

Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF071117\  
 Data File : BF096645.D  
 Acq On : 11 Jul 2017 15:37  
 Operator : SJ/JU  
 Sample : I4118-01  
 Misc :  
 ALS Vial : 12 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 NAA-PIPE-SAND

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-BF070117.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         | 3.022       | 157           | 159         | 171          | rBV      | 34605          | 82332         | 2.78%           | 0.305%        |
| 2         | 4.875       | 469           | 474         | 481          | rBV      | 466589         | 640586        | 21.60%          | 2.376%        |
| 3         | 5.299       | 541           | 546         | 549          | rBV      | 2677177        | 2673522       | 90.14%          | 9.917%        |
| 4         | 6.328       | 715           | 721         | 724          | rBV      | 2601134        | 2761283       | 93.10%          | 10.243%       |
| 5         | 6.457       | 738           | 743         | 746          | rBV      | 2675944        | 2788240       | 94.01%          | 10.343%       |
| 6         | 6.681       | 778           | 781         | 785          | rBV      | 874742         | 736040        | 24.82%          | 2.730%        |
| 7         | 6.840       | 804           | 808         | 812          | rBV      | 2328626        | 2160034       | 72.83%          | 8.012%        |
| 8         | 7.245       | 871           | 877         | 880          | rBV      | 1910713        | 1863416       | 62.83%          | 6.912%        |
| 9         | 7.351       | 889           | 895         | 901          | rBV      | 45738          | 55490         | 1.87%           | 0.206%        |
| 10        | 7.963       | 995           | 999         | 1003         | rBV      | 1142892        | 1032393       | 34.81%          | 3.829%        |
| 11        | 9.045       | 1177          | 1183        | 1186         | rBV      | 2980921        | 2966013       | 100.00%         | 11.002%       |
| 12        | 9.434       | 1244          | 1249        | 1253         | rBV      | 662935         | 612763        | 20.66%          | 2.273%        |
| 13        | 9.716       | 1292          | 1297        | 1301         | rBV      | 1191029        | 1071064       | 36.11%          | 3.973%        |
| 14        | 10.163      | 1370          | 1373        | 1376         | rVB      | 40819          | 32900         | 1.11%           | 0.122%        |
| 15        | 10.504      | 1426          | 1431        | 1434         | rBV      | 1473833        | 1580666       | 53.29%          | 5.863%        |
| 16        | 10.633      | 1450          | 1453        | 1463         | rBV      | 64069          | 73908         | 2.49%           | 0.274%        |
| 17        | 11.080      | 1525          | 1529        | 1532         | rBV2     | 68436          | 58278         | 1.96%           | 0.216%        |
| 18        | 11.192      | 1544          | 1548        | 1552         | rBV      | 1116103        | 1007695       | 33.97%          | 3.738%        |
| 19        | 11.504      | 1597          | 1601        | 1606         | rBV      | 38791          | 34025         | 1.15%           | 0.126%        |
| 20        | 11.733      | 1637          | 1640        | 1643         | rBV      | 61066          | 55536         | 1.87%           | 0.206%        |
| 21        | 12.780      | 1813          | 1818        | 1822         | rBV      | 2349733        | 2524031       | 85.10%          | 9.362%        |
| 22        | 13.680      | 1968          | 1971        | 1979         | rBV      | 180416         | 187909        | 6.34%           | 0.697%        |
| 23        | 13.821      | 1991          | 1995        | 1999         | rBV      | 953955         | 866118        | 29.20%          | 3.213%        |
| 24        | 14.674      | 2136          | 2140        | 2144         | rVB      | 387604         | 358523        | 12.09%          | 1.330%        |
| 25        | 15.221      | 2227          | 2233        | 2238         | rBV      | 506523         | 626445        | 21.12%          | 2.324%        |
| 26        | 15.668      | 2304          | 2309        | 2313         | rBV3     | 27224          | 40459         | 1.36%           | 0.150%        |
| 27        | 16.121      | 2383          | 2386        | 2392         | rVB4     | 17366          | 36307         | 1.22%           | 0.135%        |
| 28        | 17.298      | 2580          | 2586        | 2594         | rBV7     | 13149          | 33001         | 1.11%           | 0.122%        |

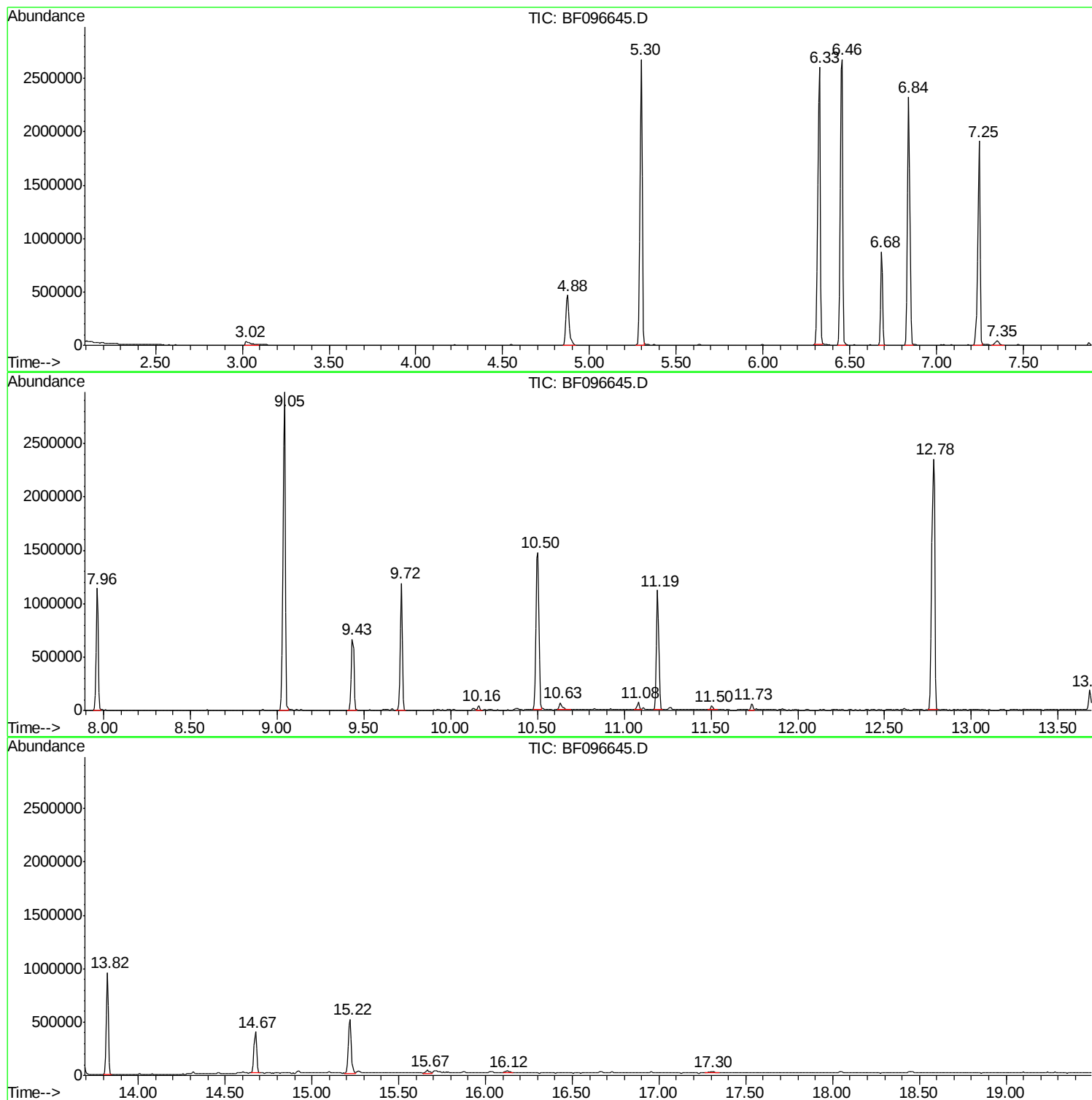
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ClientSampleId :  
NAA-PIPE-SAND

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF070117.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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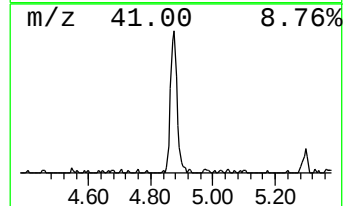
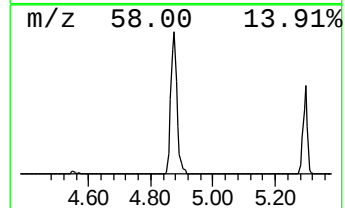
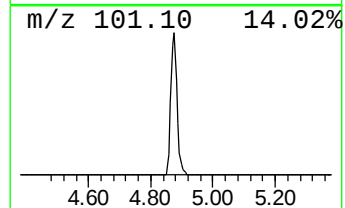
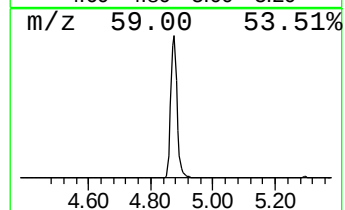
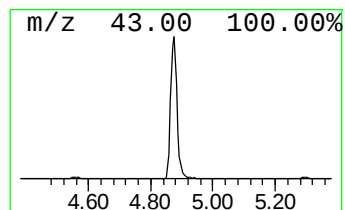
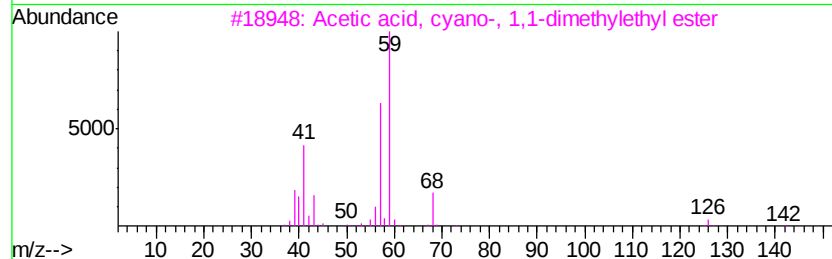
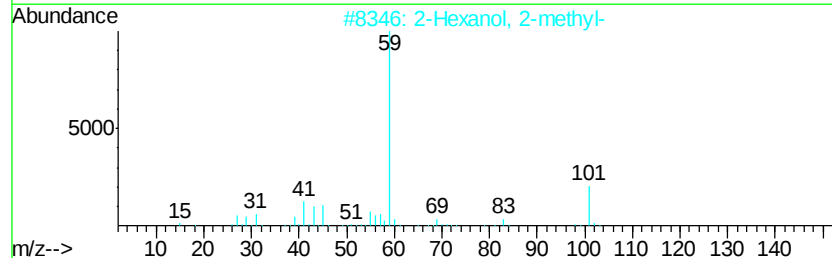
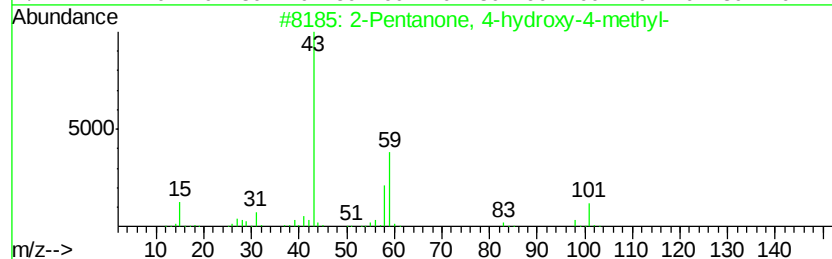
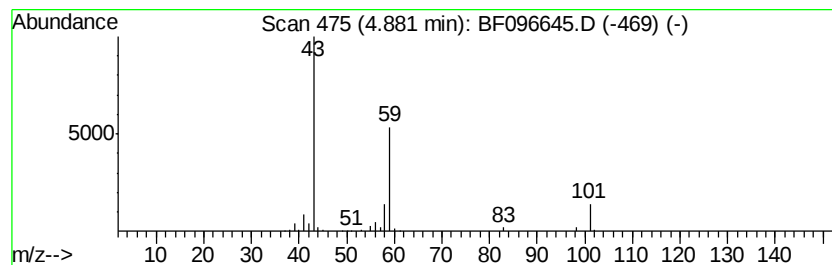
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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

| R.T. | EstConc  | Area   | Relative to ISTD       | R.T. |
|------|----------|--------|------------------------|------|
| 4.88 | 17.41 ng | 640586 | 1,4-Dichlorobenzene-d4 | 6.68 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2  | 000123-42-2 | 50   |
| 2    |    |   | 2-Hexanol, 2-methyl-                | 116 | C7H16O   | 000625-23-0 | 28   |
| 3    |    |   | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 25   |
| 4    |    |   | 2,3-Butanedione, monooxime          | 101 | C4H7NO2  | 000057-71-6 | 9    |
| 5    |    |   | Ethanol, pentamethyl-               | 116 | C7H16O   | 000594-83-2 | 9    |



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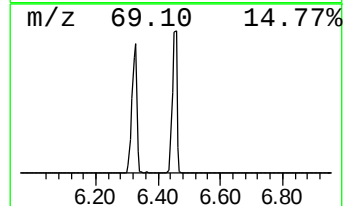
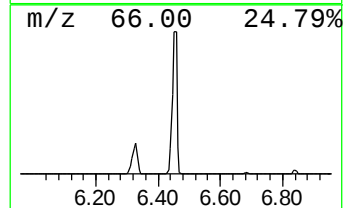
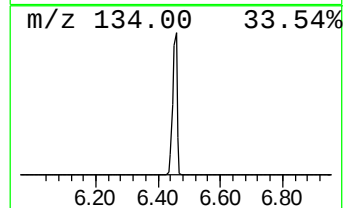
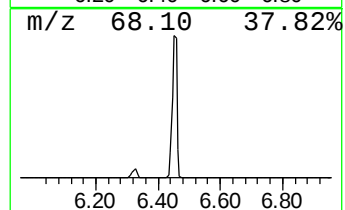
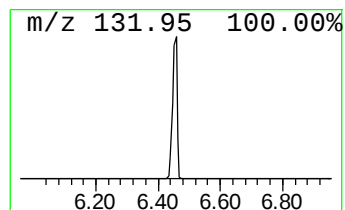
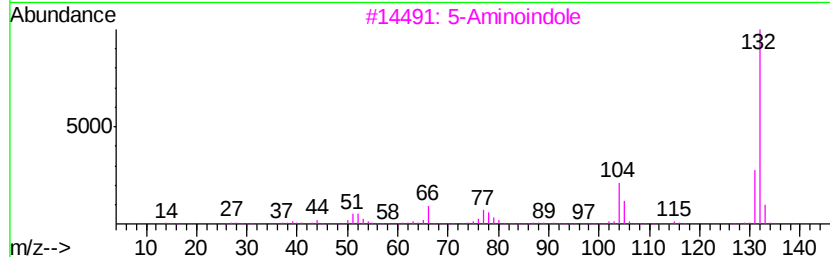
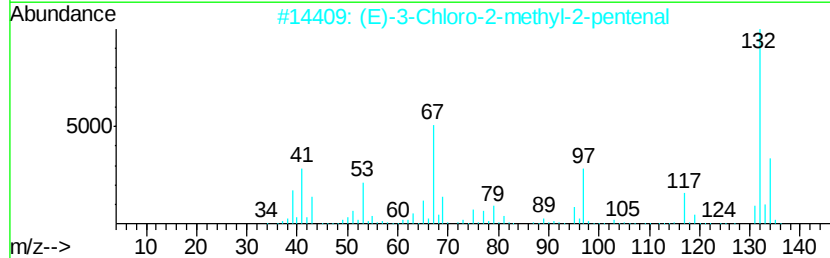
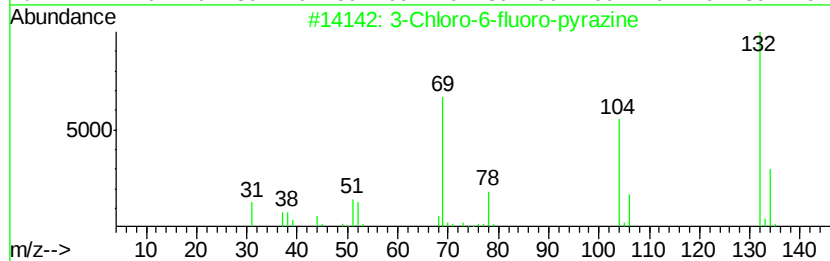
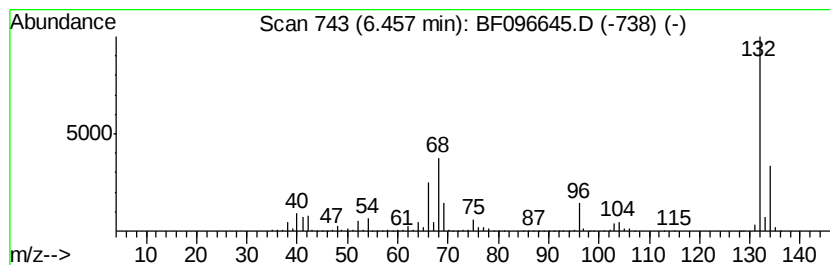
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 unknown6.46 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.46 | 75.76 ng | 2788240 | 1,4-Dichlorobenzene-d4 | 6.68 |

| Hit# | of                        | 5                          | Tentative ID | MW           | MolForm      | CAS# | Qual |
|------|---------------------------|----------------------------|--------------|--------------|--------------|------|------|
| 1    | 3                         | Chloro-6-fluoro-pyrazine   | 132          | C4H2ClFN2    | 1000146-10-7 | 35   |      |
| 2    | (E)-3                     | Chloro-2-methyl-2-pentenal | 132          | C6H9ClO      | 031357-76-3  | 17   |      |
| 3    | 5                         | Aminoindole                | 132          | C8H8N2       | 005192-03-0  | 12   |      |
| 4    | Tranylcypromine-propionyl | 189                        | C12H15NO     | 1000123-86-3 | 12           |      |      |
| 5    | 1,3,5                     | Trifluorobenzene           | 132          | C6H3F3       | 000372-38-3  | 9    |      |



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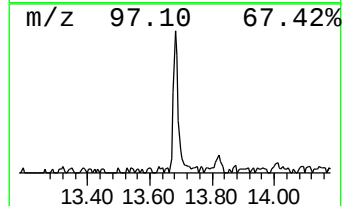
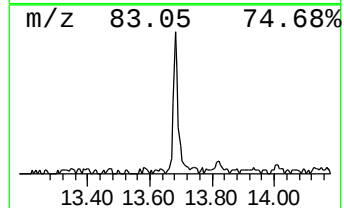
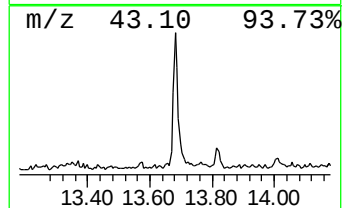
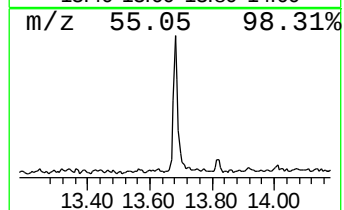
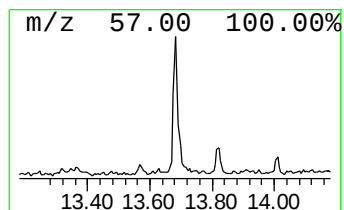
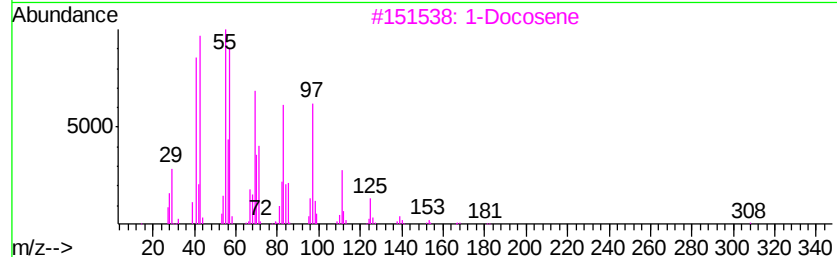
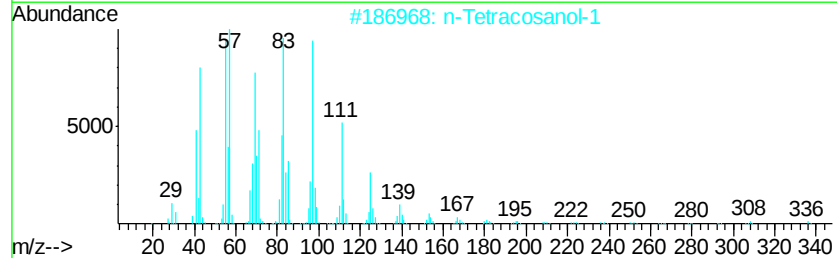
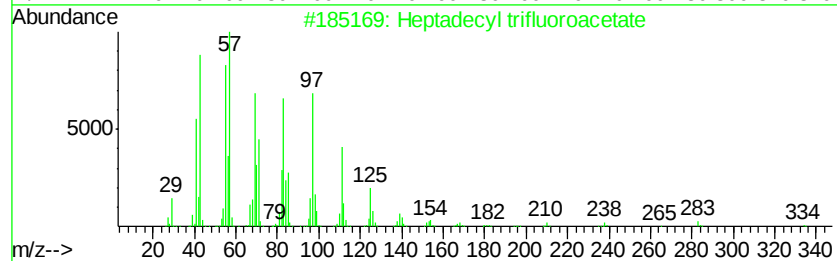
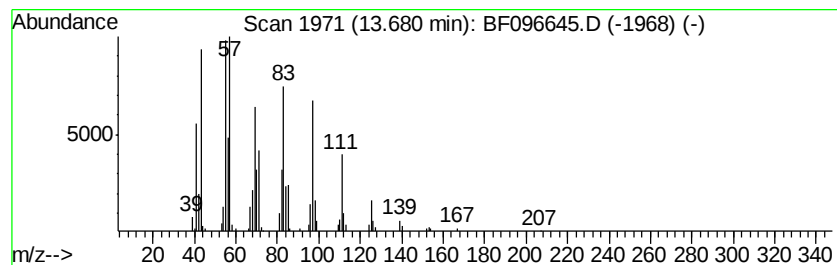
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ClientSampleId :  
NAA-PIPE-SAND

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

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Peak Number 5 Heptadecyl trifluoroacetate Concentration Rank 5

| R.T.      | EstConc                     | Area   | Relative to ISTD | R.T.         |      |
|-----------|-----------------------------|--------|------------------|--------------|------|
| 13.68     | 4.34 ng                     | 187909 | Chrysene-d12     | 13.82        |      |
| Hit# of 5 | Tentative ID                | MW     | MolForm          | CAS#         | Qual |
| 1         | Heptadecyl trifluoroacetate | 352    | C19H35F3O2       | 1000351-87-0 | 94   |
| 2         | n-Tetracosanol-1            | 354    | C24H50O          | 000506-51-4  | 93   |
| 3         | 1-Docosene                  | 308    | C22H44           | 001599-67-3  | 93   |
| 4         | Behenic alcohol             | 326    | C22H46O          | 000661-19-8  | 93   |
| 5         | 1-Heneicosanol              | 312    | C21H44O          | 015594-90-8  | 93   |



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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF070117.M  
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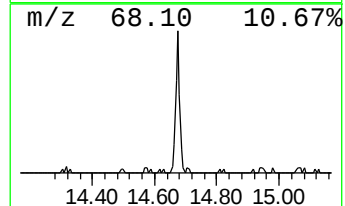
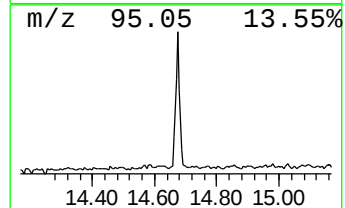
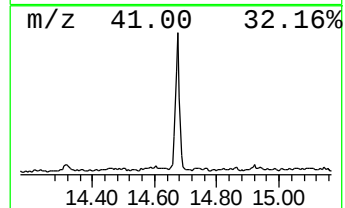
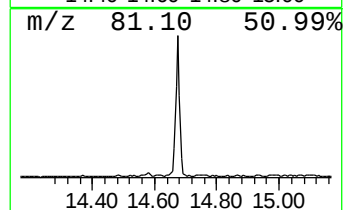
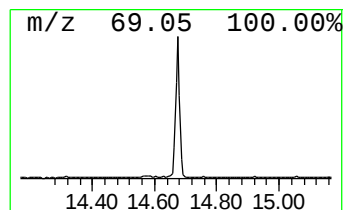
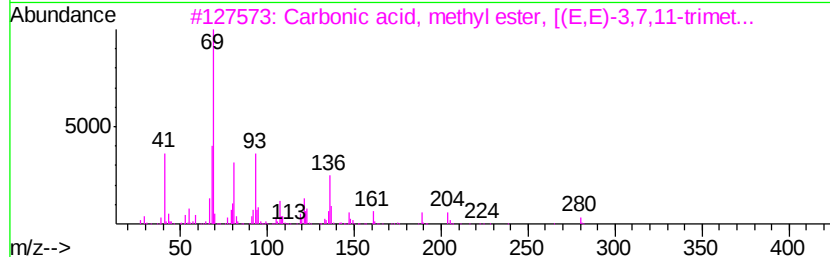
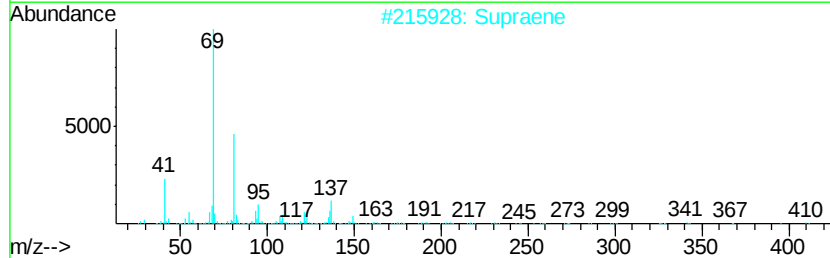
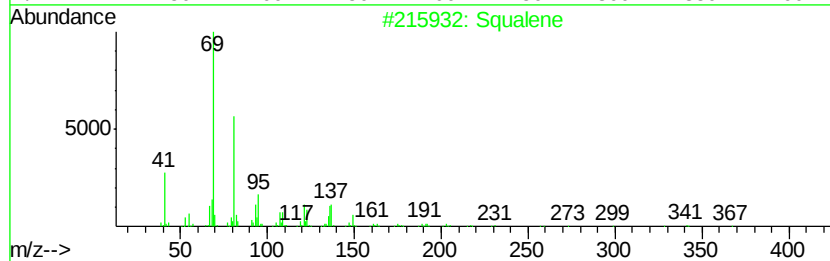
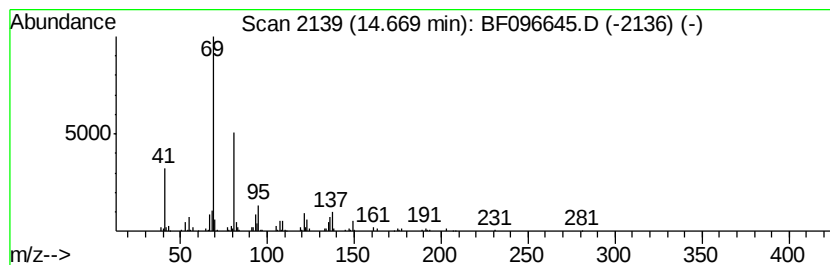
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Peak Number 6 Squalene Concentration Rank 4

| R.T.  | EstConc  | Area   | Relative to ISTD | R.T.  |
|-------|----------|--------|------------------|-------|
| 14.67 | 11.45 ng | 358523 | Perylene-d12     | 15.22 |

| Hit# | of | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|------|----|-------------------------------------|-----|----------|--------------|------|
| 1    | 5  | Squalene                            | 410 | C30H50   | 000111-02-4  | 91   |
| 2    |    | Supraene                            | 410 | C30H50   | 007683-64-9  | 91   |
| 3    |    | Carbonic acid, methyl ester, [(E... | 280 | C17H28O3 | 1000164-38-7 | 72   |
| 4    |    | 1,5-Heptadiene, 3,3,6-trimethyl-    | 138 | C10H18   | 035387-63-4  | 50   |
| 5    |    | Methanone, dicyclopropyl-           | 110 | C7H10O   | 001121-37-5  | 47   |



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| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                      |       |         |       |          | #                     | RT    | Resp   | Conc |
| 2-Pentanone, 4-hy... | 4.88  | 17.4    | ng    | 640586   | 1                     | 6.68  | 736040 | 20.0 |
| unknown6.46          | 6.46  | 75.8    | ng    | 2788240  | 1                     | 6.68  | 736040 | 20.0 |
| Heptadecyl triflu... | 13.68 | 4.3     | ng    | 187909   | 5                     | 13.82 | 866118 | 20.0 |
| Squalene             | 14.67 | 11.4    | ng    | 358523   | 6                     | 15.22 | 626445 | 20.0 |