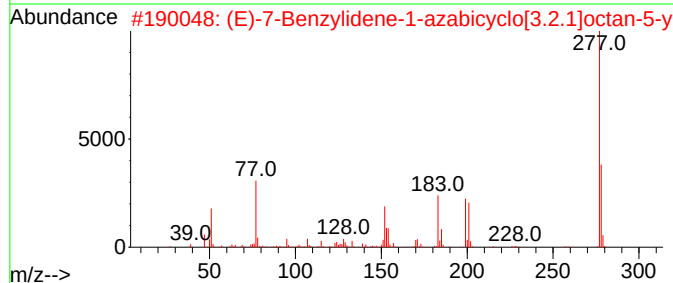
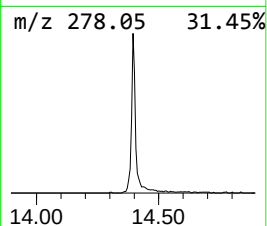
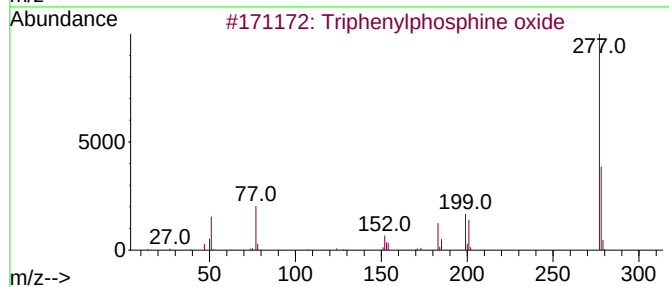
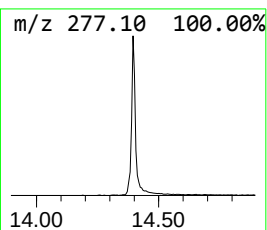
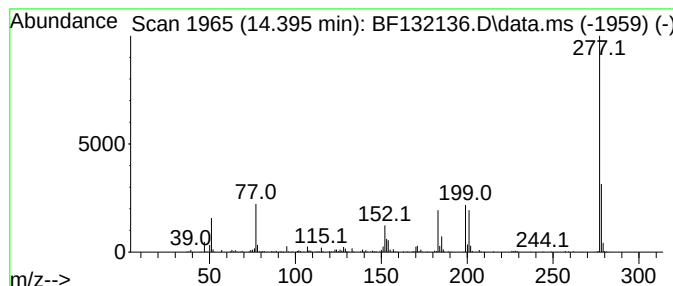
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 7 Triphenylphosphine oxide Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 14.395 | 6.23 ng | 478153 | Chrysene-d12     | 14.307 |

| Hit# | of | 5 | Tentative ID                         | MW  | MolForm     | CAS#         | Qual |
|------|----|---|--------------------------------------|-----|-------------|--------------|------|
| 1    |    |   | Triphenylphosphine oxide             | 278 | C18H15OP    | 000791-28-6  | 94   |
| 2    |    |   | (E)-7-Benzylidene-1-azabicyclo[3...] | 293 | C15H19N03S  | 1000483-83-4 | 91   |
| 3    |    |   | Formaldehyde, (triphenylphosphor...  | 304 | C19H17N2P   | 015990-54-2  | 64   |
| 4    |    |   | Carbazol-1-one, 1,2,3,4-tetrahyd...  | 277 | C18H15N02   | 299962-12-2  | 38   |
| 5    |    |   | 3-(3,4-Dichlorophenyl)-2-thioxo-...  | 277 | C9H5Cl2NOS2 | 017046-34-3  | 25   |



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Operator : CG\JU  
Sample : 01190-08  
Misc :  
ALS Vial : 17 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PE-7

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF011823.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 |
| 2-Pentanone, 4-... | 5.349  | 37.3    | ng    | 2262200  | 1                     | 7.095  | 1214620 | 20.0 |
| Benzophenone       | 10.860 | 2.3     | ng    | 205380   | 3                     | 10.148 | 1757610 | 20.0 |
| n-Hexadecanoic ... | 12.154 | 6.0     | ng    | 573916   | 4                     | 11.642 | 1908290 | 20.0 |
| Octadecanoic acid  | 12.942 | 2.1     | ng    | 202396   | 4                     | 11.642 | 1908290 | 20.0 |
| Hexadecanoic ac... | 13.042 | 2.6     | ng    | 196589   | 5                     | 14.307 | 1536010 | 20.0 |
| n-Heptadecanol-1   | 14.177 | 6.4     | ng    | 489215   | 5                     | 14.307 | 1536010 | 20.0 |
| Triphenylphosph... | 14.395 | 6.2     | ng    | 478153   | 5                     | 14.307 | 1536010 | 20.0 |