

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121217\  
 Data File : BF101358.D  
 Acq On : 13 Dec 2017 5:04  
 Operator : SJ/JU  
 Sample : I6764-04  
 Misc :  
 ALS Vial : 31 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 MAP-1-E(0-1)

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-BF113017.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         | 5.045       | 500           | 503         | 513          | rBV      | 34545          | 46972         | 4.45%           | 0.566%        |
| 2         | 5.445       | 567           | 571         | 588          | rBV      | 885313         | 862197        | 81.64%          | 10.397%       |
| 3         | 6.463       | 740           | 744         | 758          | rBV      | 872631         | 951584        | 90.11%          | 11.475%       |
| 4         | 6.598       | 763           | 767         | 770          | rBV      | 1072202        | 930374        | 88.10%          | 11.219%       |
| 5         | 6.822       | 802           | 805         | 813          | rBB      | 301993         | 243846        | 23.09%          | 2.940%        |
| 6         | 6.981       | 828           | 832         | 835          | rBV      | 840901         | 727881        | 68.92%          | 8.777%        |
| 7         | 7.392       | 898           | 902         | 913          | rBV      | 533923         | 512123        | 48.49%          | 6.175%        |
| 8         | 8.104       | 1020          | 1023        | 1042         | rBB      | 349552         | 309297        | 29.29%          | 3.730%        |
| 9         | 9.180       | 1202          | 1206        | 1209         | rBV      | 1328017        | 1056053       | 100.00%         | 12.734%       |
| 10        | 9.575       | 1267          | 1273        | 1279         | rBB      | 98220          | 82286         | 7.79%           | 0.992%        |
| 11        | 9.780       | 1305          | 1308        | 1312         | rVB      | 33295          | 23454         | 2.22%           | 0.283%        |
| 12        | 9.863       | 1318          | 1322        | 1329         | rVB      | 364198         | 308086        | 29.17%          | 3.715%        |
| 13        | 10.280      | 1390          | 1393        | 1396         | rVB      | 38942          | 29420         | 2.79%           | 0.355%        |
| 14        | 10.657      | 1453          | 1457        | 1465         | rBV      | 485333         | 450395        | 42.65%          | 5.431%        |
| 15        | 10.757      | 1470          | 1474        | 1482         | rVV      | 24506          | 28422         | 2.69%           | 0.343%        |
| 16        | 11.357      | 1572          | 1576        | 1579         | rBV      | 326790         | 278184        | 26.34%          | 3.354%        |
| 17        | 12.574      | 1780          | 1783        | 1788         | rBV      | 41852          | 33110         | 3.14%           | 0.399%        |
| 18        | 12.804      | 1820          | 1822        | 1829         | rVB      | 36604          | 28839         | 2.73%           | 0.348%        |
| 19        | 12.939      | 1841          | 1845        | 1849         | rBV      | 861092         | 805848        | 76.31%          | 9.717%        |
| 20        | 13.498      | 1936          | 1940        | 1946         | rBV7     | 7349           | 13220         | 1.25%           | 0.159%        |
| 21        | 13.827      | 1994          | 1996        | 2000         | rVB      | 29774          | 29702         | 2.81%           | 0.358%        |
| 22        | 14.010      | 2022          | 2027        | 2030         | rBV      | 263997         | 271320        | 25.69%          | 3.272%        |
| 23        | 15.057      | 2202          | 2205        | 2207         | rBV2     | 21004          | 25022         | 2.37%           | 0.302%        |
| 24        | 15.427      | 2265          | 2268        | 2270         | rVB      | 14308          | 14041         | 1.33%           | 0.169%        |
| 25        | 15.486      | 2271          | 2278        | 2283         | rBV      | 159936         | 202359        | 19.16%          | 2.440%        |
| 26        | 15.892      | 2344          | 2347        | 2351         | rVB6     | 11665          | 14696         | 1.39%           | 0.177%        |
| 27        | 16.586      | 2463          | 2465        | 2471         | rVB7     | 11405          | 14206         | 1.35%           | 0.171%        |

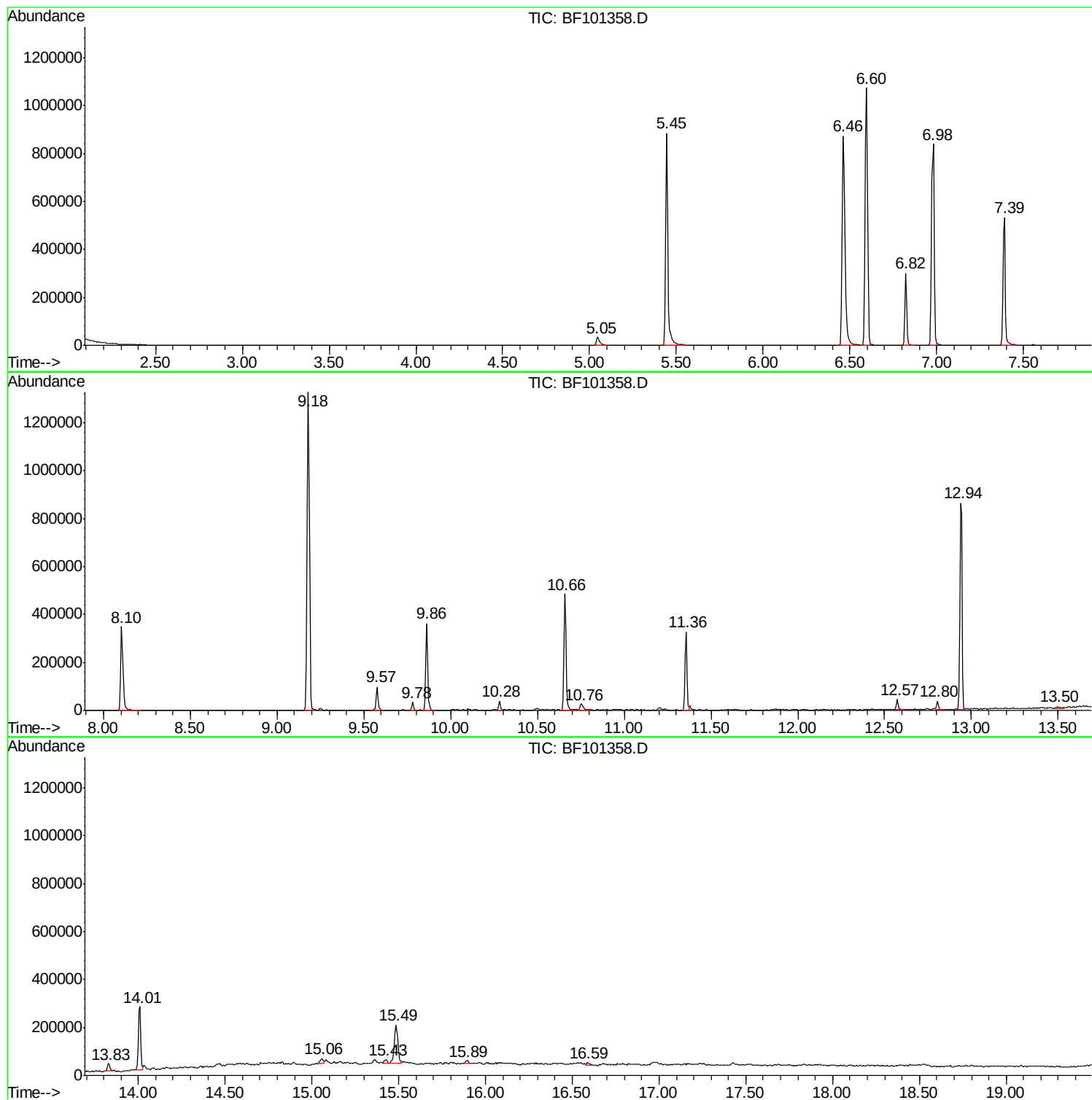
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ClientSampleId :  
MAP-1-E(0-1)

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF113017.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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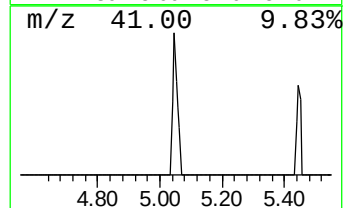
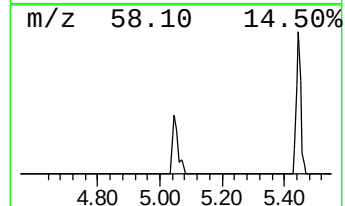
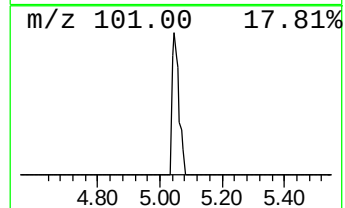
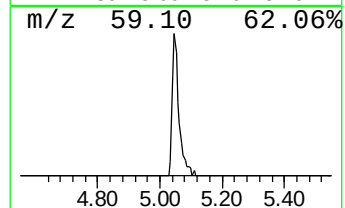
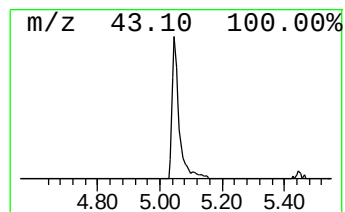
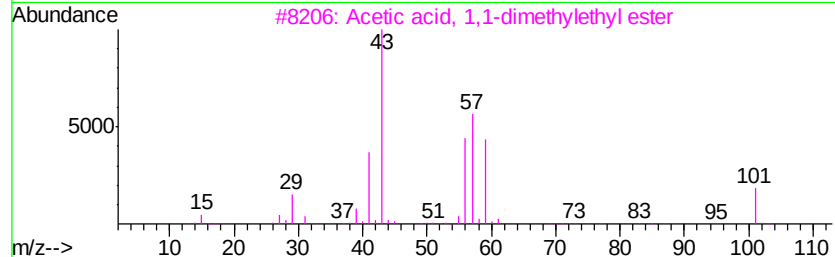
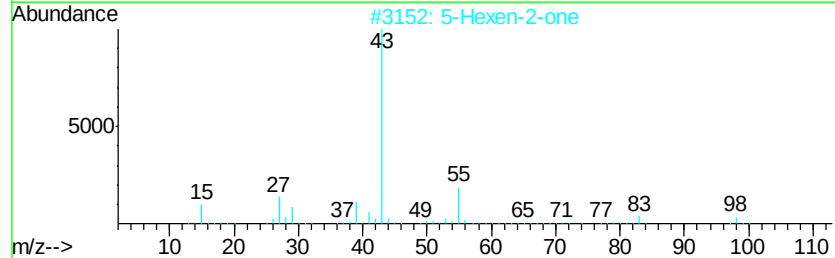
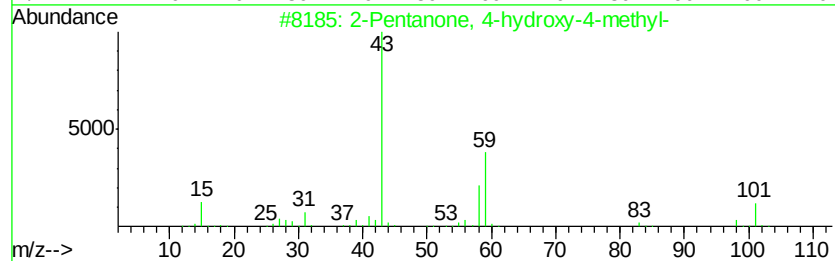
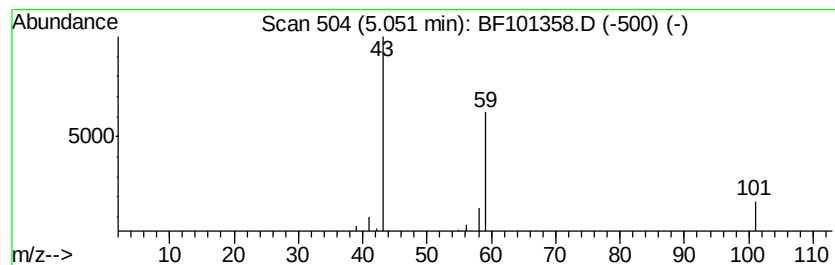
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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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. |
|------|---------|-------|------------------------|------|
| 5.05 | 3.85 ng | 46972 | 1,4-Dichlorobenzene-d4 | 6.82 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|---------|-------------|------|
| 1    |    |   | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2 | 000123-42-2 | 56   |
| 2    |    |   | 5-Hexen-2-one                       | 98  | C6H10O  | 000109-49-9 | 9    |
| 3    |    |   | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 9    |
| 4    |    |   | 1-Propen-2-ol, acetate              | 100 | C5H8O2  | 000108-22-5 | 9    |
| 5    |    |   | Diacetamide                         | 101 | C4H7NO2 | 000625-77-4 | 7    |



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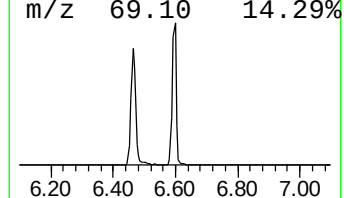
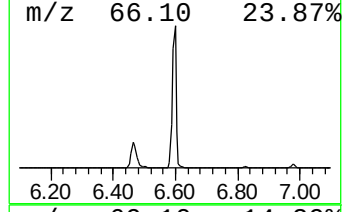
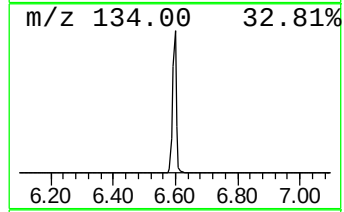
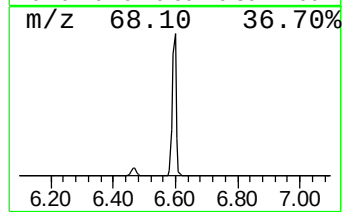
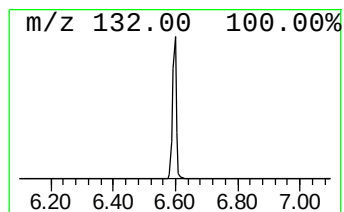
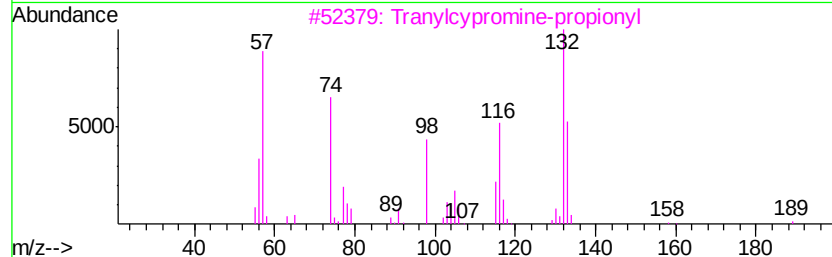
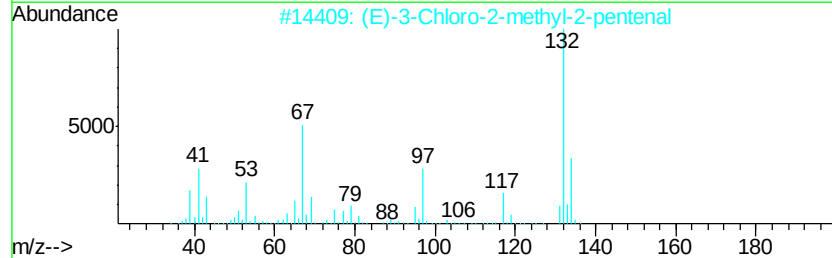
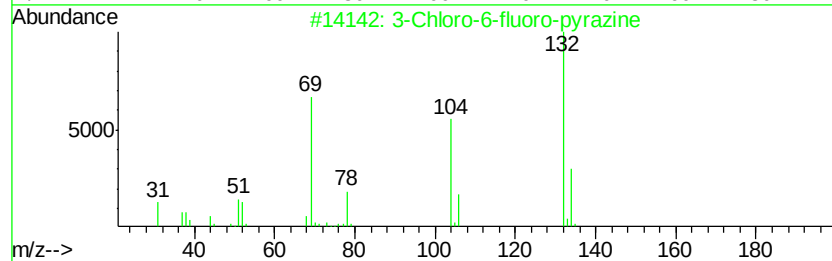
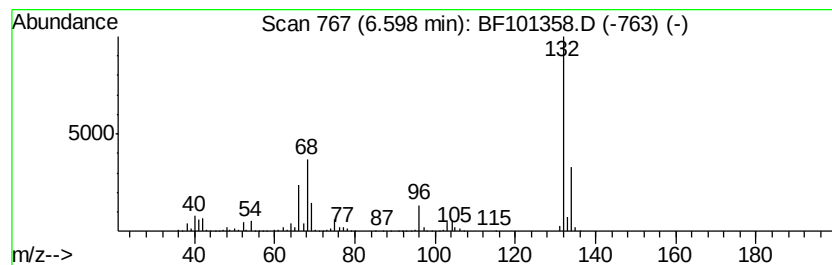
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TIC Integration Parameters: LSCINT.P

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Peak Number 2 unknown6.60 Concentration Rank 1

| R.T. | EstConc  | Area   | Relative to ISTD       | R.T. |
|------|----------|--------|------------------------|------|
| 6.60 | 76.31 ng | 930374 | 1,4-Dichlorobenzene-d4 | 6.82 |

| Hit# | of | Tentative ID                     | MW  | MolForm   | CAS#         | Qual |
|------|----|----------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 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    |    | Tranvlcypropine-propionyl        | 189 | C12H15NO  | 1000123-86-3 | 12   |
| 4    |    | 5-Aminoindole                    | 132 | C8H8N2    | 005192-03-0  | 12   |
| 5    |    | 1-Methylpyrrolo[1,2-a]pyrazine   | 132 | C8H8N2    | 064608-59-9  | 9    |



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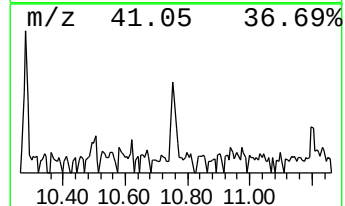
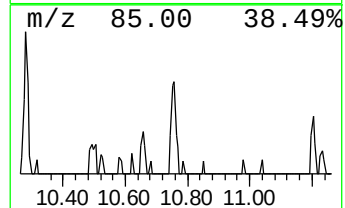
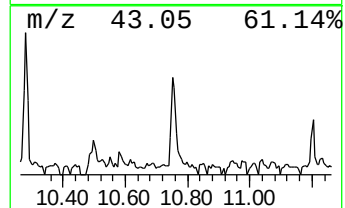
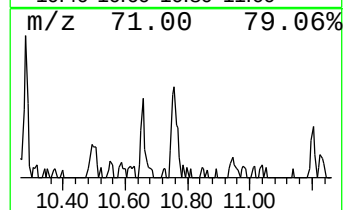
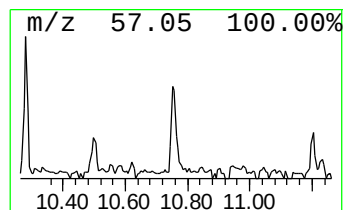
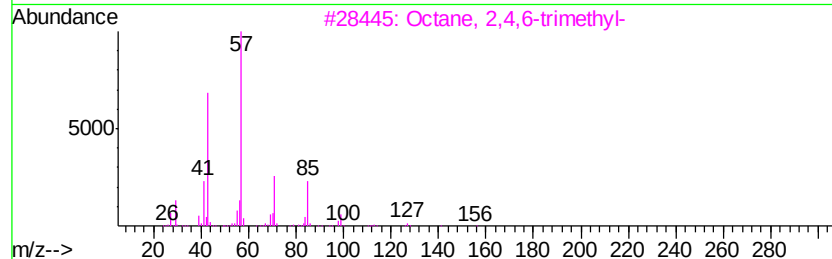
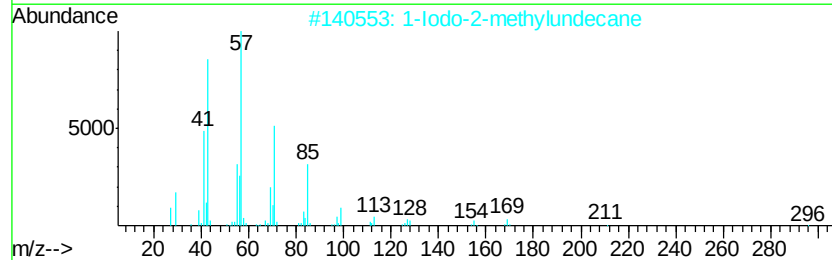
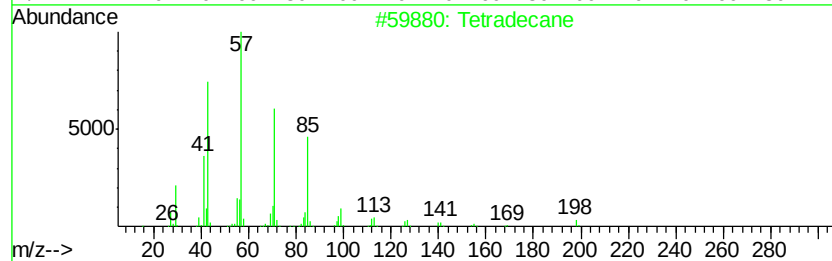
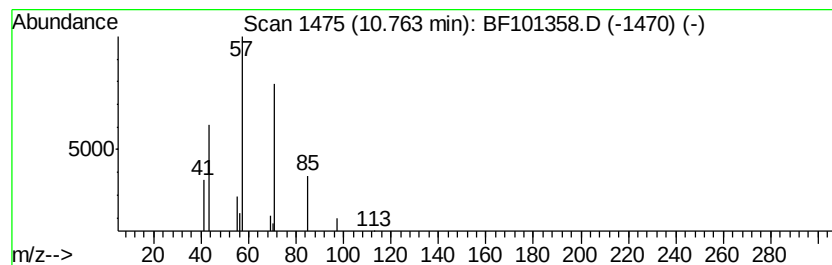
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 Tetradecane Concentration Rank 5

| R.T.  | EstConc | Area  | Relative to ISTD | R.T.  |
|-------|---------|-------|------------------|-------|
| 10.76 | 2.04 ng | 28422 | Phenanthrene-d10 | 11.36 |

| Hit# of 5 | Tentative ID             | MW  | MolForm | CAS#        | Qual |
|-----------|--------------------------|-----|---------|-------------|------|
| 1         | Tetradecane              | 198 | C14H30  | 000629-59-4 | 78   |
| 2         | 1-Iodo-2-methylundecane  | 296 | C12H25I | 073105-67-6 | 74   |
| 3         | Octane, 2,4,6-trimethyl- | 156 | C11H24  | 062016-37-9 | 72   |
| 4         | Pentadecane              | 212 | C15H32  | 000629-62-9 | 59   |
| 5         | Hexadecane               | 226 | C16H34  | 000544-76-3 | 59   |



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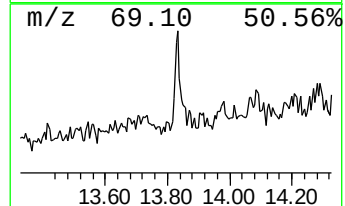
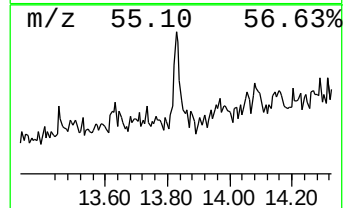
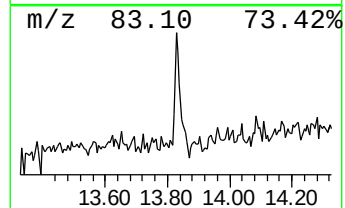
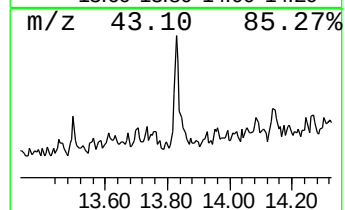
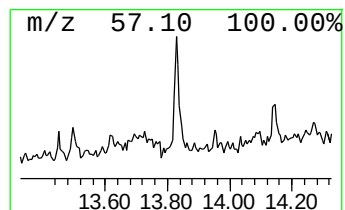
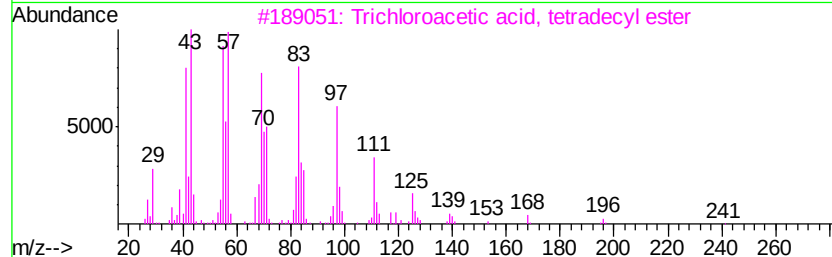
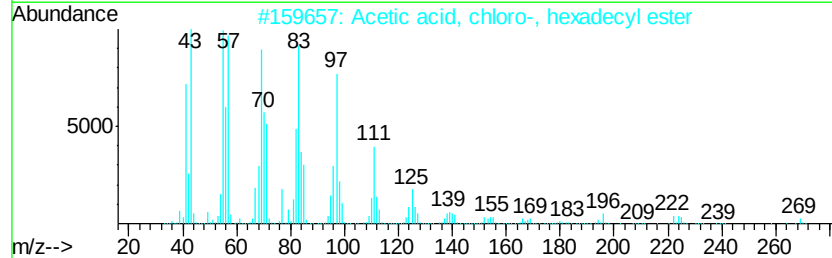
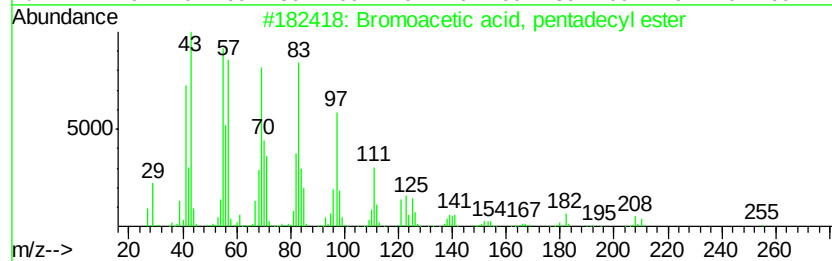
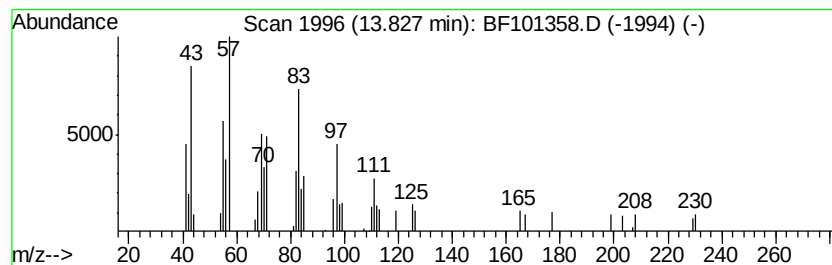
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ClientSampleId :  
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\*\*\*\*\*  
Peak Number 5 Bromoacetic acid, pentadecyl... Concentration Rank 4

| R.T.    | EstConc | Area                                | Relative to ISTD | R.T.        |             |      |
|---------|---------|-------------------------------------|------------------|-------------|-------------|------|
| 13.83   | 2.19 ng | 29702                               | Chrysene-d12     | 14.01       |             |      |
| Hit# of | 5       | Tentative ID                        | MW               | MolForm     | CAS#        | Qual |
| 1       |         | Bromoacetic acid, pentadecyl ester  | 348              | C17H33BrO2  | 131143-01-6 | 76   |
| 2       |         | Acetic acid, chloro-, hexadecyl ... | 318              | C18H35ClO2  | 052132-58-8 | 70   |
| 3       |         | Trichloroacetic acid, tetradecyl... | 358              | C16H29Cl3O2 | 074339-52-9 | 70   |
| 4       |         | n-Pentadecanol                      | 228              | C15H32O     | 000629-76-5 | 70   |
| 5       |         | Trichloroacetic acid, hexadecyl ... | 386              | C18H33Cl3O2 | 074339-54-1 | 70   |



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| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                      |       |         |       |          | #                     | RT    | Resp   | Conc |
| 2-Pentanone, 4-hy... | 5.05  | 3.9     | ng    | 46972    | 1                     | 6.82  | 243846 | 20.0 |
| unknown6.60          | 6.60  | 76.3    | ng    | 930374   | 1                     | 6.82  | 243846 | 20.0 |
| Tetradecane          | 10.76 | 2.0     | ng    | 28422    | 4                     | 11.36 | 278184 | 20.0 |
| Bromoacetic acid,... | 13.83 | 2.2     | ng    | 29702    | 5                     | 14.01 | 271320 | 20.0 |