

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011918\  
 Data File : BF102242.D  
 Acq On : 20 Jan 2018 2:52  
 Operator : SJ/JU  
 Sample : J1114-11  
 Misc :  
 ALS Vial : 18 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 SB-26-2.0-2.5

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-BF010918.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         | 4.928       | 479           | 483         | 494          | rVB      | 204523         | 298513        | 7.54%           | 0.903%        |
| 2         | 5.334       | 547           | 552         | 555          | rBV      | 3408741        | 3825672       | 96.62%          | 11.567%       |
| 3         | 6.363       | 721           | 727         | 730          | rBV      | 3416129        | 3873293       | 97.82%          | 11.711%       |
| 4         | 6.492       | 744           | 749         | 752          | rBV      | 3927625        | 3834123       | 96.83%          | 11.593%       |
| 5         | 6.716       | 784           | 787         | 791          | rBV      | 1014363        | 828947        | 20.94%          | 2.506%        |
| 6         | 6.875       | 810           | 814         | 817          | rBV      | 3277847        | 2959883       | 74.75%          | 8.949%        |
| 7         | 7.286       | 878           | 884         | 887          | rBV      | 2472225        | 2470917       | 62.40%          | 7.471%        |
| 8         | 7.998       | 1001          | 1005        | 1009         | rBV      | 1256271        | 1106103       | 27.93%          | 3.344%        |
| 9         | 9.080       | 1183          | 1189        | 1192         | rBV      | 4158145        | 3959613       | 100.00%         | 11.972%       |
| 10        | 9.469       | 1251          | 1255        | 1258         | rBV      | 352862         | 320116        | 8.08%           | 0.968%        |
| 11        | 9.686       | 1283          | 1292        | 1295         | rBV      | 114888         | 96376         | 2.43%           | 0.291%        |
| 12        | 9.751       | 1299          | 1303        | 1307         | rVB2     | 1261359        | 1148071       | 28.99%          | 3.471%        |
| 13        | 10.186      | 1373          | 1377        | 1380         | rVB      | 141359         | 121069        | 3.06%           | 0.366%        |
| 14        | 10.404      | 1409          | 1414        | 1416         | rBV      | 39581          | 49968         | 1.26%           | 0.151%        |
| 15        | 10.545      | 1431          | 1438        | 1441         | rBV      | 2413599        | 2248421       | 56.78%          | 6.798%        |
| 16        | 10.657      | 1454          | 1457        | 1465         | rBV      | 131552         | 126772        | 3.20%           | 0.383%        |
| 17        | 11.239      | 1552          | 1556        | 1559         | rBV      | 1115665        | 1025178       | 25.89%          | 3.100%        |
| 18        | 12.645      | 1791          | 1795        | 1798         | rBV      | 93507          | 72190         | 1.82%           | 0.218%        |
| 19        | 12.821      | 1821          | 1825        | 1829         | rBV      | 2707176        | 2773985       | 70.06%          | 8.387%        |
| 20        | 13.351      | 1912          | 1915        | 1917         | rBV      | 56479          | 46219         | 1.17%           | 0.140%        |
| 21        | 13.715      | 1973          | 1977        | 1986         | rBV      | 277489         | 273236        | 6.90%           | 0.826%        |
| 22        | 13.868      | 1999          | 2003        | 2007         | rBV      | 828865         | 713625        | 18.02%          | 2.158%        |
| 23        | 14.345      | 2079          | 2084        | 2091         | rBV2     | 43179          | 67638         | 1.71%           | 0.205%        |
| 24        | 15.292      | 2240          | 2245        | 2249         | rBV      | 637822         | 749181        | 18.92%          | 2.265%        |
| 25        | 15.774      | 2324          | 2327        | 2334         | rVB6     | 28653          | 43567         | 1.10%           | 0.132%        |
| 26        | 17.209      | 2568          | 2571        | 2580         | rVB9     | 21890          | 40991         | 1.04%           | 0.124%        |

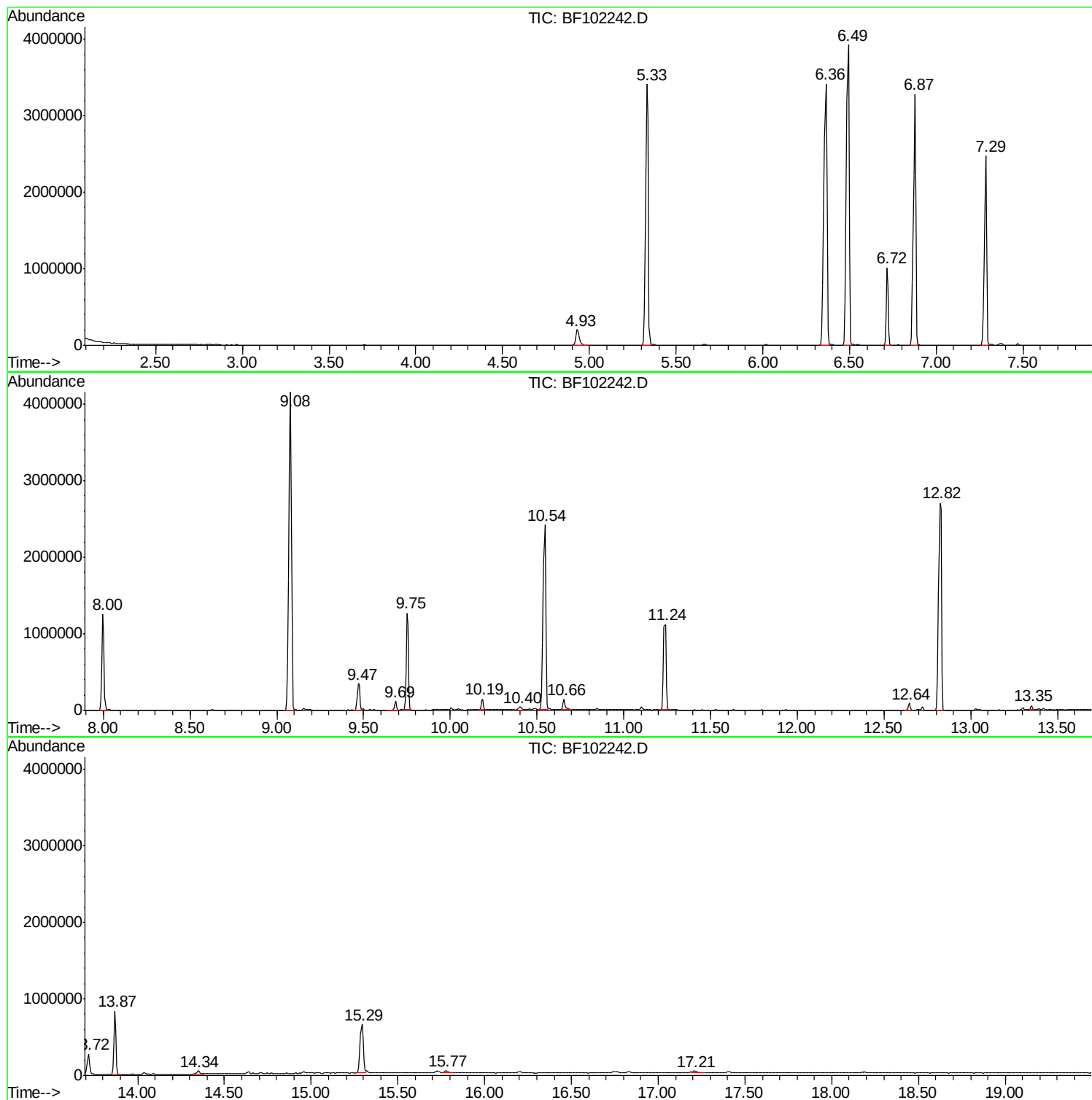
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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF010918.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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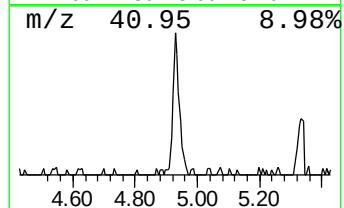
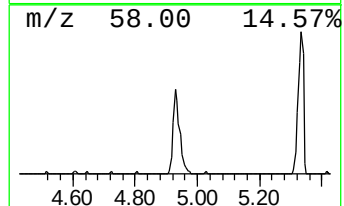
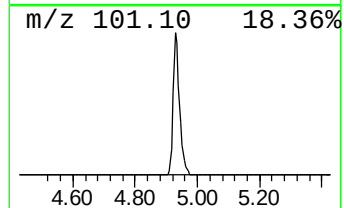
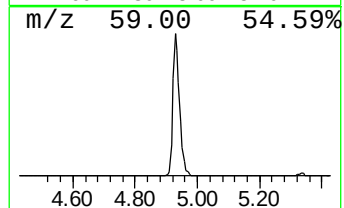
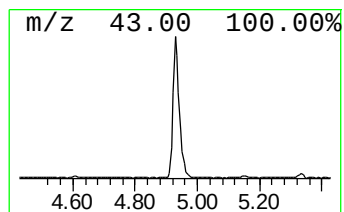
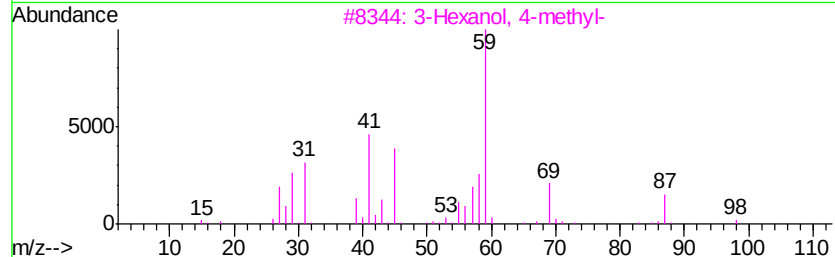
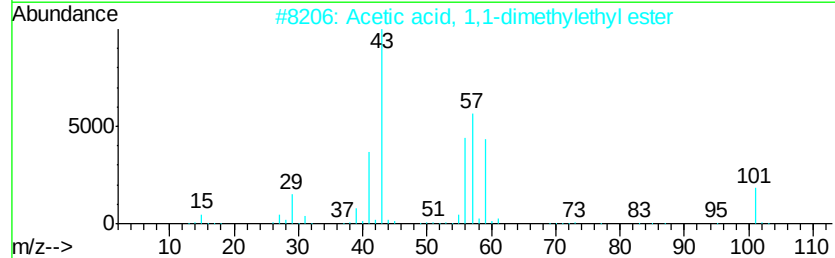
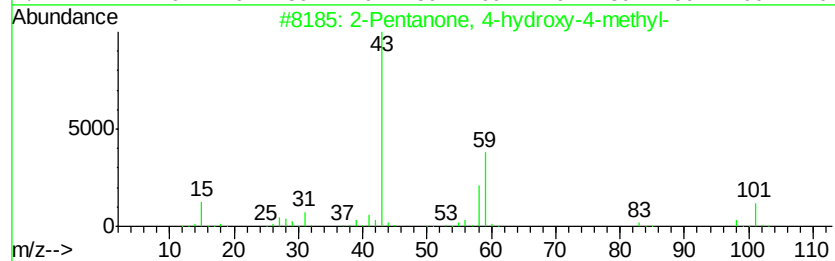
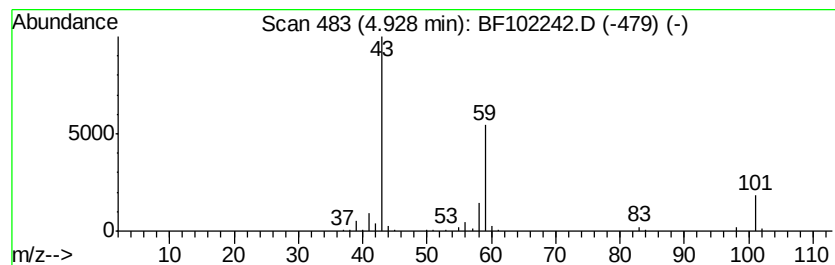
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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

| R.T. | EstConc | Area   | Relative to ISTD       | R.T. |
|------|---------|--------|------------------------|------|
| 4.93 | 7.20 ng | 298513 | 1,4-Dichlorobenzene-d4 | 6.72 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2  | 000123-42-2 | 64   |
| 2    |    |   | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2  | 000540-88-5 | 39   |
| 3    |    |   | 3-Hexanol, 4-methyl-                | 116 | C7H16O   | 000615-29-2 | 33   |
| 4    |    |   | Propane, 2-methyl-2-(1-methyleth... | 116 | C7H16O   | 017348-59-3 | 33   |
| 5    |    |   | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 23   |



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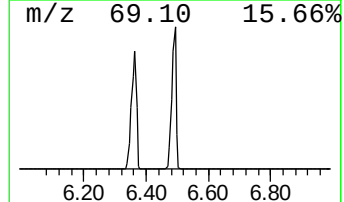
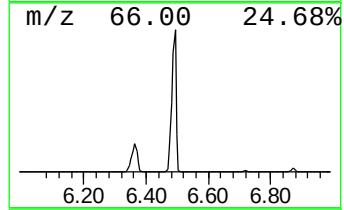
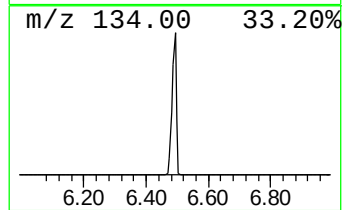
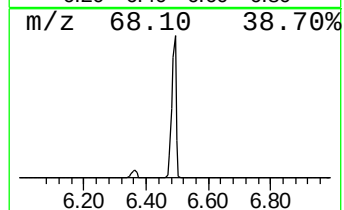
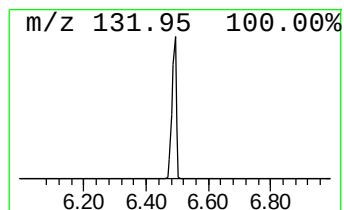
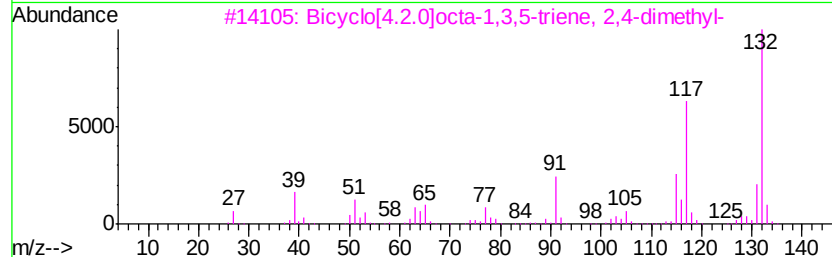
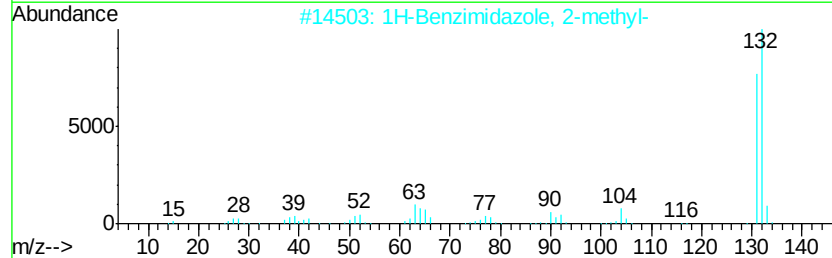
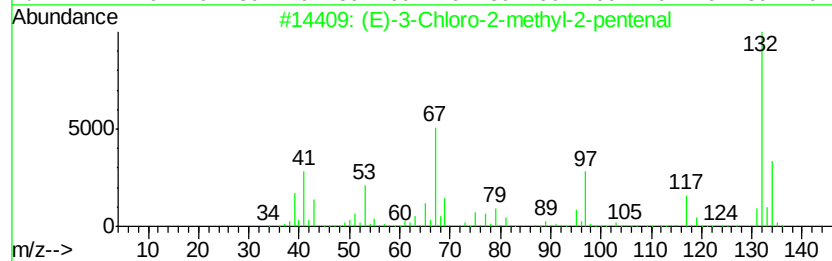
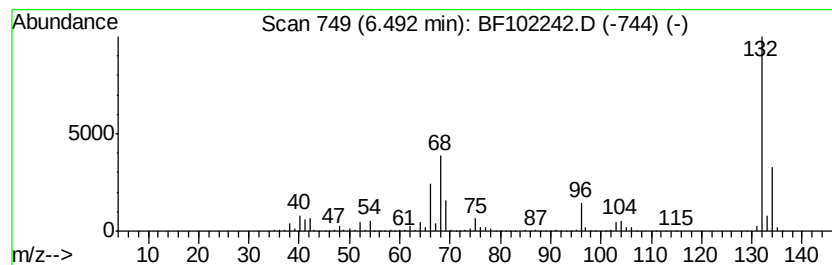
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 unknown6.49 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.49 | 92.51 ng | 3834120 | 1,4-Dichlorobenzene-d4 | 6.72 |

| Hit# | of | Tentative ID                        | MW  | MolForm   | CAS#        | Qual |
|------|----|-------------------------------------|-----|-----------|-------------|------|
| 1    | 5  | (E)-3-Chloro-2-methyl-2-pentenal    | 132 | C6H9ClO   | 031357-76-3 | 27   |
| 2    |    | 1H-Benzimidazole, 2-methyl-         | 132 | C8H8N2    | 000615-15-6 | 10   |
| 3    |    | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12    | 028749-81-7 | 9    |
| 4    |    | 5-Fluoro-2-chloropyrimidine         | 132 | C4H2ClFN2 | 062802-42-0 | 9    |
| 5    |    | 4-Methylpyrrolo[1,2-a]pyrazine      | 132 | C8H8N2    | 064608-60-2 | 9    |



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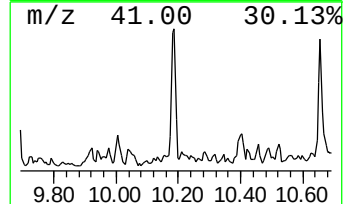
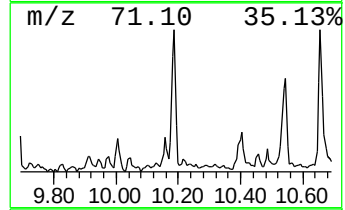
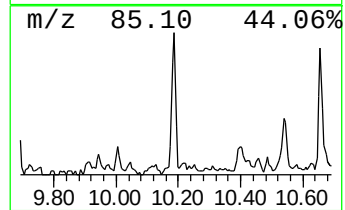
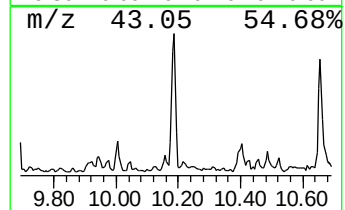
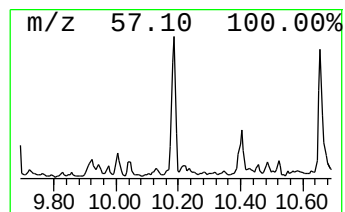
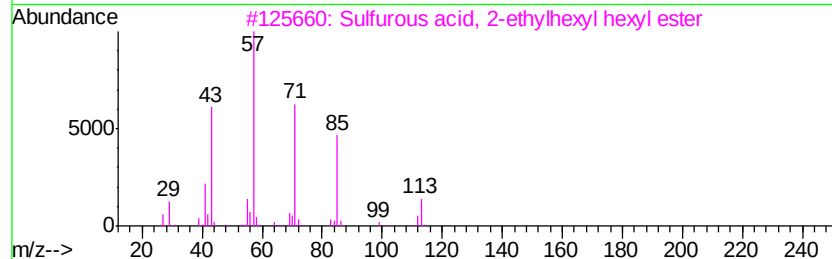
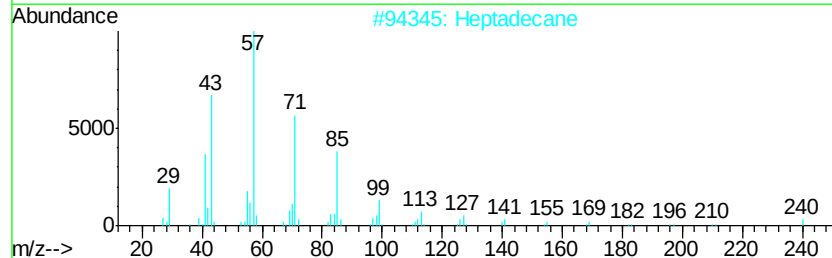
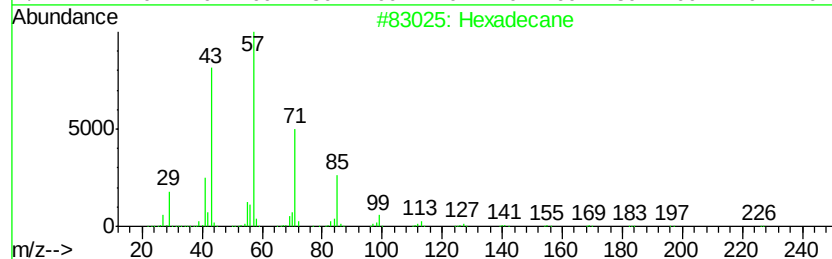
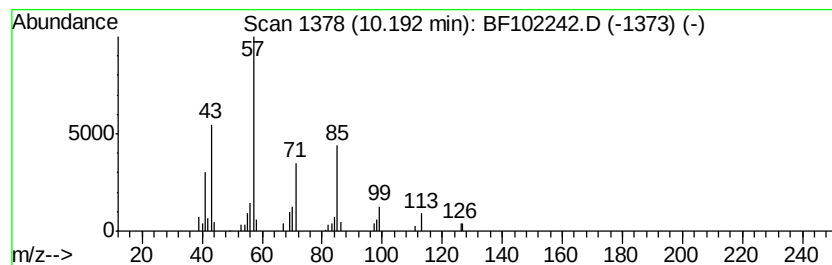
Instrument :  
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Peak Number 4 Hexadecane Concentration Rank 6

| R.T.      | EstConc                             | Area   | Relative to ISTD | R.T.         |      |
|-----------|-------------------------------------|--------|------------------|--------------|------|
| 10.19     | 2.11 ng                             | 121069 | Acenaphthene-d10 | 9.75         |      |
| Hit# of 5 | Tentative ID                        | MW     | MolForm          | CAS#         | Qual |
| 1         | Hexadecane                          | 226    | C16H34           | 000544-76-3  | 90   |
| 2         | Heptadecane                         | 240    | C17H36           | 000629-78-7  | 80   |
| 3         | Sulfurous acid, 2-ethylhexyl hex... | 278    | C14H30O3S        | 1000309-20-2 | 80   |
| 4         | Decane, 2,3,5-trimethyl-            | 184    | C13H28           | 062238-11-3  | 78   |
| 5         | Sulfurous acid, pentadecyl 2-pro... | 334    | C18H38O3S        | 1000309-12-6 | 78   |



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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF010918.M  
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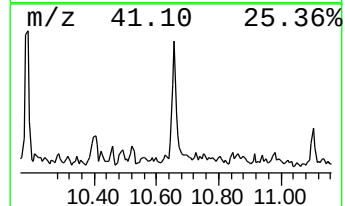
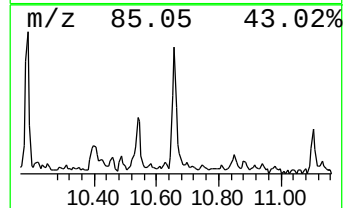
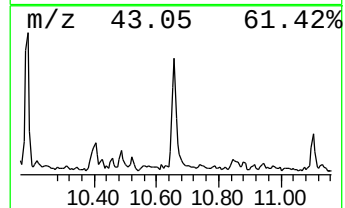
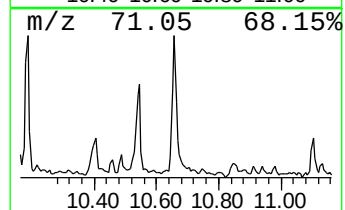
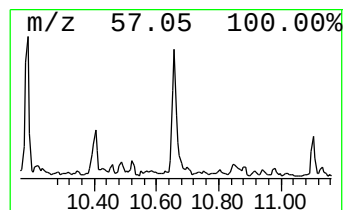
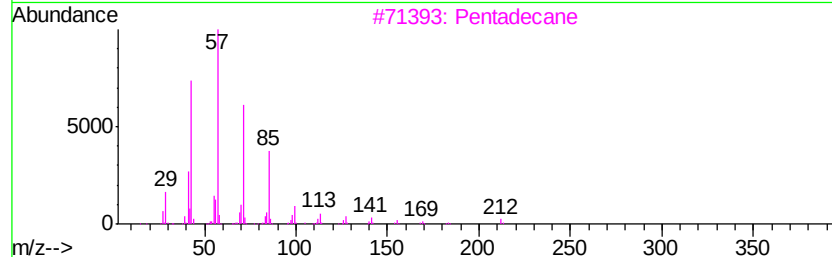
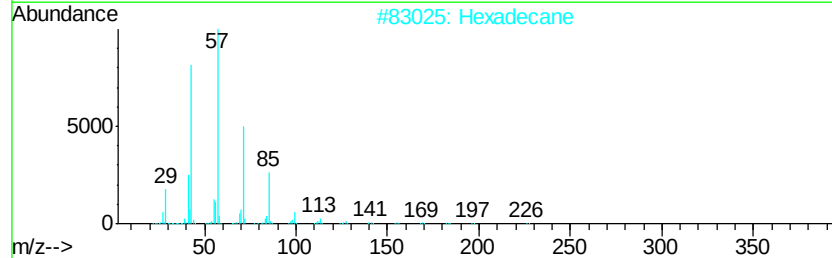
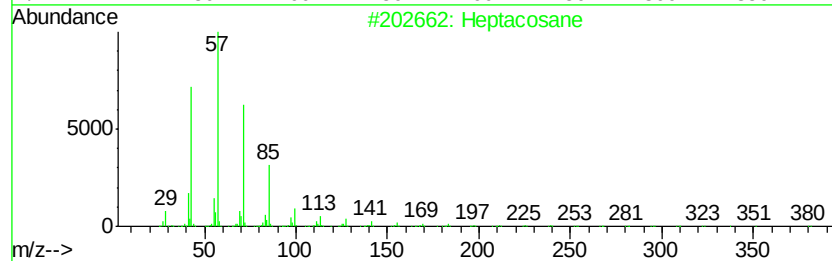
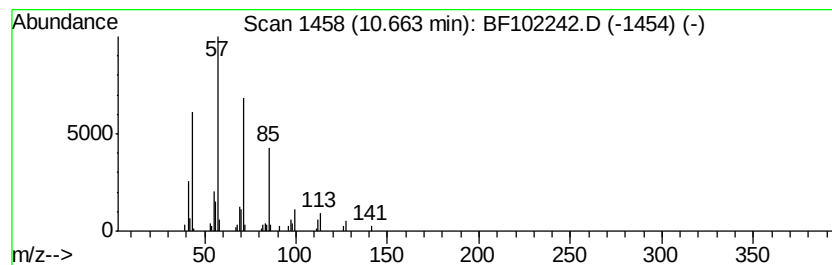
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Peak Number 5 Heptacosane Concentration Rank 5

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 10.66 | 2.47 ng | 126772 | Phenanthrene-d10 | 11.24 |

| Hit# of | 5                                   | Tentative ID | MW  | MolForm | CAS#        | Qual |
|---------|-------------------------------------|--------------|-----|---------|-------------|------|
| 1       | Heptacosane                         |              | 380 | C27H56  | 000593-49-7 | 91   |
| 2       | Hexadecane                          |              | 226 | C16H34  | 000544-76-3 | 90   |
| 3       | Pentadecane                         |              | 212 | C15H32  | 000629-62-9 | 90   |
| 4       | Heptadecane, 2,6,10,15-tetramethyl- |              | 296 | C21H44  | 054833-48-6 | 87   |
| 5       | Eicosane                            |              | 282 | C20H42  | 000112-95-8 | 83   |



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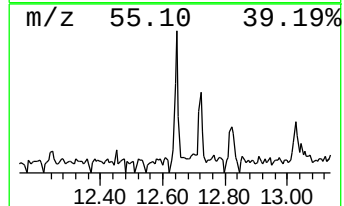
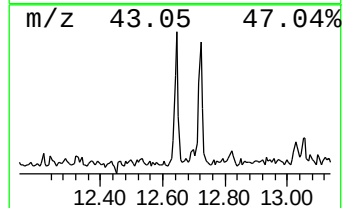
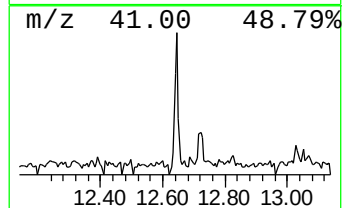
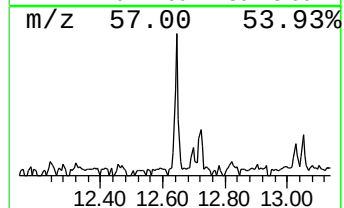
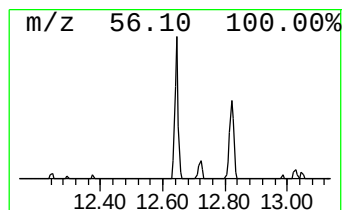
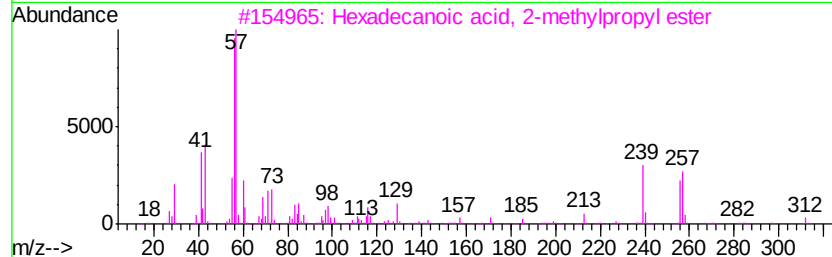
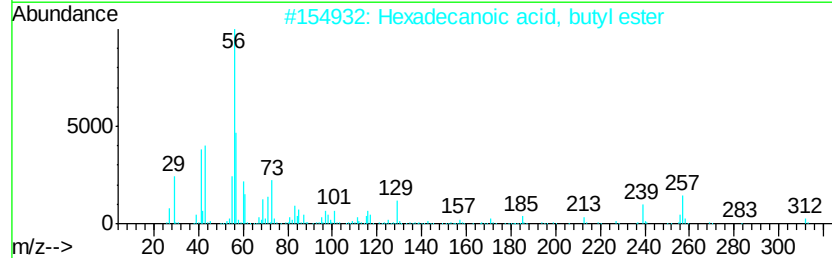
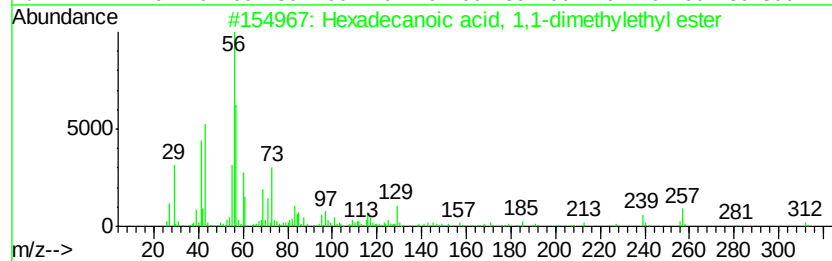
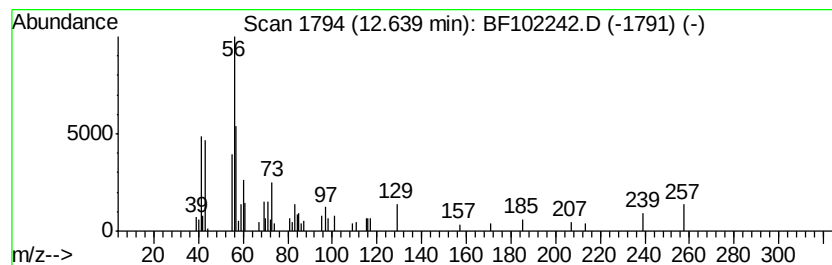
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 6 Hexadecanoic acid, 1,1-dime... Concentration Rank 7

| R.T.  | EstConc | Area  | Relative to ISTD | R.T.  |
|-------|---------|-------|------------------|-------|
| 12.64 | 2.02 ng | 72190 | Chrysene-d12     | 13.87 |

| Hit# | of | Tentative ID                         | MW  | MolForm  | CAS#        | Qual |
|------|----|--------------------------------------|-----|----------|-------------|------|
| 1    | 5  | Hexadecanoic acid, 1,1-dimethyle...  | 312 | C20H40O2 | 031158-91-5 | 91   |
| 2    |    | Hexadecanoic acid, butyl ester       | 312 | C20H40O2 | 000111-06-8 | 91   |
| 3    |    | Hexadecanoic acid, 2-methylpropyl... | 312 | C20H40O2 | 000110-34-9 | 59   |
| 4    |    | 5-Methyl-5-hexen-3-ol                | 114 | C7H14O   | 067760-89-8 | 35   |
| 5    |    | Pentadecane, 8-methylene-            | 224 | C16H32   | 055668-09-2 | 32   |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011918\  
 Data File : BF102242.D  
 Acq On : 20 Jan 2018 2:52  
 Operator : SJ/JU  
 Sample : J1114-11  
 Misc :  
 ALS Vial : 18 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 SB-26-2.0-2.5

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF010918.M  
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

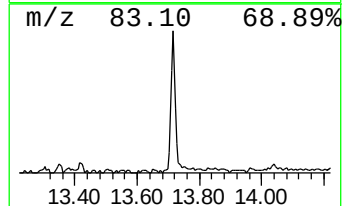
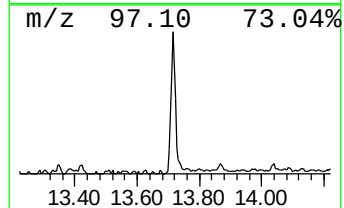
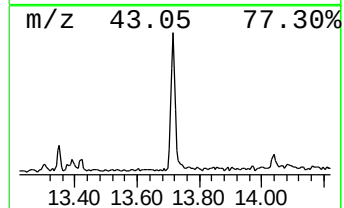
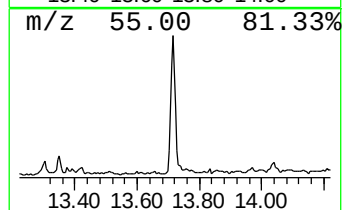
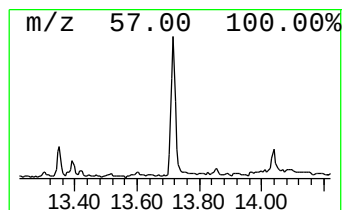
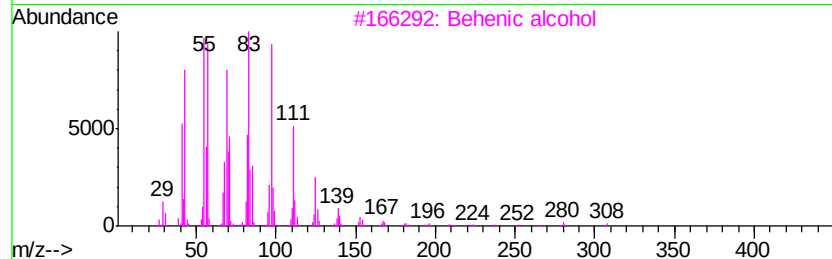
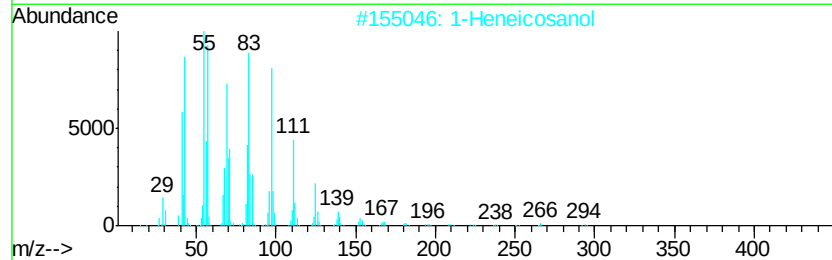
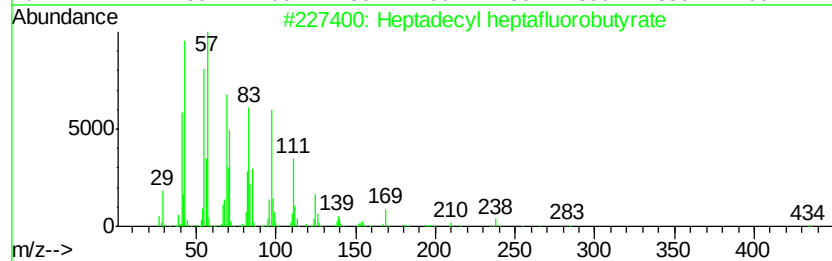
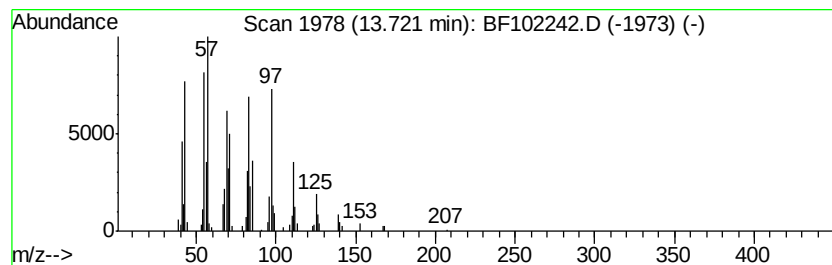
TIC Library : C:\DATABASE\NIST11.L  
 TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
 Peak Number 7 Heptadecyl heptafluorobutyrate Concentration Rank 3

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 13.72 | 7.66 ng | 273236 | Chrysene-d12     | 13.87 |

| Hit# | of | Tentative ID                   | MW  | MolForm    | CAS#         | Qual |
|------|----|--------------------------------|-----|------------|--------------|------|
| 1    | 5  | Heptadecyl heptafluorobutyrate | 452 | C21H35F7O2 | 959085-66-6  | 95   |
| 2    |    | 1-Heneicosanol                 | 312 | C21H44O    | 015594-90-8  | 95   |
| 3    |    | Behenic alcohol                | 326 | C22H46O    | 000661-19-8  | 95   |
| 4    |    | Octacosanol                    | 410 | C28H58O    | 000557-61-9  | 94   |
| 5    |    | Heptacosyl acetate             | 438 | C29H58O2   | 1000351-78-2 | 94   |





Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF011918\  
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Acq On : 20 Jan 2018 2:52  
Operator : SJ/JU  
Sample : J1114-11  
Misc :  
ALS Vial : 18 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
SB-26-2.0-2.5

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF010918.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... | 4.93  | 7.2     | ng    | 298513   | 1                     | 6.72  | 828947  | 20.0 |
| unknown6.49          | 6.49  | 92.5    | ng    | 3834120  | 1                     | 6.72  | 828947  | 20.0 |
| Hexadecane           | 10.19 | 2.1     | ng    | 121069   | 3                     | 9.75  | 1148070 | 20.0 |
| Heptacosane          | 10.66 | 2.5     | ng    | 126772   | 4                     | 11.24 | 1025180 | 20.0 |
| Hexadecanoic acid... | 12.64 | 2.0     | ng    | 72190    | 5                     | 13.87 | 713625  | 20.0 |
| Heptadecyl heptaf... | 13.72 | 7.7     | ng    | 273236   | 5                     | 13.87 | 713625  | 20.0 |