

Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF111517\  
 Data File : BF100595.D  
 Acq On : 15 Nov 2017 18:26  
 Operator : SJ/JU  
 Sample : I6454-01  
 Misc :  
 ALS Vial : 19 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 N-NARANJITO-S001-0001-01

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-BF110817.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         | 5.116       | 510           | 515         | 528          | rBV      | 397260         | 545891        | 19.66%          | 2.306%        |
| 2         | 5.504       | 574           | 581         | 584          | rBV      | 2544648        | 2715803       | 97.80%          | 11.473%       |
| 3         | 6.510       | 746           | 752         | 755          | rBV      | 2462226        | 2776980       | 100.00%         | 11.731%       |
| 4         | 6.651       | 771           | 776         | 780          | rBV      | 2612032        | 2714065       | 97.73%          | 11.466%       |
| 5         | 6.881       | 812           | 815         | 819          | rVB      | 880954         | 761473        | 27.42%          | 3.217%        |
| 6         | 7.040       | 838           | 842         | 845          | rVB      | 2341168        | 2113120       | 76.09%          | 8.927%        |
| 7         | 7.445       | 905           | 911         | 914          | rBV      | 1768502        | 1751712       | 63.08%          | 7.400%        |
| 8         | 8.163       | 1029          | 1033        | 1037         | rBV      | 1161685        | 967938        | 34.86%          | 4.089%        |
| 9         | 9.239       | 1210          | 1216        | 1219         | rBV      | 3091791        | 2720837       | 97.98%          | 11.494%       |
| 10        | 9.628       | 1278          | 1282        | 1285         | rBV      | 170801         | 124535        | 4.48%           | 0.526%        |
| 11        | 9.916       | 1327          | 1331        | 1335         | rBV      | 1008770        | 923212        | 33.25%          | 3.900%        |
| 12        | 10.628      | 1448          | 1452        | 1455         | rBV      | 74441          | 56459         | 2.03%           | 0.239%        |
| 13        | 10.704      | 1461          | 1465        | 1469         | rBV      | 1447424        | 1296830       | 46.70%          | 5.478%        |
| 14        | 11.404      | 1580          | 1584        | 1587         | rBV      | 866685         | 708041        | 25.50%          | 2.991%        |
| 15        | 12.986      | 1849          | 1853        | 1856         | rBV      | 1861202        | 1656137       | 59.64%          | 6.996%        |
| 16        | 13.869      | 2000          | 2003        | 2011         | rBV      | 107134         | 119719        | 4.31%           | 0.506%        |
| 17        | 14.039      | 2028          | 2032        | 2035         | rBV      | 854535         | 701585        | 25.26%          | 2.964%        |
| 18        | 15.145      | 2216          | 2220        | 2223         | rBV      | 35472          | 36697         | 1.32%           | 0.155%        |
| 19        | 15.516      | 2277          | 2283        | 2291         | rBV      | 596505         | 750141        | 27.01%          | 3.169%        |
| 20        | 15.968      | 2355          | 2360        | 2364         | rBV      | 43579          | 59119         | 2.13%           | 0.250%        |
| 21        | 16.480      | 2441          | 2447        | 2455         | rBV2     | 36741          | 71995         | 2.59%           | 0.304%        |
| 22        | 17.080      | 2544          | 2549        | 2557         | rVB2     | 24751          | 46359         | 1.67%           | 0.196%        |
| 23        | 17.786      | 2665          | 2669        | 2680         | rVB8     | 20918          | 52742         | 1.90%           | 0.223%        |

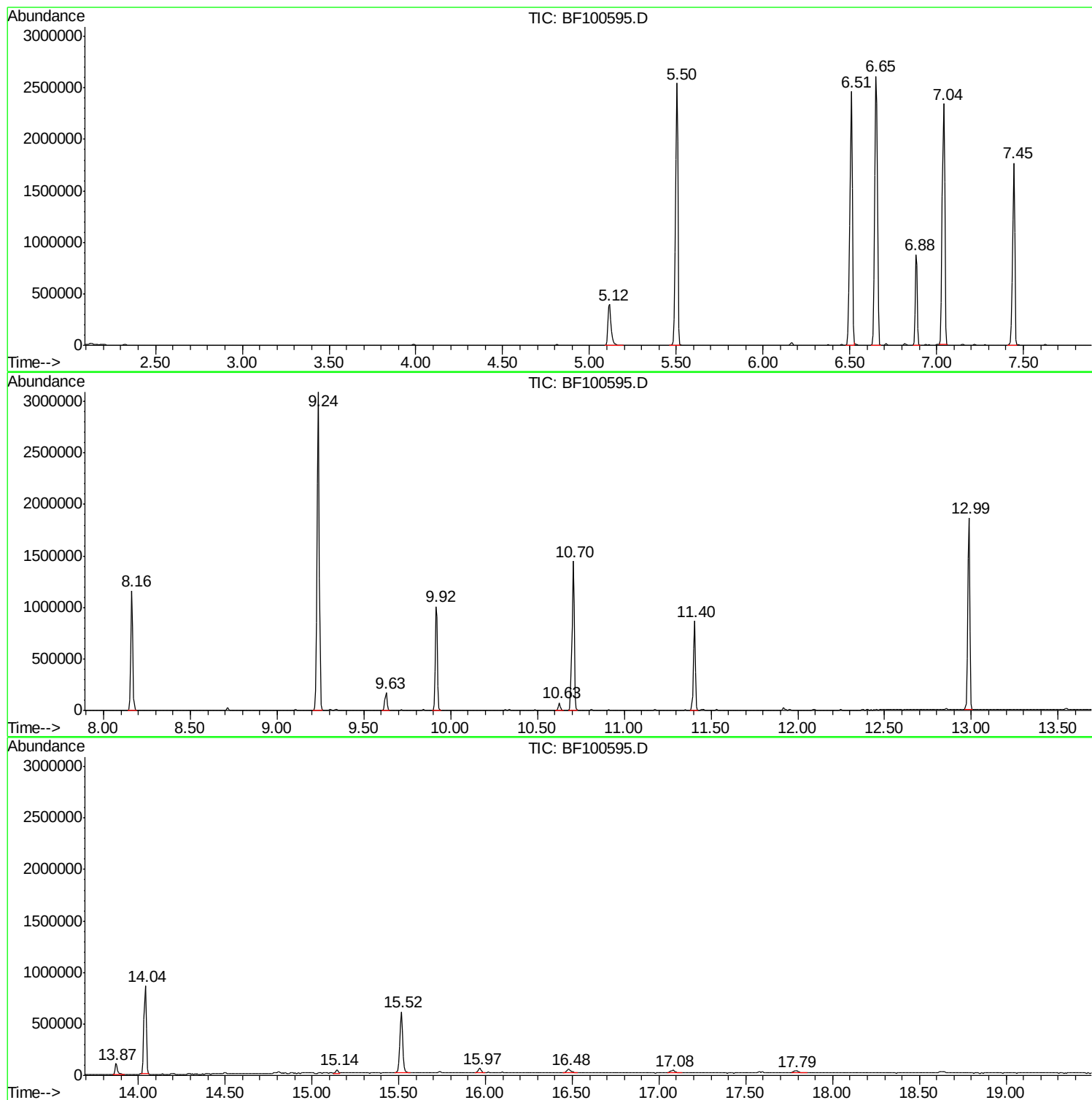
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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF110817.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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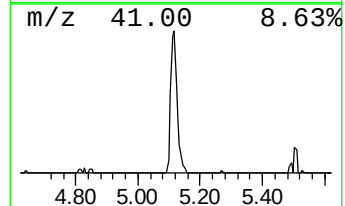
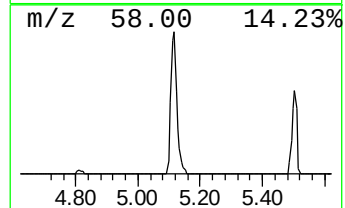
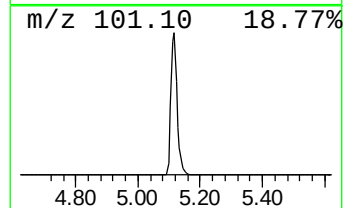
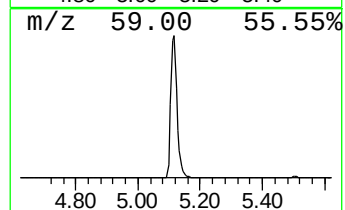
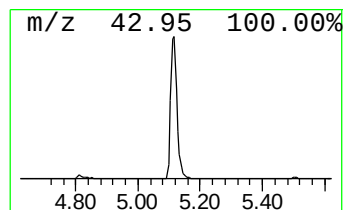
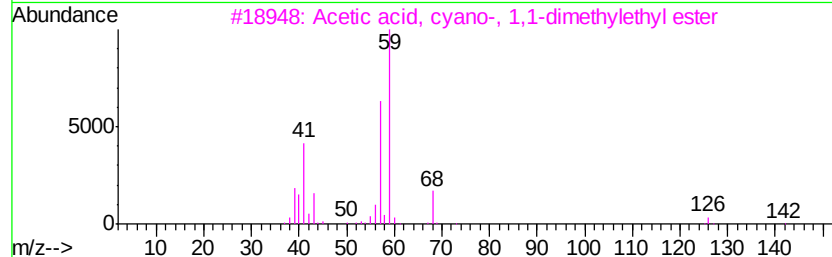
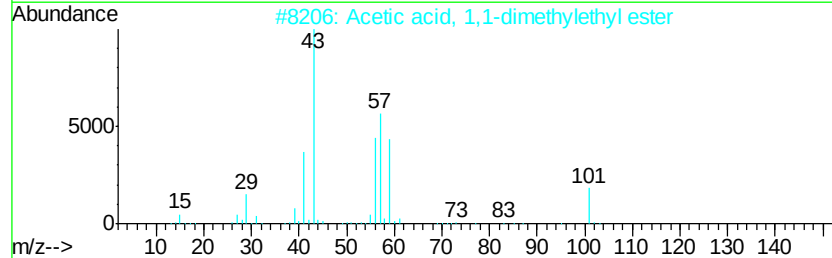
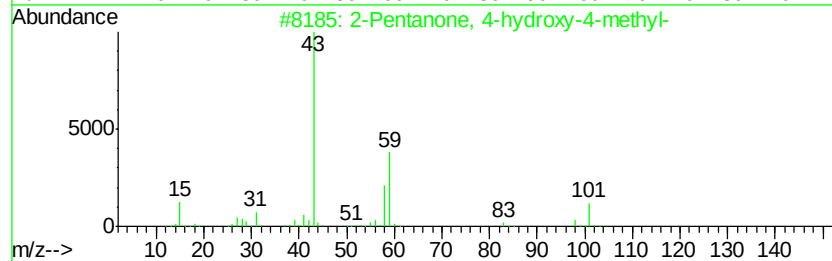
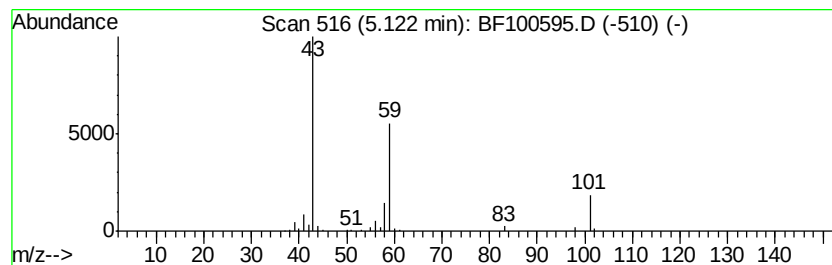
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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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. |
|------|----------|--------|------------------------|------|
| 5.12 | 14.34 ng | 545891 | 1,4-Dichlorobenzene-d4 | 6.88 |

| 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, 1,1-dimethylethyl e... | 116 | C6H12O2  | 000540-88-5 | 39   |
| 3    |    |   | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 23   |
| 4    |    |   | 2,3-Butanedione, monooxime          | 101 | C4H7NO2  | 000057-71-6 | 9    |
| 5    |    |   | 5-Oxohexanenitrile                  | 111 | C6H9NO   | 010412-98-3 | 9    |



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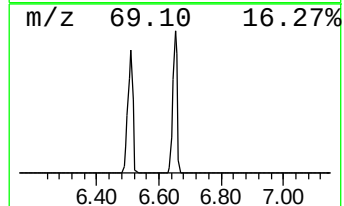
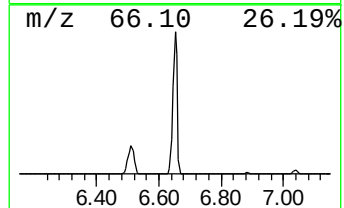
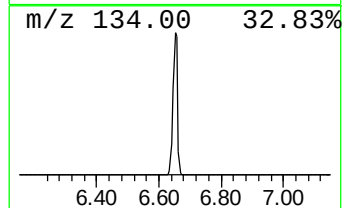
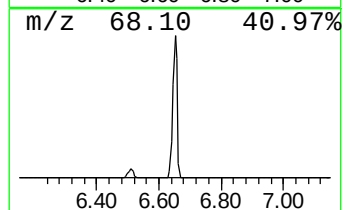
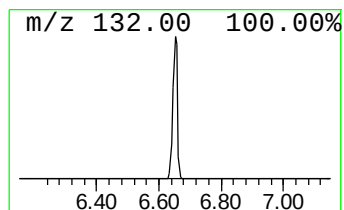
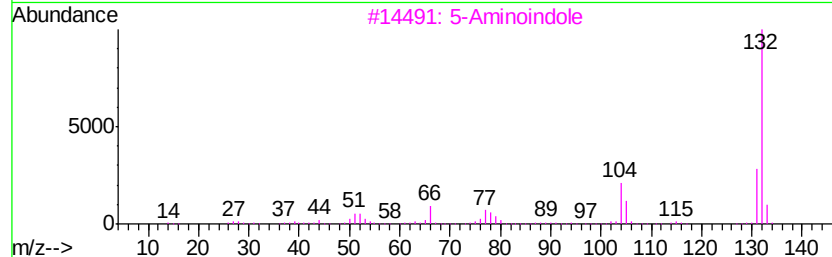
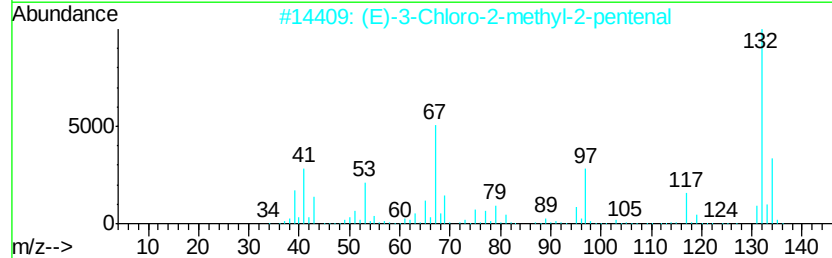
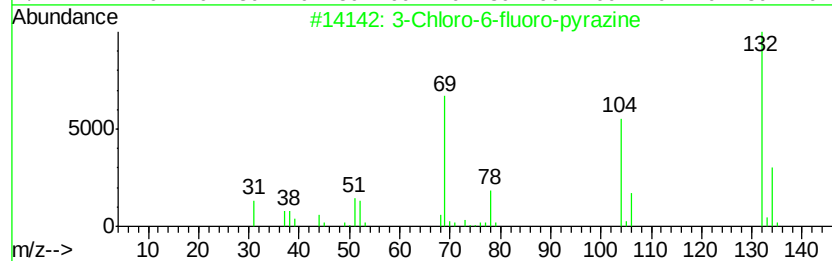
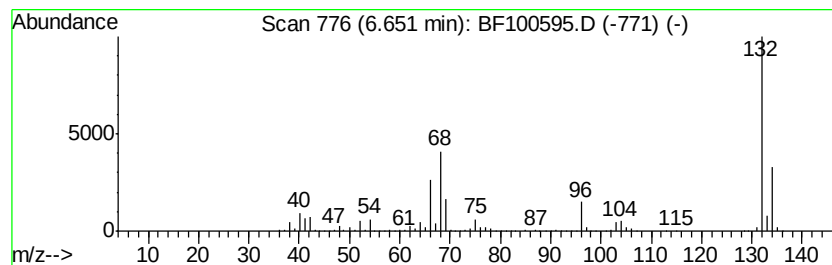
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Peak Number 2 unknown6.65 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.65 | 71.28 ng | 2714070 | 1,4-Dichlorobenzene-d4 | 6.88 |

| Hit# | of | Tentative ID                     | MW  | MolForm   | CAS#         | Qual |
|------|----|----------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 3-Chloro-6-fluoro-pyrazine       | 132 | C4H2ClFN2 | 1000146-10-7 | 27   |
| 2    |    | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO   | 031357-76-3  | 12   |
| 3    |    | 5-Aminoindole                    | 132 | C8H8N2    | 005192-03-0  | 12   |
| 4    |    | Tranlylcypromine-propionyl       | 189 | C12H15NO  | 1000123-86-3 | 10   |
| 5    |    | 4-Methylpyrrolo[1,2-a]pyrazine   | 132 | C8H8N2    | 064608-60-2  | 9    |



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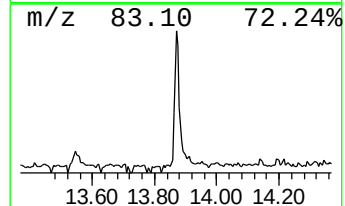
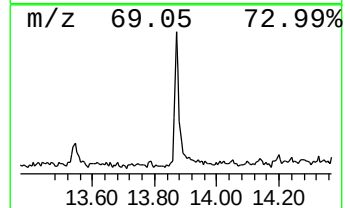
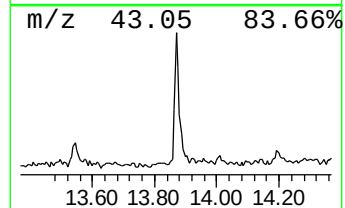
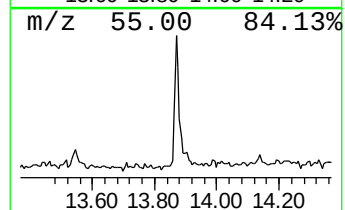
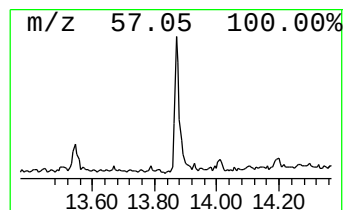
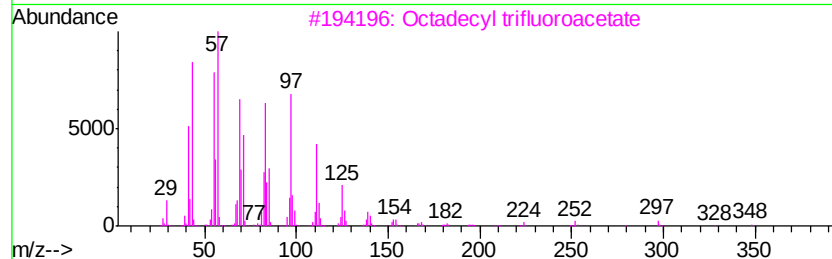
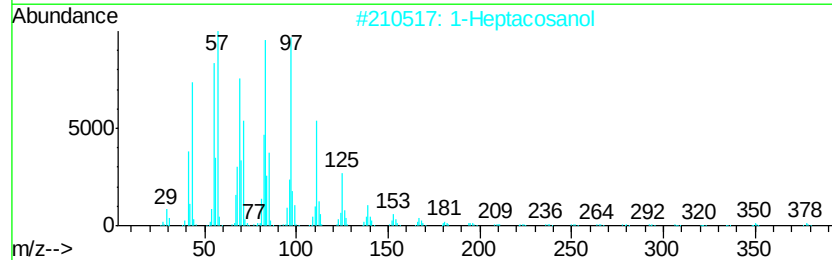
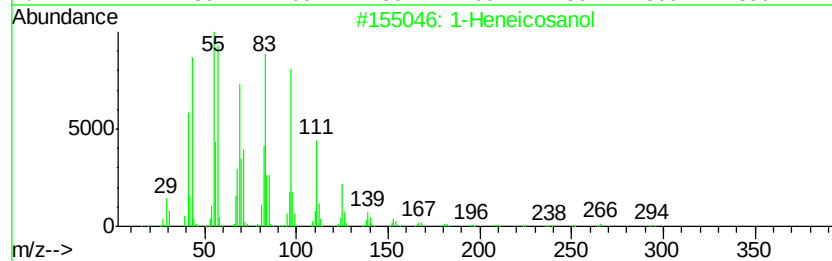
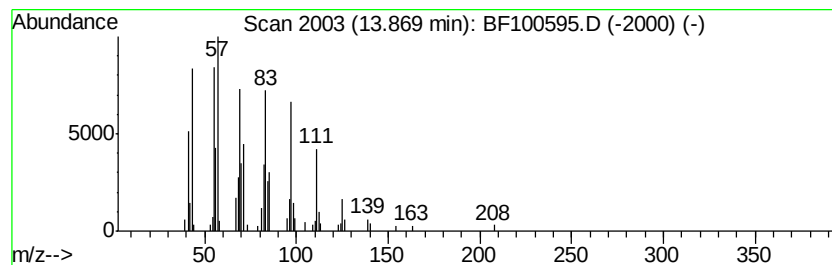
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ClientSampleId :  
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Peak Number 4 1-Heneicosanol Concentration Rank 4

| R.T.  | EstConc | Area   | Relative to ISTD            |     | R.T.       |              |      |
|-------|---------|--------|-----------------------------|-----|------------|--------------|------|
| 13.87 | 3.41 ng | 119719 | Chrysene-d12                |     | 14.04      |              |      |
| Hit#  | of      | 5      | Tentative ID                | MW  | MolForm    | CAS#         | Qual |
| 1     |         |        | 1-Heneicosanol              | 312 | C21H44O    | 015594-90-8  | 93   |
| 2     |         |        | 1-Heptacosanol              | 396 | C27H56O    | 002004-39-9  | 91   |
| 3     |         |        | Octadecyl trifluoroacetate  | 366 | C20H37F3O2 | 079392-43-1  | 91   |
| 4     |         |        | Heptadecyl trifluoroacetate | 352 | C19H35F3O2 | 1000351-87-0 | 91   |
| 5     |         |        | n-Tetracosanol-1            | 354 | C24H50O    | 000506-51-4  | 91   |



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| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                      |       |         |       |          | #                     | RT    | Resp   | Conc |
| 2-Pentanone, 4-hy... | 5.12  | 14.3    | ng    | 545891   | 1                     | 6.88  | 761473 | 20.0 |
| unknown6.65          | 6.65  | 71.3    | ng    | 2714070  | 1                     | 6.88  | 761473 | 20.0 |
| 1-Heneicosanol       | 13.87 | 3.4     | ng    | 119719   | 5                     | 14.04 | 701585 | 20.0 |