

Data Path : Z:\HPCHEM1\BNA F\DATA\BF082417\  
 Data File : BF098009.D  
 Acq On : 24 Aug 2017 18:37  
 Operator : SJ/JU  
 Sample : I4925-03  
 Misc :  
 ALS Vial : 10 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 RWB-1

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-BF081517.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         | 4.934       | 480           | 484         | 493          | rVB      | 195083         | 267726        | 8.69%           | 1.036%        |
| 2         | 5.345       | 549           | 554         | 557          | rBV      | 2823851        | 2825182       | 91.73%          | 10.936%       |
| 3         | 6.375       | 723           | 729         | 741          | rBV      | 2831639        | 3079871       | 100.00%         | 11.922%       |
| 4         | 6.504       | 746           | 751         | 755          | rBV      | 2685538        | 2788874       | 90.55%          | 10.795%       |
| 5         | 6.739       | 787           | 791         | 794          | rBV      | 815154         | 751489        | 24.40%          | 2.909%        |
| 6         | 6.892       | 813           | 817         | 820          | rBV      | 2108047        | 1801582       | 58.50%          | 6.974%        |
| 7         | 7.298       | 881           | 886         | 889          | rBV      | 1643831        | 1679510       | 54.53%          | 6.501%        |
| 8         | 8.022       | 1004          | 1009        | 1012         | rBV      | 1067308        | 967463        | 31.41%          | 3.745%        |
| 9         | 9.098       | 1186          | 1192        | 1195         | rBV      | 2345885        | 2142504       | 69.56%          | 8.293%        |
| 10        | 9.492       | 1254          | 1259        | 1262         | rBV      | 616270         | 512610        | 16.64%          | 1.984%        |
| 11        | 9.769       | 1301          | 1306        | 1310         | rBV      | 1008776        | 993714        | 32.26%          | 3.846%        |
| 12        | 10.557      | 1435          | 1440        | 1444         | rBV      | 1631539        | 1574361       | 51.12%          | 6.094%        |
| 13        | 10.680      | 1458          | 1461        | 1470         | rVB      | 45636          | 47694         | 1.55%           | 0.185%        |
| 14        | 11.251      | 1554          | 1558        | 1561         | rBV      | 1159384        | 1032193       | 33.51%          | 3.995%        |
| 15        | 11.274      | 1561          | 1562        | 1565         | rVB      | 64756          | 34009         | 1.10%           | 0.132%        |
| 16        | 11.480      | 1592          | 1597        | 1603         | rBV3     | 49609          | 56760         | 1.84%           | 0.220%        |
| 17        | 12.298      | 1733          | 1736        | 1741         | rBV      | 286096         | 297764        | 9.67%           | 1.153%        |
| 18        | 12.357      | 1744          | 1746        | 1748         | rVB2     | 42595          | 31475         | 1.02%           | 0.122%        |
| 19        | 12.457      | 1758          | 1763        | 1767         | rBV      | 251801         | 226945        | 7.37%           | 0.878%        |
| 20        | 12.686      | 1796          | 1802        | 1805         | rBV      | 241450         | 264773        | 8.60%           | 1.025%        |
| 21        | 12.839      | 1824          | 1828        | 1831         | rVB      | 1842740        | 1708724       | 55.48%          | 6.614%        |
| 22        | 13.051      | 1861          | 1864        | 1867         | rBV3     | 48789          | 57648         | 1.87%           | 0.223%        |
| 23        | 13.286      | 1901          | 1904        | 1908         | rBV      | 89996          | 80922         | 2.63%           | 0.313%        |
| 24        | 13.733      | 1976          | 1980        | 1987         | rVB2     | 101949         | 133446        | 4.33%           | 0.517%        |
| 25        | 13.880      | 2000          | 2005        | 2008         | rBV      | 964304         | 1043595       | 33.88%          | 4.040%        |
| 26        | 13.904      | 2008          | 2009        | 2015         | rVB      | 115647         | 103927        | 3.37%           | 0.402%        |
| 27        | 14.733      | 2147          | 2150        | 2155         | rVB2     | 29217          | 33068         | 1.07%           | 0.128%        |
| 28        | 14.892      | 2173          | 2177        | 2187         | rVB      | 92333          | 171947        | 5.58%           | 0.666%        |
| 29        | 14.986      | 2189          | 2193        | 2200         | rBV4     | 31809          | 54253         | 1.76%           | 0.210%        |
| 30        | 15.180      | 2222          | 2226        | 2229         | rBV      | 47595          | 55520         | 1.80%           | 0.215%        |
| 31        | 15.233      | 2232          | 2235        | 2241         | rVB      | 72333          | 84348         | 2.74%           | 0.326%        |
| 32        | 15.298      | 2241          | 2246        | 2251         | rBV2     | 575125         | 691526        | 22.45%          | 2.677%        |
| 33        | 15.756      | 2319          | 2324        | 2328         | rBV      | 38580          | 57545         | 1.87%           | 0.223%        |
| 34        | 15.798      | 2328          | 2331        | 2339         | rVB9     | 16124          | 31911         | 1.04%           | 0.124%        |

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Misc :  
ALS Vial : 10 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
RWB-1

Integration Parameters: rteint.p  
Integrator: RTE  
Smoothing : ON Filtering: 5  
Sampling : 1 Min Area: 3 % of largest Peak  
Start Thrs: 0.2 Max Peaks: 100  
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >  
Peak separation: 5

Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF081517.M  
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

|    |        |      |      |      |      |       |       |       |        |
|----|--------|------|------|------|------|-------|-------|-------|--------|
| 35 | 16.656 | 2472 | 2477 | 2486 | rVB2 | 27478 | 57811 | 1.88% | 0.224% |
| 36 | 17.068 | 2543 | 2547 | 2556 | rVB2 | 24880 | 54166 | 1.76% | 0.210% |
| 37 | 17.745 | 2657 | 2662 | 2669 | rBV7 | 19179 | 37662 | 1.22% | 0.146% |

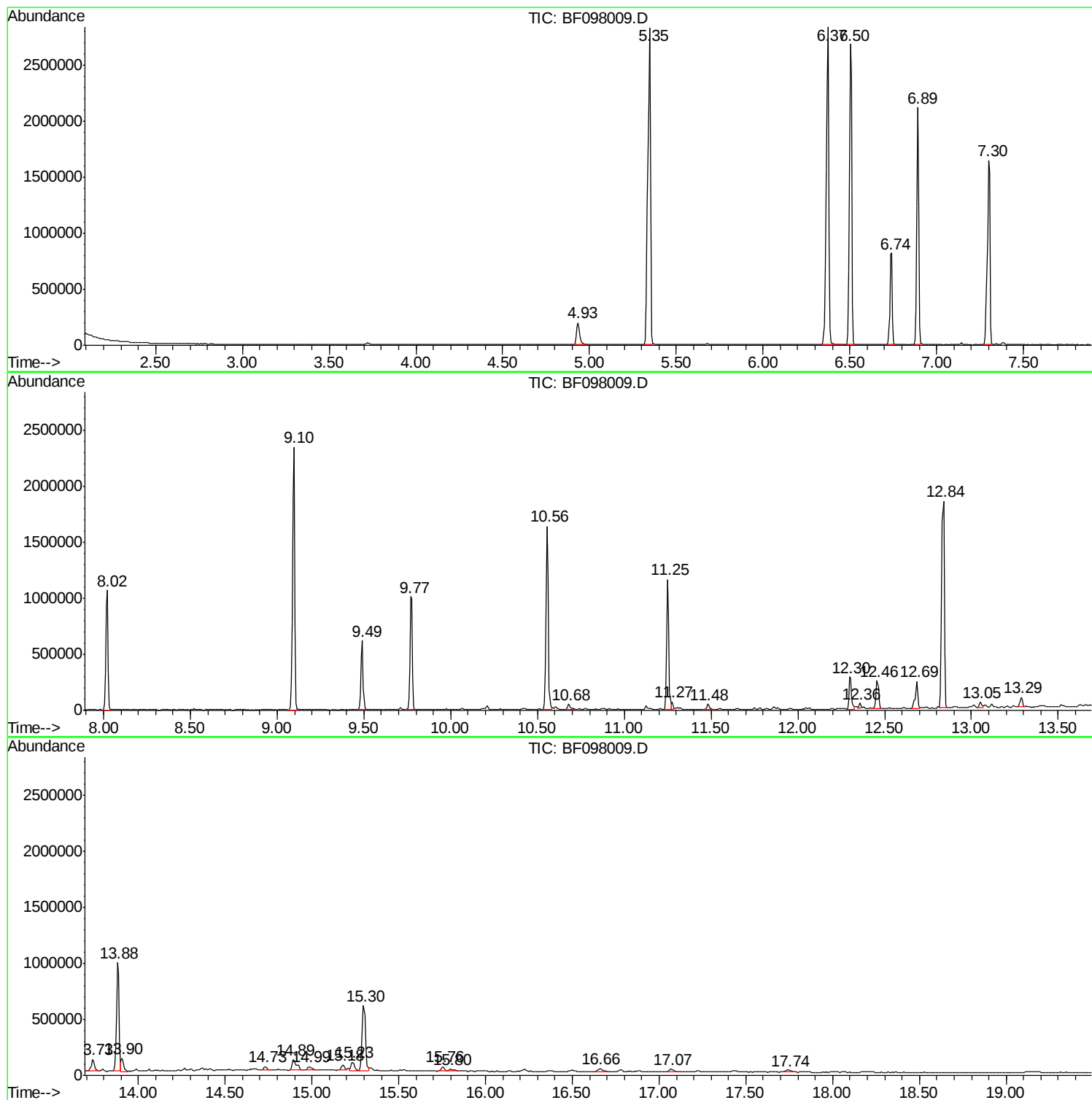
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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF081517.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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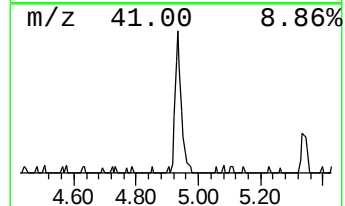
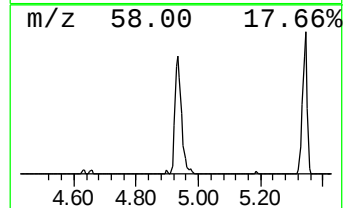
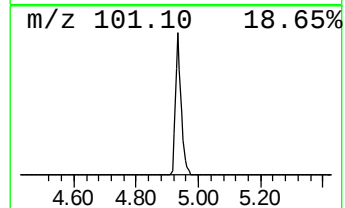
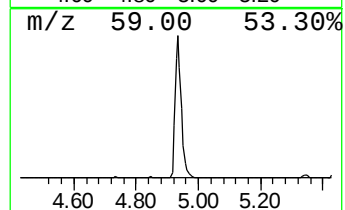
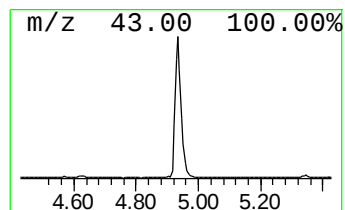
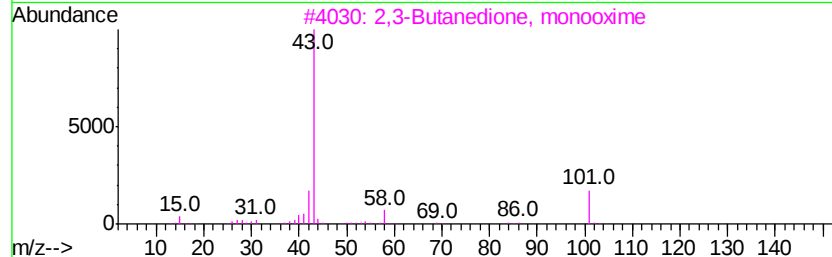
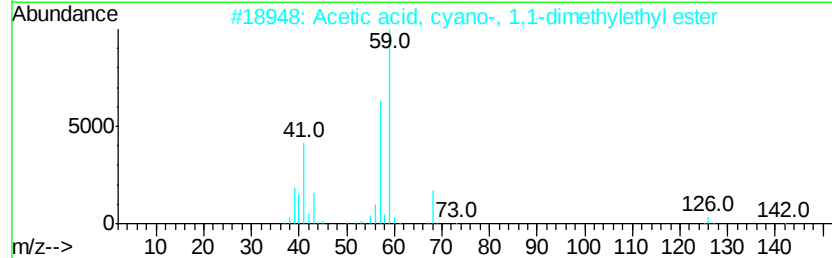
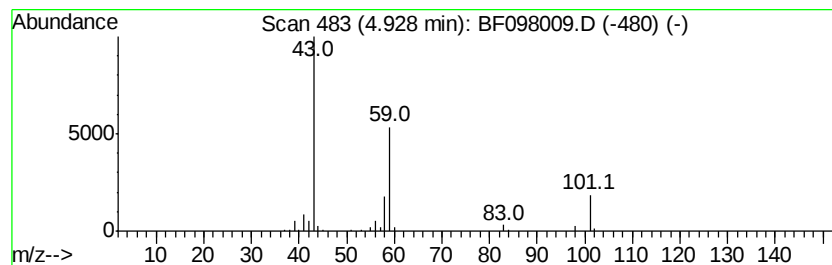
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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

| R.T. | EstConc | Area   | Relative to ISTD       | R.T. |
|------|---------|--------|------------------------|------|
| 4.93 | 7.13 ng | 267726 | 1,4-Dichlorobenzene-d4 | 6.74 |

| Hit# | of | Tentative ID                         | MW  | MolForm  | CAS#        | Qual |
|------|----|--------------------------------------|-----|----------|-------------|------|
| 1    | 5  | 2-Pentanone, 4-hydroxy-4-methyl-     | 116 | C6H12O2  | 000123-42-2 | 72   |
| 2    |    | Acetic acid, cyano-, 1,1-dimethyl... | 141 | C7H11NO2 | 001116-98-9 | 25   |
| 3    |    | 2,3-Butanedione, monooxime           | 101 | C4H7NO2  | 000057-71-6 | 9    |
| 4    |    | Acetone                              | 58  | C3H6O    | 000067-64-1 | 9    |
| 5    |    | Acetic acid, 1,1-dimethylethyl e...  | 116 | C6H12O2  | 000540-88-5 | 9    |



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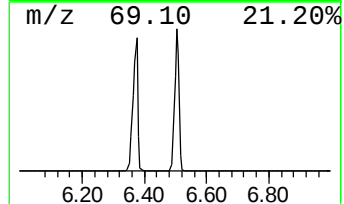
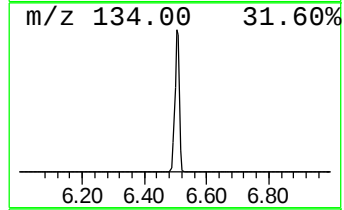
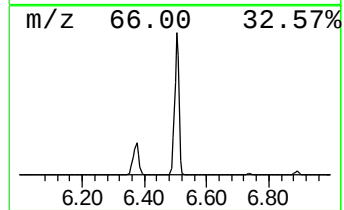
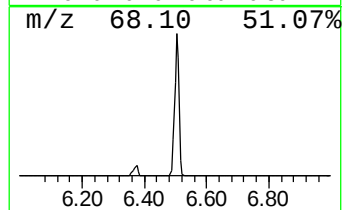
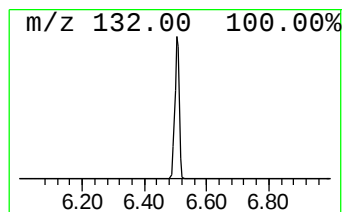
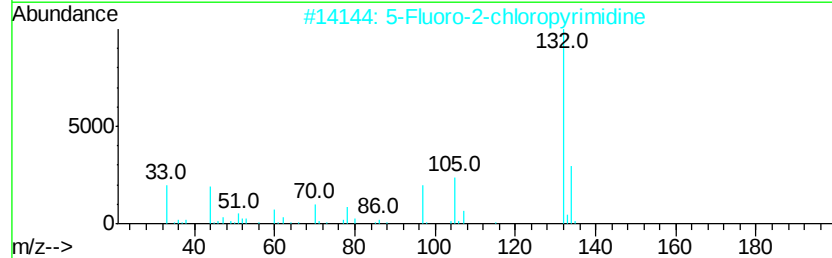
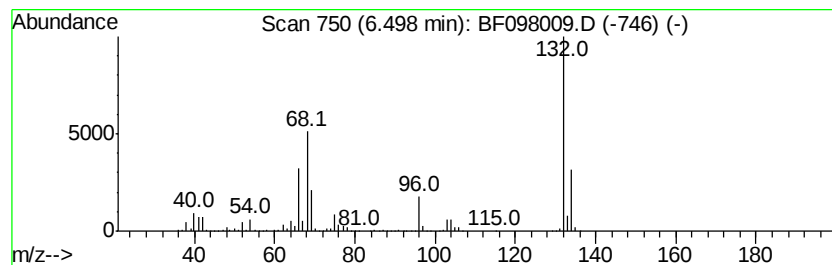
Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF081517.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 2 unknown6.50 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.50 | 74.22 ng | 2788870 | 1,4-Dichlorobenzene-d4 | 6.74 |

| Hit# | of | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|-------------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 3-Chloro-6-fluoro-pyrazine          | 132 | C4H2ClFN2 | 1000146-10-7 | 27   |
| 2    |    | 5-Fluoro-2-chloropyrimidine         | 132 | C4H2ClFN2 | 062802-42-0  | 12   |
| 3    |    | Tranvlcyproline-propionyl           | 189 | C12H15NO  | 1000123-86-3 | 10   |
| 4    |    | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12    | 028749-81-7  | 9    |
| 5    |    | Benzene, 1-ethenyl-3,5-dimethyl-    | 132 | C10H12    | 005379-20-4  | 9    |



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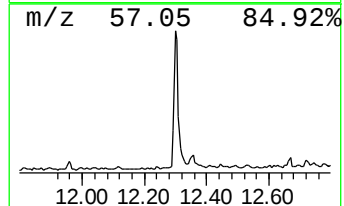
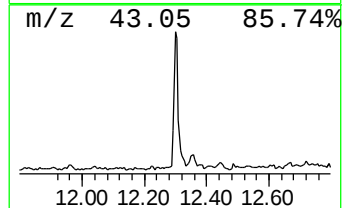
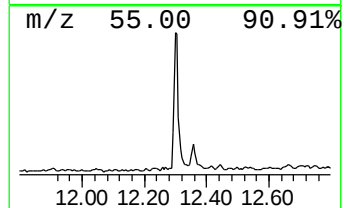
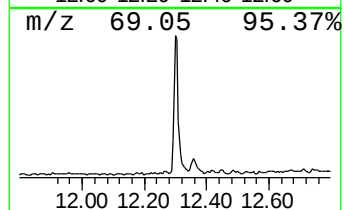
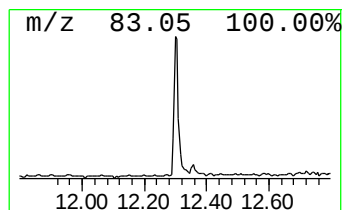
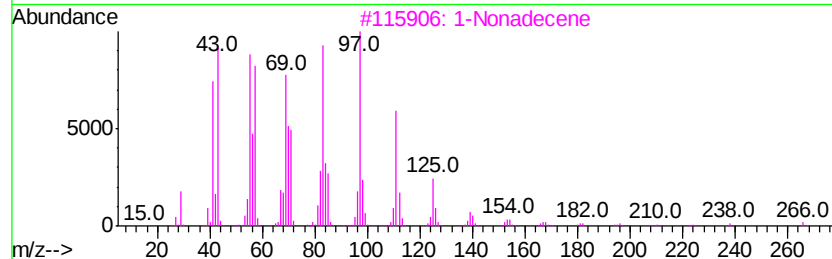
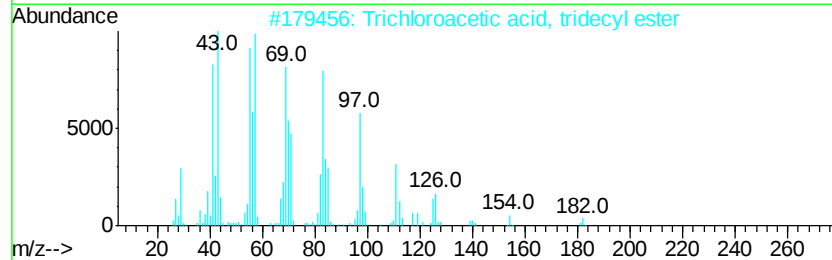
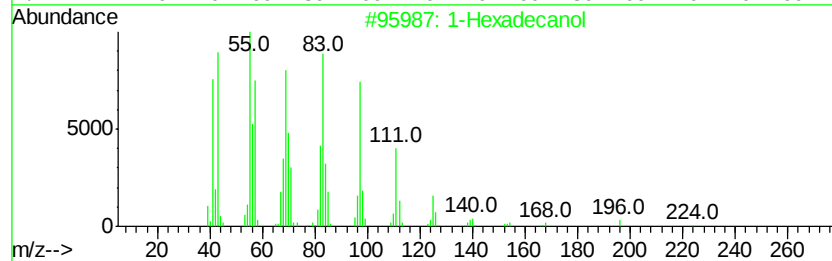
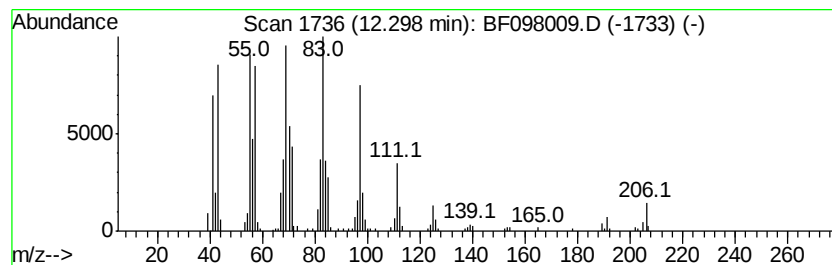
Instrument :  
BNA\_F  
ClientSampleId :  
RWB-1

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF081517.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 4 1-Hexadecanol Concentration Rank 4

| R.T.      | EstConc                             | Area   | Relative to ISTD | R.T.         |      |
|-----------|-------------------------------------|--------|------------------|--------------|------|
| 12.30     | 5.77 ng                             | 297764 | Phenanthrene-d10 | 11.25        |      |
| Hit# of 5 | Tentative ID                        | MW     | MolForm          | CAS#         | Qual |
| 1         | 1-Hexadecanol                       | 242    | C16H34O          | 036653-82-4  | 93   |
| 2         | Trichloroacetic acid, tridecyl e... | 344    | C15H27Cl3O2      | 074339-51-8  | 91   |
| 3         | 1-Nonadecene                        | 266    | C19H38           | 018435-45-5  | 91   |
| 4         | 9-Eicosene, (E)-                    | 280    | C20H40           | 074685-29-3  | 91   |
| 5         | Dichloroacetic acid, tridecyl ester | 310    | C15H28Cl2O2      | 1000280-48-3 | 91   |



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Instrument :  
BNA\_F  
ClientSampleId :  
RWB-1

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF081517.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

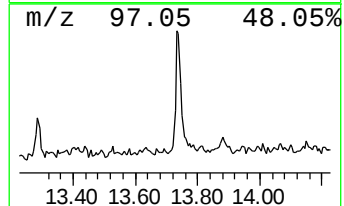
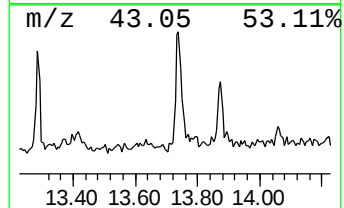
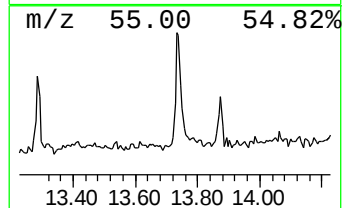
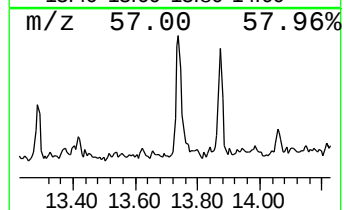
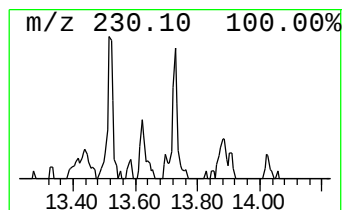
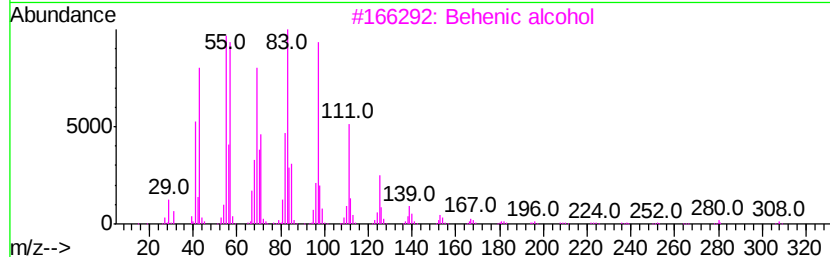
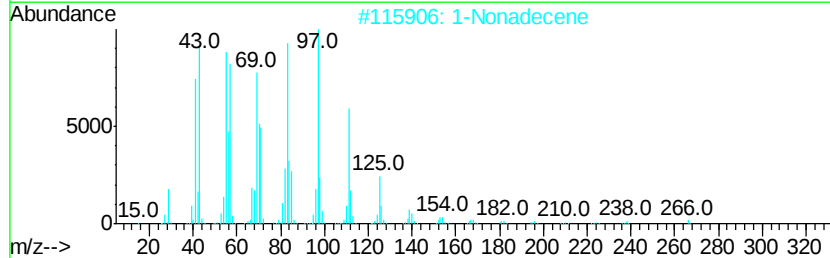
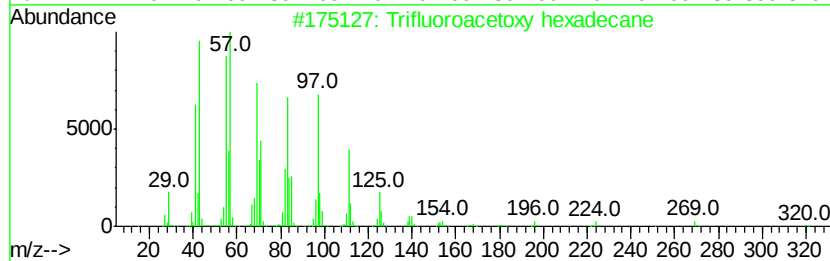
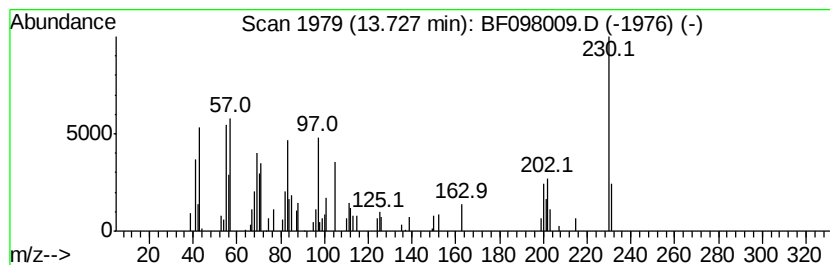
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 Trifluoroacetoxy hexadecane Concentration Rank 5

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 13.73 | 2.56 ng | 133446 | Chrysene-d12     | 13.89 |

| Hit# of | 5 | Tentative ID                | MW  | MolForm    | CAS#        | Qual |
|---------|---|-----------------------------|-----|------------|-------------|------|
| 1       |   | Trifluoroacetoxy hexadecane | 338 | C18H33F3O2 | 006222-03-3 | 91   |
| 2       |   | 1-Nonadecene                | 266 | C19H38     | 018435-45-5 | 87   |
| 3       |   | Behenic alcohol             | 326 | C22H46O    | 000661-19-8 | 87   |
| 4       |   | 1-Hexadecanol               | 242 | C16H34O    | 036653-82-4 | 87   |
| 5       |   | n-Tetracosanol-1            | 354 | C24H50O    | 000506-51-4 | 87   |



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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  | 7.1     | ng    | 267726   | 1                     | 6.74  | 751489  | 20.0 |
| unknown6.50          | 6.50  | 74.2    | ng    | 2788870  | 1                     | 6.74  | 751489  | 20.0 |
| 1-Hexadecanol        | 12.30 | 5.8     | ng    | 297764   | 4                     | 11.25 | 1032190 | 20.0 |
| Trifluoroacetoxy ... | 13.73 | 2.6     | ng    | 133446   | 5                     | 13.89 | 1043600 | 20.0 |