

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF110922\  
 Data File : BF131105.D  
 Acq On : 10 Nov 2022 00:35  
 Operator : CG\JU  
 Sample : N5360-17  
 Misc :  
 ALS Vial : 14 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 DISSOLVED-20221172-COMP-07-MODIFIED-ELUTRIATE

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-BF110922.M  
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131105.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         | 2.158       | 6             | 12          | 20           | rVB      | 1422535        | 1781068       | 75.66%          | 12.795%       |
| 2         | 5.105       | 509           | 513         | 519          | rVB      | 171377         | 170310        | 7.23%           | 1.223%        |
| 3         | 5.504       | 577           | 581         | 593          | rBV      | 1107680        | 949907        | 40.35%          | 6.824%        |
| 4         | 6.510       | 749           | 752         | 762          | rBV      | 860265         | 742035        | 31.52%          | 5.331%        |
| 5         | 6.887       | 813           | 816         | 820          | rBV      | 574753         | 518391        | 22.02%          | 3.724%        |
| 6         | 7.457       | 908           | 913         | 916          | rVB      | 1460964        | 1335880       | 56.75%          | 9.597%        |
| 7         | 8.175       | 1031          | 1035        | 1038         | rBV      | 808252         | 660058        | 28.04%          | 4.742%        |
| 8         | 9.251       | 1213          | 1218        | 1221         | rBV      | 2839227        | 2354162       | 100.00%         | 16.912%       |
| 9         | 9.645       | 1282          | 1285        | 1288         | rBV      | 33084          | 27590         | 1.17%           | 0.198%        |
| 10        | 9.934       | 1325          | 1334        | 1337         | rBV      | 891541         | 753290        | 32.00%          | 5.411%        |
| 11        | 10.028      | 1347          | 1350        | 1353         | rBV      | 68726          | 51624         | 2.19%           | 0.371%        |
| 12        | 10.722      | 1464          | 1468        | 1472         | rBV      | 1532771        | 1441781       | 61.24%          | 10.357%       |
| 13        | 11.422      | 1584          | 1587        | 1591         | rBV      | 854285         | 743210        | 31.57%          | 5.339%        |
| 14        | 11.804      | 1649          | 1652        | 1655         | rBV2     | 59306          | 45606         | 1.94%           | 0.328%        |
| 15        | 13.010      | 1853          | 1857        | 1860         | rBV      | 1269694        | 1035488       | 43.99%          | 7.439%        |
| 16        | 13.927      | 2010          | 2013        | 2022         | rVB3     | 35498          | 69663         | 2.96%           | 0.500%        |
| 17        | 14.069      | 2034          | 2037        | 2041         | rBV      | 662979         | 553916        | 23.53%          | 3.979%        |
| 18        | 14.163      | 2048          | 2053        | 2057         | rBV      | 84190          | 87257         | 3.71%           | 0.627%        |
| 19        | 14.916      | 2178          | 2181        | 2185         | rVB      | 39039          | 41931         | 1.78%           | 0.301%        |
| 20        | 15.563      | 2286          | 2291        | 2300         | rBV      | 447728         | 557154        | 23.67%          | 4.002%        |

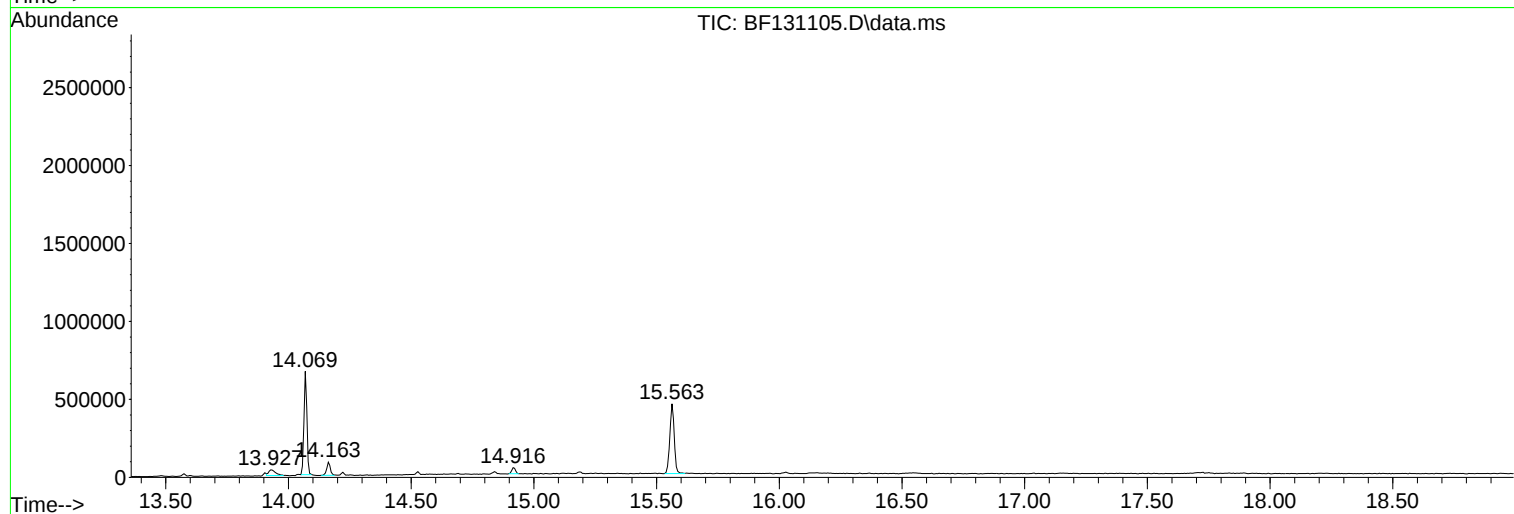
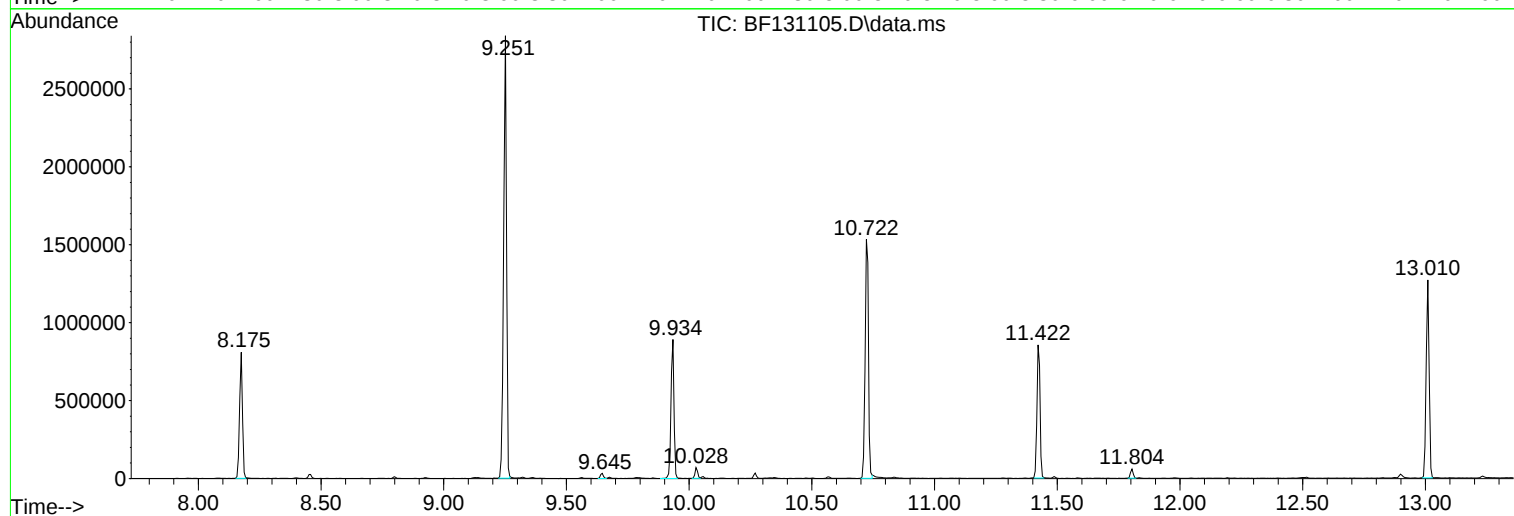
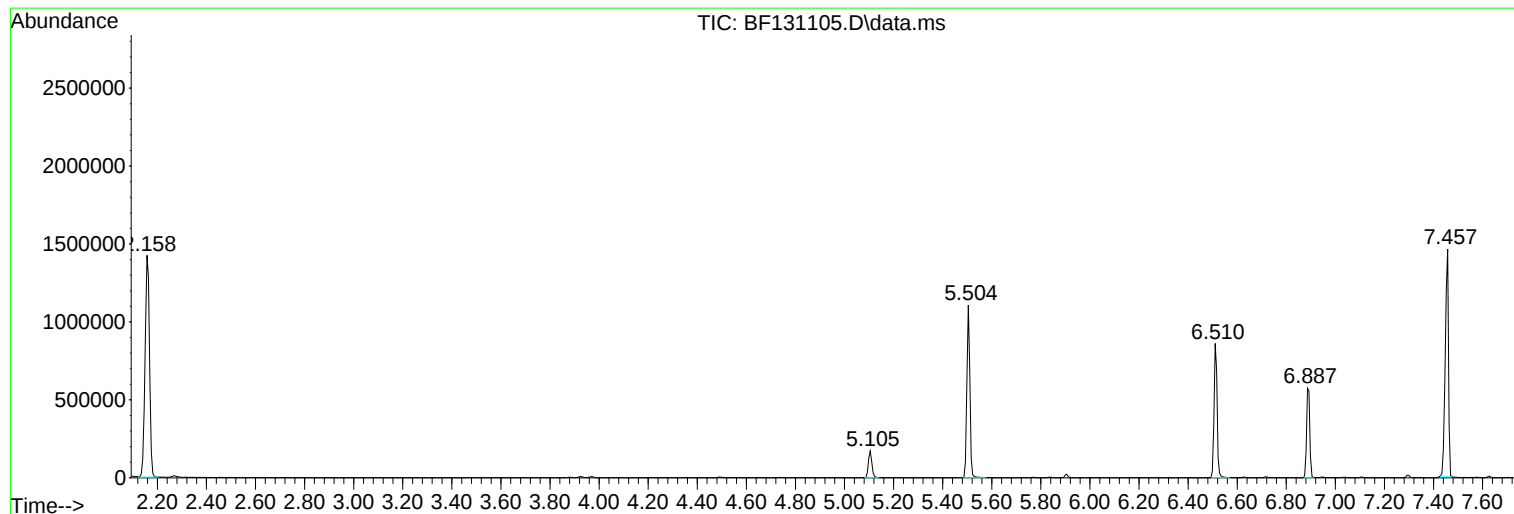
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Misc :  
ALS Vial : 14 Sample Multiplier: 1

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BNA\_F  
ClientSampleId :  
DISSOLVED-20221172-COMP-07-MODIFIED-ELUTRIATE

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF110922.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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

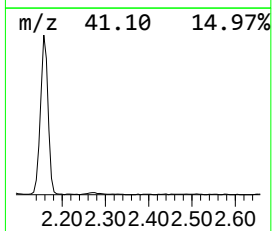
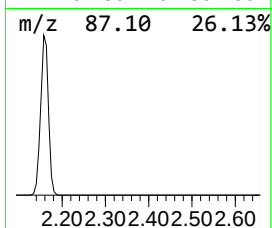
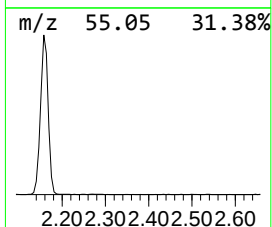
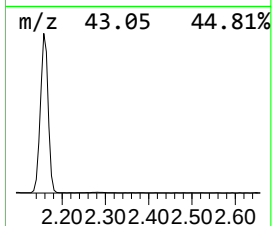
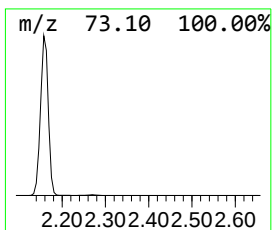
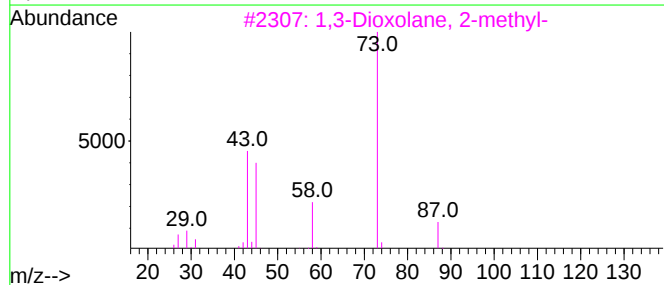
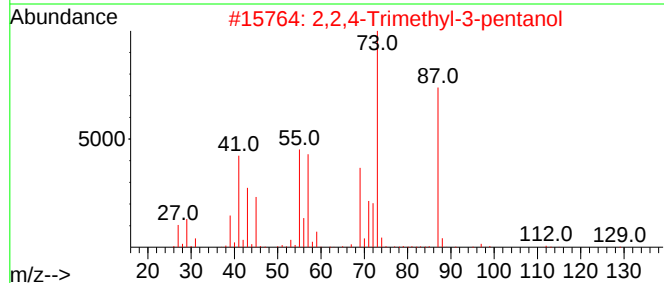
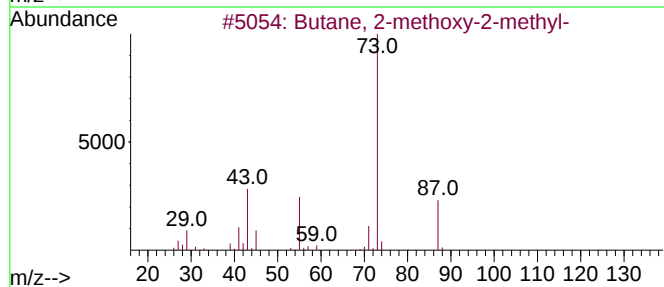
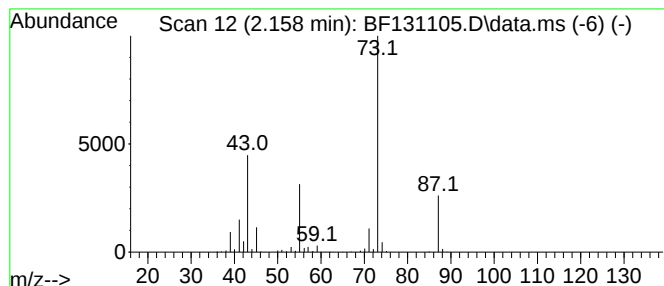
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

| R.T.  | EstConc  | Area    | Relative to ISTD       | R.T.  |
|-------|----------|---------|------------------------|-------|
| 2.158 | 68.72 ng | 1781070 | 1,4-Dichlorobenzene-d4 | 6.893 |

| Hit# | of | 5 | Tentative ID                | MW  | MolForm | CAS#        | Qual |
|------|----|---|-----------------------------|-----|---------|-------------|------|
| 1    |    |   | Butane, 2-methoxy-2-methyl- | 102 | C6H14O  | 000994-05-8 | 83   |
| 2    |    |   | 2,2,4-Trimethyl-3-pentanol  | 130 | C8H18O  | 005162-48-1 | 40   |
| 3    |    |   | 1,3-Dioxolane, 2-methyl-    | 88  | C4H8O2  | 000497-26-7 | 23   |
| 4    |    |   | Pentane, 3-methoxy-         | 102 | C6H14O  | 036839-67-5 | 12   |
| 5    |    |   | Acetamide, N-ethyl-         | 87  | C4H9NO  | 000625-50-3 | 9    |



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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF110922.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

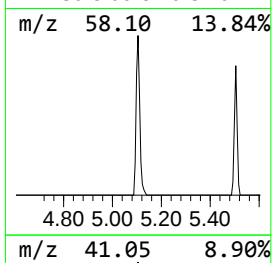
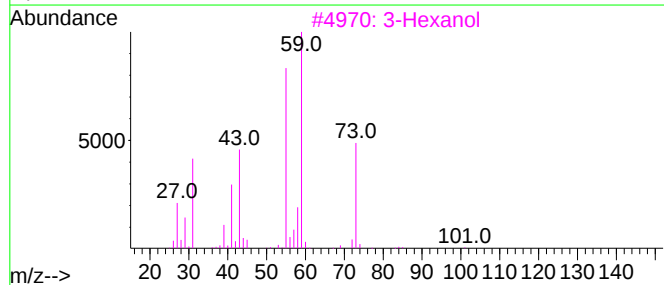
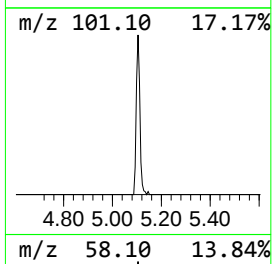
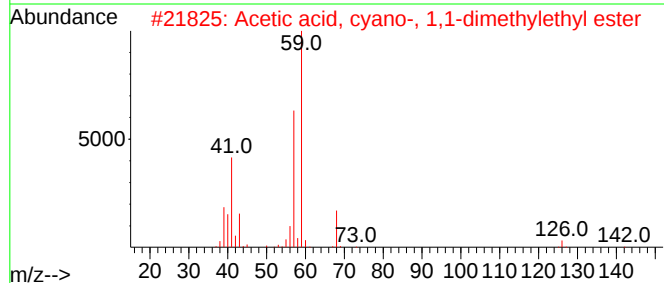
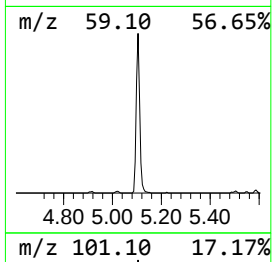
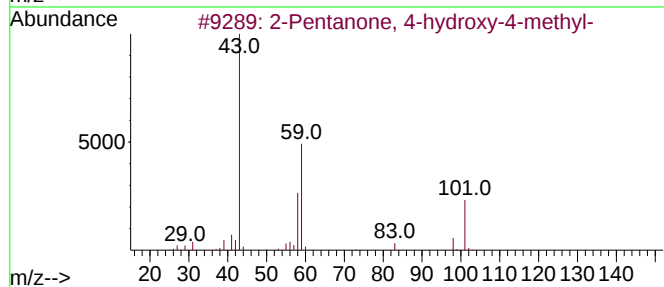
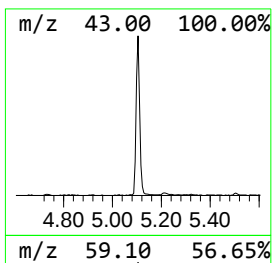
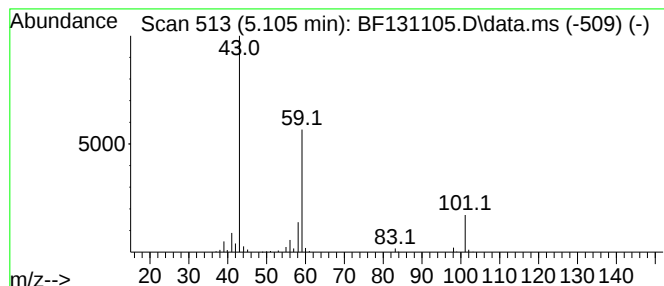
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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

| R.T.  | EstConc | Area   | Relative to ISTD       | R.T.  |
|-------|---------|--------|------------------------|-------|
| 5.105 | 6.57 ng | 170310 | 1,4-Dichlorobenzene-d4 | 6.893 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2  | 000123-42-2 | 40   |
| 2    |    |   | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 37   |
| 3    |    |   | 3-Hexanol                           | 102 | C6H14O   | 000623-37-0 | 33   |
| 4    |    |   | 3-Hexanol, 4-methyl-                | 116 | C7H16O   | 000615-29-2 | 33   |
| 5    |    |   | 2,3-Butanedione, monooxime          | 101 | C4H7NO2  | 000057-71-6 | 27   |



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Sample : N5360-17  
Misc :  
ALS Vial : 14 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF110922.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

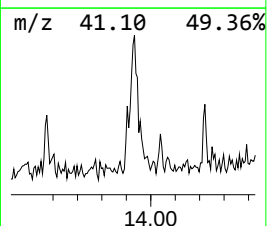
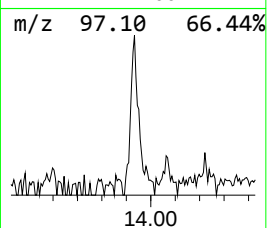
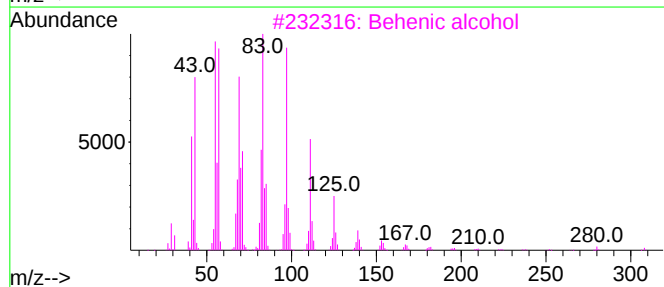
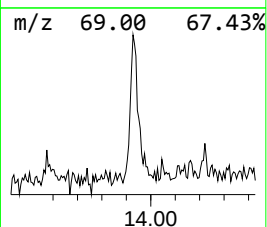
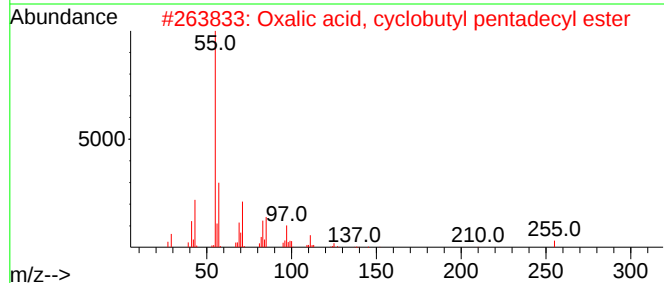
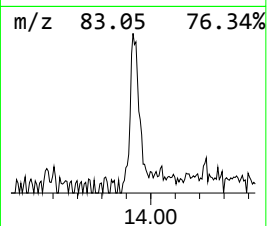
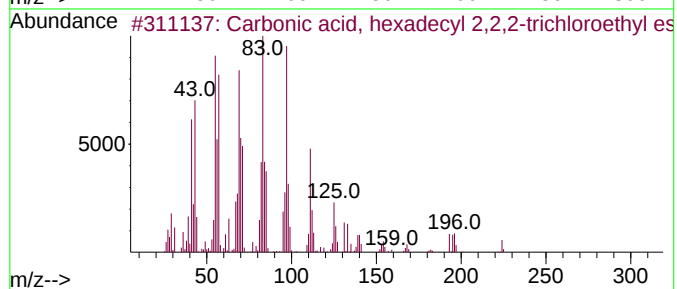
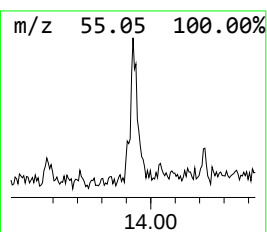
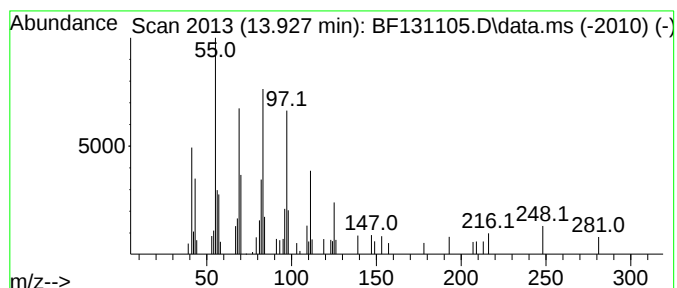
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 Carbonic acid, hexadecyl 2,... Concentration Rank 4

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 13.928 | 2.52 ng | 69663 | Chrysene-d12     | 14.069 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm     | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|-------------|--------------|------|
| 1    |    |   | Carbonic acid, hexadecyl 2,2,2-t... | 416 | C19H35Cl3O3 | 1000314-56-2 | 64   |
| 2    |    |   | Oxalic acid, cyclobutyl pentadec... | 354 | C21H38O4    | 1010309-70-5 | 59   |
| 3    |    |   | Behenic alcohol                     | 326 | C22H46O     | 000661-19-8  | 59   |
| 4    |    |   | Decane, 5,6-bis(2,2-dimethylprop... | 278 | C20H38      | 073002-85-4  | 50   |
| 5    |    |   | 1-Hexacosanol                       | 382 | C26H54O     | 000506-52-5  | 47   |



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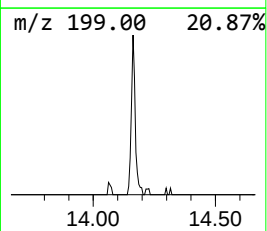
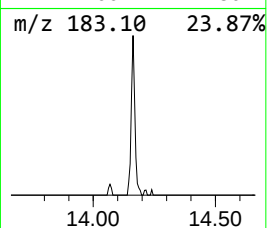
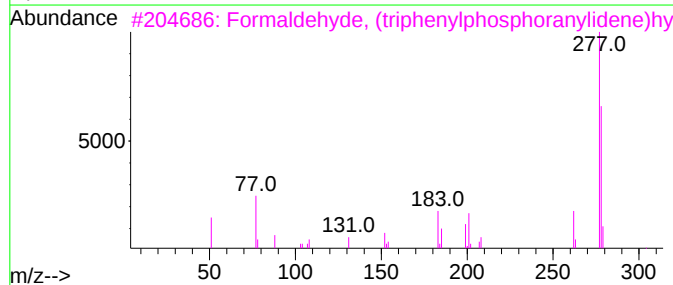
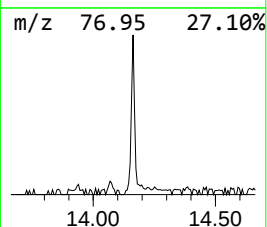
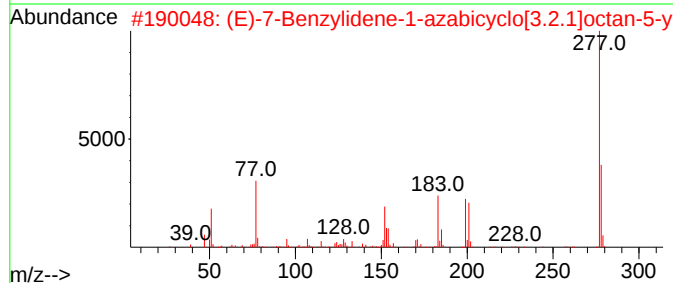
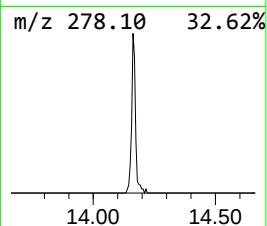
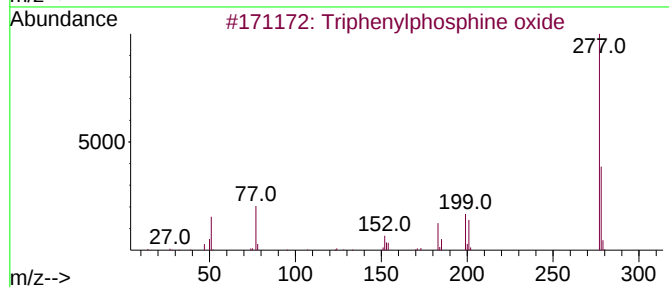
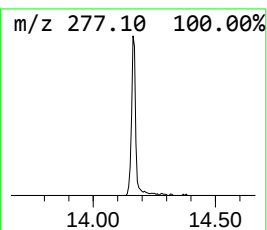
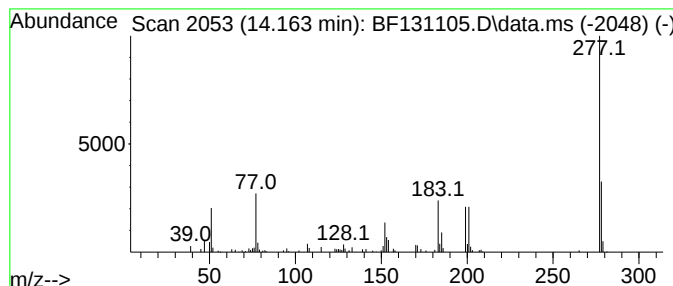
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TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 Triphenylphosphine oxide Concentration Rank 3

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 14.163 | 3.15 ng | 87257 | Chrysene-d12     | 14.069 |

| Hit# | of | 5 | Tentative ID                         | MW  | MolForm    | CAS#         | Qual |
|------|----|---|--------------------------------------|-----|------------|--------------|------|
| 1    |    |   | Triphenylphosphine oxide             | 278 | C18H15OP   | 000791-28-6  | 98   |
| 2    |    |   | (E)-7-Benzylidene-1-azabicyclo[3...] | 293 | C15H19N03S | 1000483-83-4 | 91   |
| 3    |    |   | Formaldehyde, (triphenylphosphor...  | 304 | C19H17N2P  | 015990-54-2  | 45   |
| 4    |    |   | Vanadium, cycloheptatrienyl-(pen...  | 277 | C17H22V    | 1000155-20-5 | 43   |
| 5    |    |   | Cobalt, (.eta.<5>-2,4-cyclopentad... | 277 | C16H15BCo  | 036682-12-9  | 38   |



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

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| Butane, 2-metho... | 2.158  | 68.7    | ng    | 1781070  | 1                     | 6.893  | 518391 | 20.0 |
| 2-Pentanone, 4-... | 5.105  | 6.6     | ng    | 170310   | 1                     | 6.893  | 518391 | 20.0 |
| Carbonic acid, ... | 13.928 | 2.5     | ng    | 69663    | 5                     | 14.069 | 553916 | 20.0 |
| Triphenylphosph... | 14.163 | 3.1     | ng    | 87257    | 5                     | 14.069 | 553916 | 20.0 |