

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF013023\  
 Data File : BF132216.D  
 Acq On : 30 Jan 2023 18:01  
 Operator : CG\JU  
 Sample : 01327-01  
 Misc :  
 ALS Vial : 6 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 N48965

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:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF012723.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132216.D\data.ms

| 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         | 5.325       | 418           | 423         | 426          | rBV      | 967982         | 921472        | 12.02%          | 2.713%        |
| 2         | 5.701       | 483           | 487         | 492          | rVB      | 1158498        | 1389874       | 18.13%          | 4.092%        |
| 3         | 6.678       | 650           | 653         | 661          | rVB      | 997696         | 860902        | 11.23%          | 2.534%        |
| 4         | 6.942       | 694           | 698         | 703          | rBV      | 120875         | 134444        | 1.75%           | 0.396%        |
| 5         | 7.078       | 717           | 721         | 725          | rBV      | 1504441        | 1197344       | 15.62%          | 3.525%        |
| 6         | 7.642       | 806           | 817         | 820          | rBV      | 3487883        | 3398970       | 44.35%          | 10.007%       |
| 7         | 8.366       | 936           | 940         | 943          | rBV      | 2017071        | 1579399       | 20.61%          | 4.650%        |
| 8         | 9.442       | 1118          | 1123        | 1126         | rBV      | 7033225        | 6591464       | 86.00%          | 19.405%       |
| 9         | 10.130      | 1236          | 1240        | 1243         | rVB      | 2389917        | 1866232       | 24.35%          | 5.494%        |
| 10        | 10.160      | 1243          | 1245        | 1249         | rBV2     | 148217         | 148179        | 1.93%           | 0.436%        |
| 11        | 10.642      | 1322          | 1327        | 1330         | rBV      | 125257         | 123263        | 1.61%           | 0.363%        |
| 12        | 10.842      | 1354          | 1361        | 1365         | rBV      | 626356         | 512148        | 6.68%           | 1.508%        |
| 13        | 10.919      | 1370          | 1374        | 1378         | rBV      | 2452365        | 2294563       | 29.94%          | 6.755%        |
| 14        | 11.630      | 1491          | 1495        | 1497         | rBV      | 2469033        | 2048942       | 26.73%          | 6.032%        |
| 15        | 11.648      | 1497          | 1498        | 1502         | rVB      | 173524         | 132350        | 1.73%           | 0.390%        |
| 16        | 12.848      | 1698          | 1702        | 1706         | rBV      | 89764          | 77277         | 1.01%           | 0.228%        |
| 17        | 13.083      | 1735          | 1742        | 1744         | rBV      | 92762          | 110095        | 1.44%           | 0.324%        |
| 18        | 13.224      | 1761          | 1766        | 1769         | rBV      | 7427367        | 7664588       | 100.00%         | 22.565%       |
| 19        | 14.113      | 1913          | 1917        | 1937         | rBV      | 131239         | 261078        | 3.41%           | 0.769%        |
| 20        | 14.289      | 1943          | 1947        | 1955         | rVB      | 1660000        | 1422192       | 18.56%          | 4.187%        |
| 21        | 15.171      | 2093          | 2097        | 2102         | rBV      | 97271          | 100951        | 1.32%           | 0.297%        |
| 22        | 15.877      | 2211          | 2217        | 2232         | rBV      | 848573         | 1131631       | 14.76%          | 3.332%        |

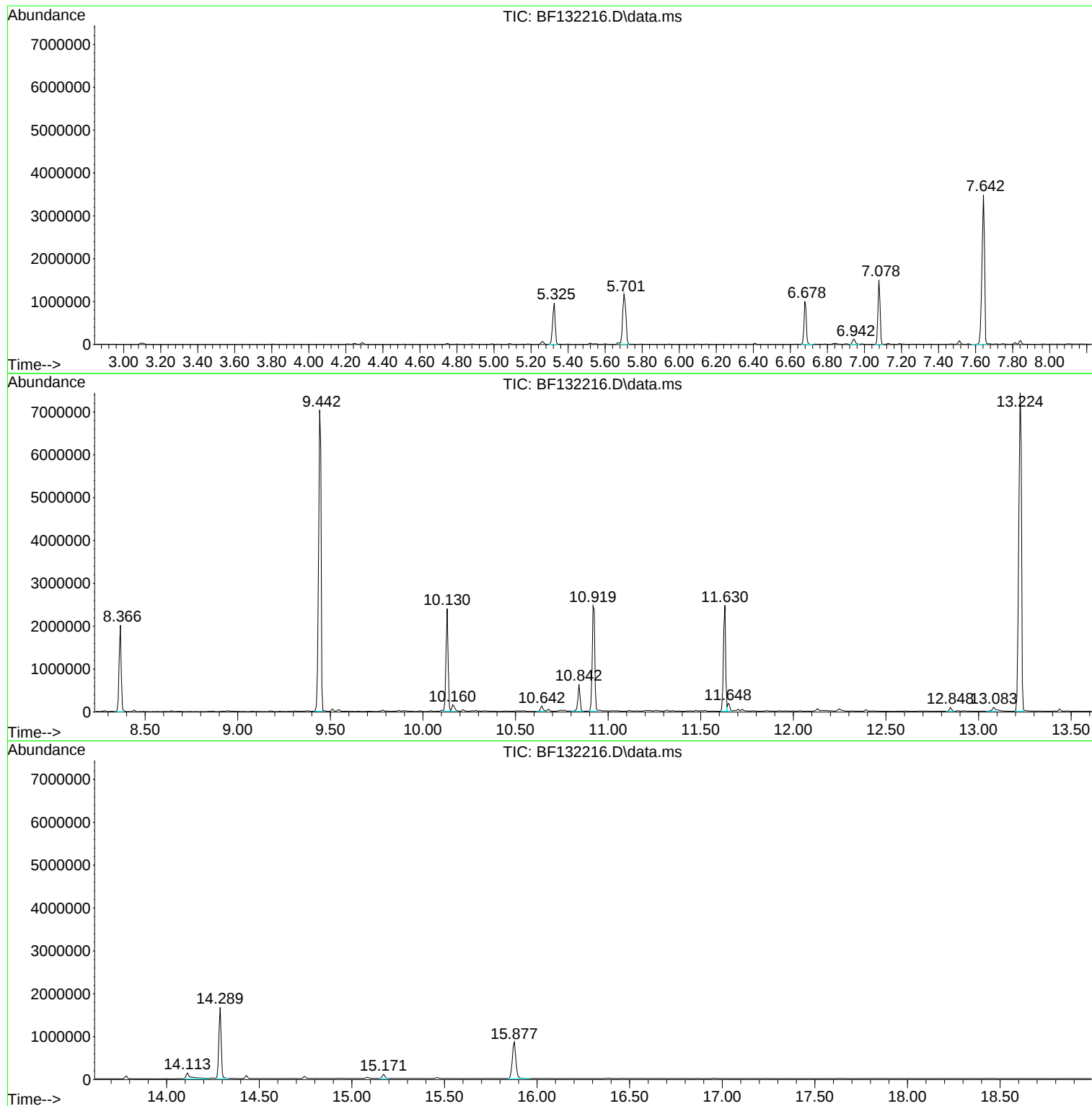
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BNA\_F  
ClientSampleId :  
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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF012723.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P



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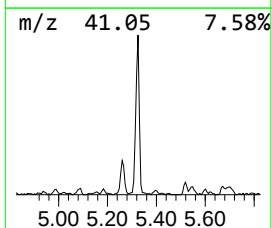
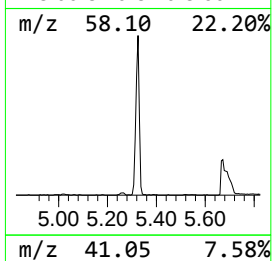
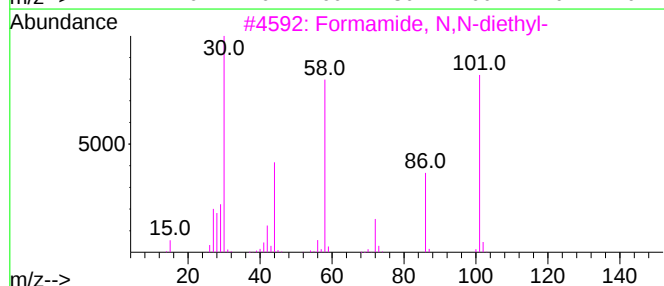
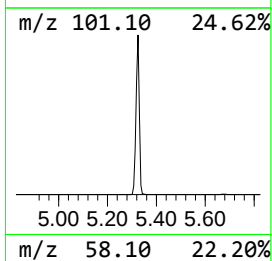
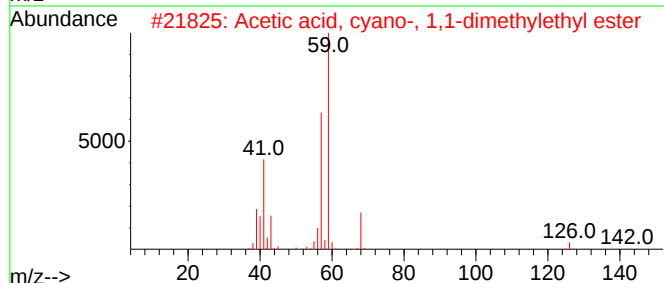
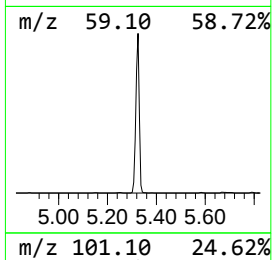
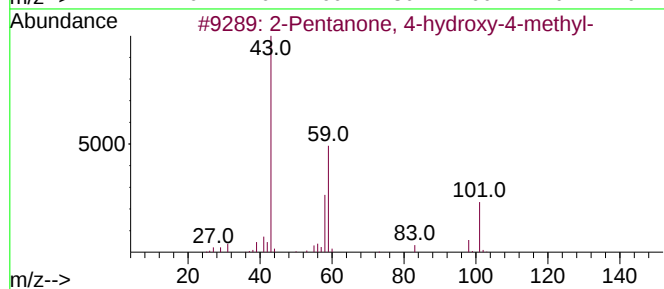
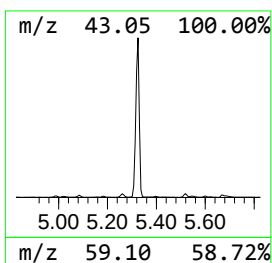
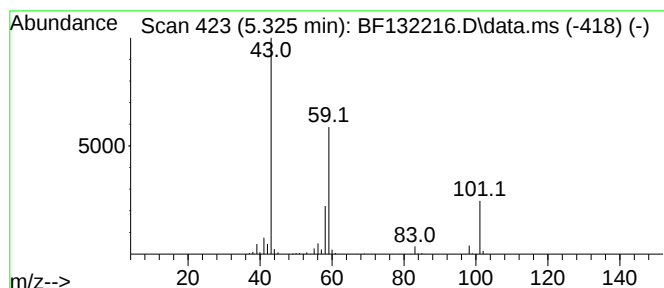
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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

| R.T.  | EstConc  | Area   | Relative to ISTD       | R.T.  |
|-------|----------|--------|------------------------|-------|
| 5.325 | 15.39 ng | 921472 | 1,4-Dichlorobenzene-d4 | 7.078 |

| 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, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 12   |
| 3    |    |   | Formamide, N,N-diethyl-             | 101 | C5H11NO  | 000617-84-5 | 9    |
| 4    |    |   | Butane, 1-ethoxy-                   | 102 | C6H14O   | 000628-81-9 | 9    |
| 5    |    |   | 5-Hexen-2-one                       | 98  | C6H10O   | 000109-49-9 | 9    |



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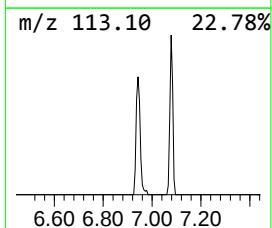
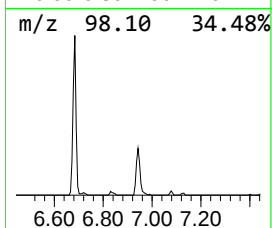
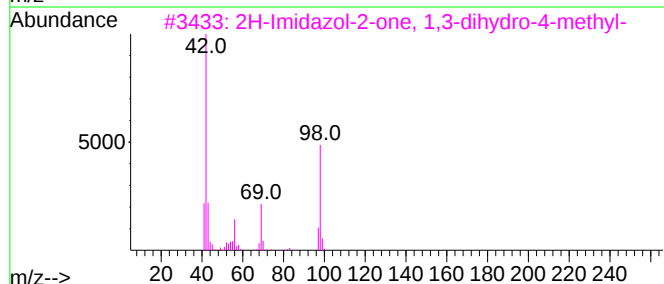
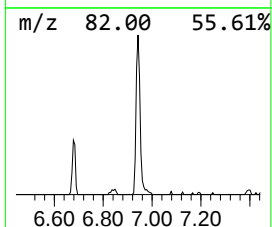
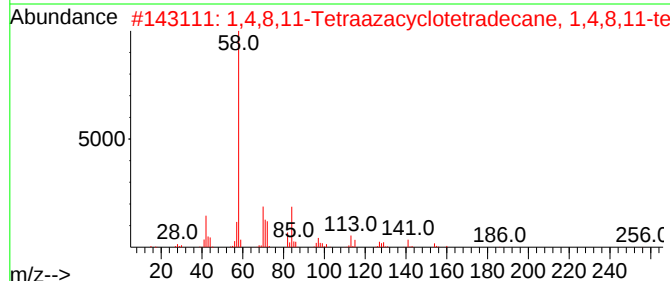
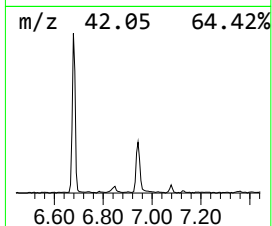
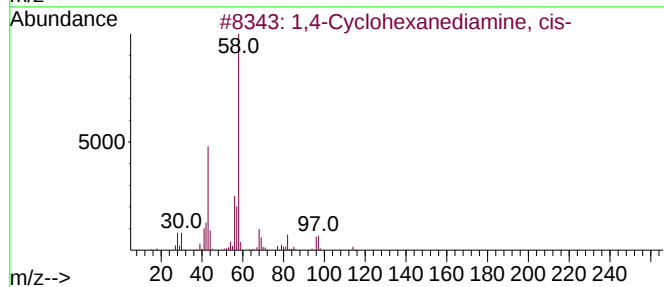
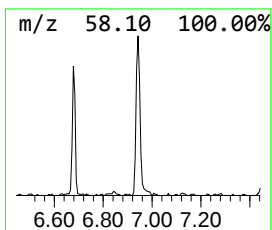
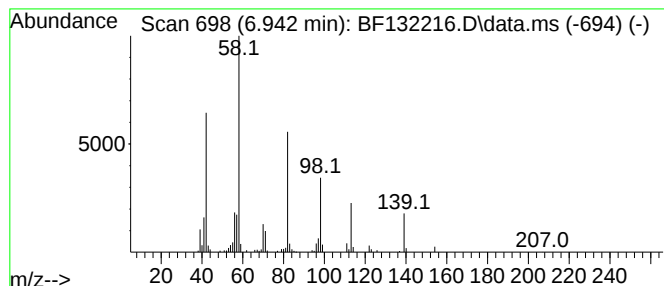
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF012723.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 unknown6.942 Concentration Rank 4

| R.T.  | EstConc | Area   | Relative to ISTD       | R.T.  |
|-------|---------|--------|------------------------|-------|
| 6.942 | 2.25 ng | 134444 | 1,4-Dichlorobenzene-d4 | 7.078 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm      | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|--------------|-------------|------|
| 1    |    |   | 1,4-Cyclohexanediamine, cis-        | 114 | C6H14N2      | 015827-56-2 | 38   |
| 2    |    |   | 1,4,8,11-Tetraazacyclotetradecan... | 256 | C14H32N4     | 041203-22-9 | 35   |
| 3    |    |   | 2H-Imidazol-2-one, 1,3-dihydro-4... | 98  | C4H6N2O      | 001192-34-3 | 18   |
| 4    |    |   | N,N'-Dipropylidene-1,1-diaminopr... | 154 | C9H18N2      | 040899-13-6 | 17   |
| 5    |    |   | O-(2-(Dimethylamino)ethyl)-2-chl... | 336 | C17H18Cl2N2O | 126551-78-8 | 16   |



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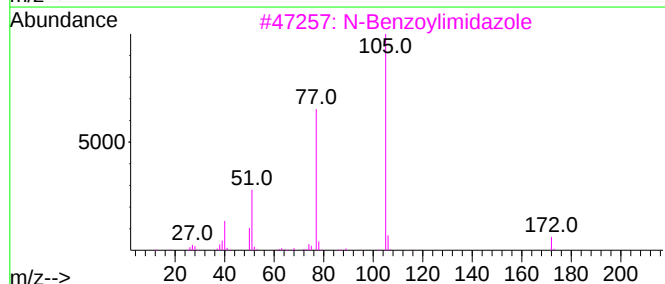
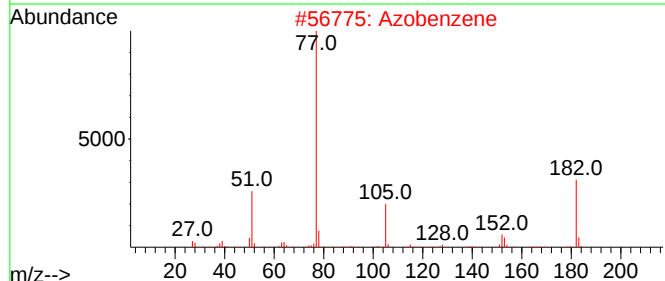
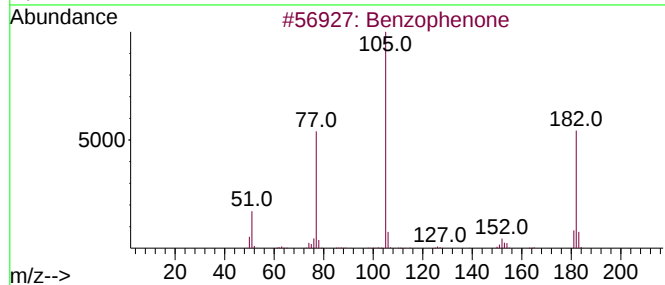
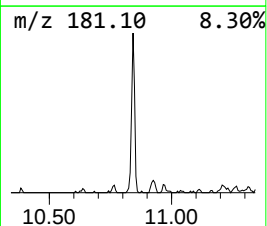
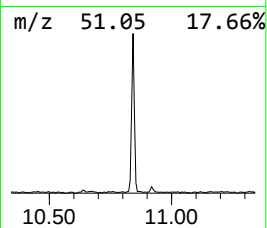
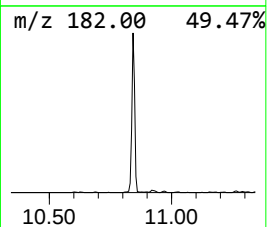
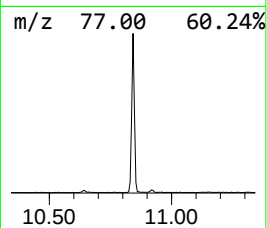
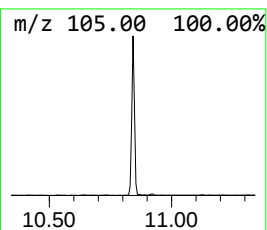
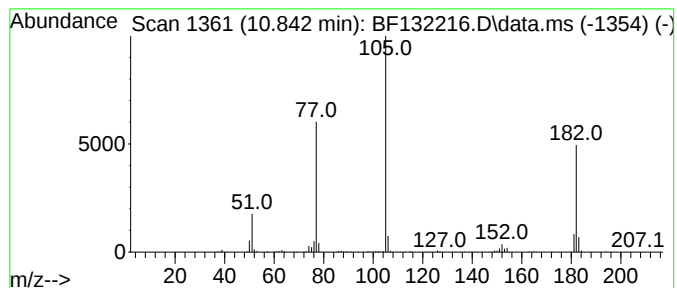
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TIC Library : C:\Database\NIST20.L  
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Peak Number 3 Benzophenone Concentration Rank 2

| R.T.      | EstConc                        | Area   | Relative to ISTD |          | R.T.        |      |
|-----------|--------------------------------|--------|------------------|----------|-------------|------|
| 10.842    | 5.49 ng                        | 512148 | Acenaphthene-d10 |          | 10.131      |      |
| Hit# of 5 | Tentative ID                   |        | MW               | MolForm  | CAS#        | Qual |
| 1         | Benzophenone                   |        | 182              | C13H10O  | 000119-61-9 | 96   |
| 2         | Azobenzene                     |        | 182              | C12H10N2 | 000103-33-3 | 59   |
| 3         | N-Benzoylimidazole             |        | 172              | C10H8N2O | 010364-94-0 | 43   |
| 4         | Benzoyl bromide                |        | 184              | C7H5BrO  | 000618-32-6 | 43   |
| 5         | Pentafluoroethyl phenyl ketone |        | 224              | C9H5F5O  | 000394-52-5 | 43   |



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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF012723.M  
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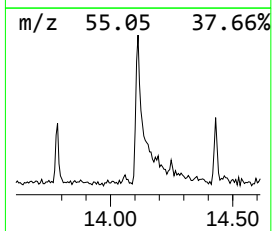
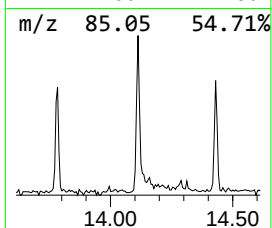
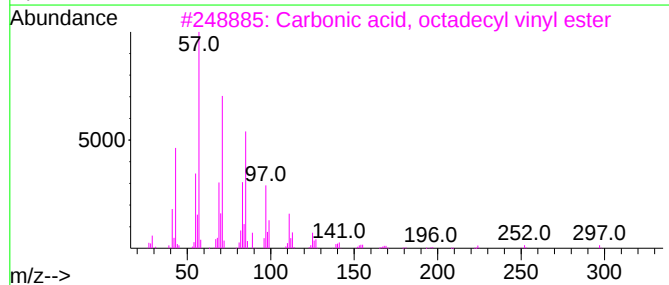
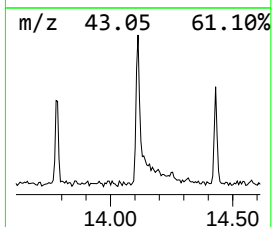
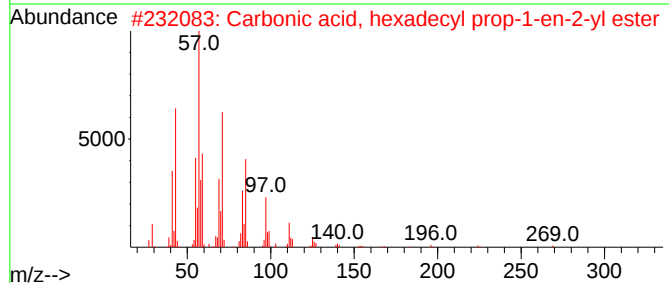
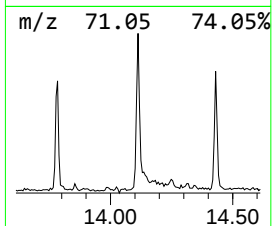
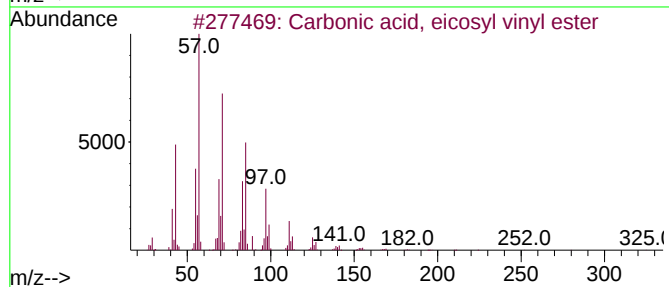
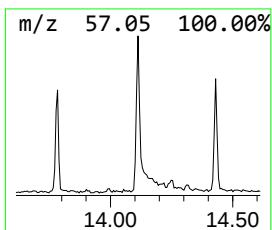
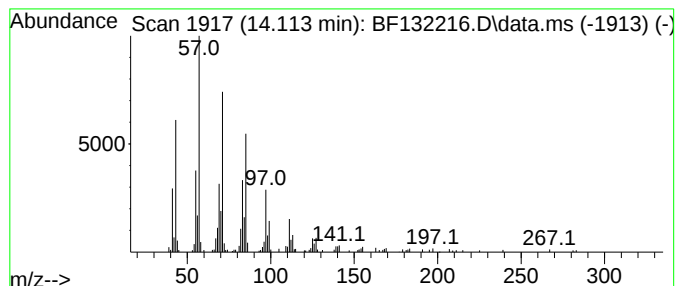
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Peak Number 4 Carbonic acid, eicosyl vinyl... Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 14.113 | 3.67 ng | 261078 | Chrysene-d12     | 14.289 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm     | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|-------------|--------------|------|
| 1    |    |   | Carbonic acid, eicosyl vinyl ester  | 368 | C23H44O3    | 1000382-54-3 | 94   |
| 2    |    |   | Carbonic acid, hexadecyl prop-1-... | 326 | C20H38O3    | 1000382-90-3 | 91   |
| 3    |    |   | Carbonic acid, octadecyl vinyl e... | 340 | C21H40O3    | 1000382-54-4 | 91   |
| 4    |    |   | 1-Octadecanesulphonyl chloride      | 352 | C18H37ClO2S | 1000342-70-4 | 91   |
| 5    |    |   | Sulfurous acid, 2-propyl tetrad...  | 320 | C17H36O3S   | 1010309-12-5 | 90   |



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| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |         |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|---------|------|
|                    |        |         |       |          | #                     | RT     | Resp    | Conc |
| 2-Pentanone, 4-... | 5.325  | 15.4    | ng    | 921472   | 1                     | 7.078  | 1197340 | 20.0 |
| unknown6.942       | 6.942  | 2.3     | ng    | 134444   | 1                     | 7.078  | 1197340 | 20.0 |
| Benzophenone       | 10.842 | 5.5     | ng    | 512148   | 3                     | 10.131 | 1866230 | 20.0 |
| Carbonic acid, ... | 14.113 | 3.7     | ng    | 261078   | 5                     | 14.289 | 1422190 | 20.0 |