

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061418\  
 Data File : BF106452.D  
 Acq On : 14 Jun 2018 19:44  
 Operator : JU/SJ  
 Sample : J3498-11  
 Misc :  
 ALS Vial : 18 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 TP-E-S

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-BF061118.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         | 4.101       | 295           | 300         | 305          | rVB      | 880815         | 1062159       | 38.64%          | 4.202%        |
| 2         | 5.201       | 483           | 487         | 494          | rBV      | 225814         | 257434        | 9.37%           | 1.018%        |
| 3         | 5.613       | 553           | 557         | 564          | rBV      | 2449805        | 2574522       | 93.66%          | 10.185%       |
| 4         | 6.607       | 723           | 726         | 742          | rVB      | 2491782        | 2574858       | 93.67%          | 10.186%       |
| 5         | 6.748       | 746           | 750         | 753          | rBV      | 2765664        | 2499773       | 90.94%          | 9.889%        |
| 6         | 6.966       | 783           | 787         | 790          | rBV      | 1011103        | 787325        | 28.64%          | 3.115%        |
| 7         | 7.125       | 809           | 814         | 817          | rBV      | 2330040        | 2065667       | 75.15%          | 8.172%        |
| 8         | 7.531       | 878           | 883         | 886          | rBV      | 1647670        | 1672812       | 60.85%          | 6.618%        |
| 9         | 8.248       | 1001          | 1005        | 1008         | rBV      | 1184376        | 952031        | 34.63%          | 3.766%        |
| 10        | 9.325       | 1183          | 1188        | 1191         | rBV      | 2869859        | 2748856       | 100.00%         | 10.874%       |
| 11        | 9.713       | 1250          | 1254        | 1259         | rBV      | 357661         | 287364        | 10.45%          | 1.137%        |
| 12        | 9.919       | 1285          | 1289        | 1293         | rVB2     | 55917          | 47724         | 1.74%           | 0.189%        |
| 13        | 10.007      | 1300          | 1304        | 1308         | rVB      | 1100516        | 911379        | 33.15%          | 3.605%        |
| 14        | 10.419      | 1371          | 1374        | 1377         | rVB      | 68190          | 58304         | 2.12%           | 0.231%        |
| 15        | 10.795      | 1434          | 1438        | 1442         | rBV      | 1378652        | 1349377       | 49.09%          | 5.338%        |
| 16        | 10.895      | 1452          | 1455        | 1461         | rBV      | 57778          | 63588         | 2.31%           | 0.252%        |
| 17        | 11.495      | 1554          | 1557        | 1560         | rBV      | 837847         | 777997        | 28.30%          | 3.078%        |
| 18        | 12.713      | 1761          | 1764        | 1767         | rBV      | 57427          | 50198         | 1.83%           | 0.199%        |
| 19        | 12.942      | 1800          | 1803        | 1805         | rBV      | 89189          | 77109         | 2.81%           | 0.305%        |
| 20        | 12.966      | 1805          | 1807        | 1810         | rVB      | 44984          | 37820         | 1.38%           | 0.150%        |
| 21        | 13.083      | 1823          | 1827        | 1830         | rBV      | 2629776        | 2341611       | 85.18%          | 9.263%        |
| 22        | 13.266      | 1856          | 1858        | 1861         | rBV3     | 24289          | 28563         | 1.04%           | 0.113%        |
| 23        | 13.971      | 1974          | 1978        | 1986         | rBV      | 209605         | 250594        | 9.12%           | 0.991%        |
| 24        | 14.148      | 2004          | 2008        | 2012         | rBV      | 943666         | 913148        | 33.22%          | 3.612%        |
| 25        | 14.613      | 2085          | 2087        | 2090         | rVB2     | 63923          | 56072         | 2.04%           | 0.222%        |
| 26        | 15.013      | 2153          | 2155        | 2159         | rVB      | 166928         | 158391        | 5.76%           | 0.627%        |
| 27        | 15.689      | 2266          | 2270        | 2278         | rVB2     | 495419         | 673409        | 24.50%          | 2.664%        |

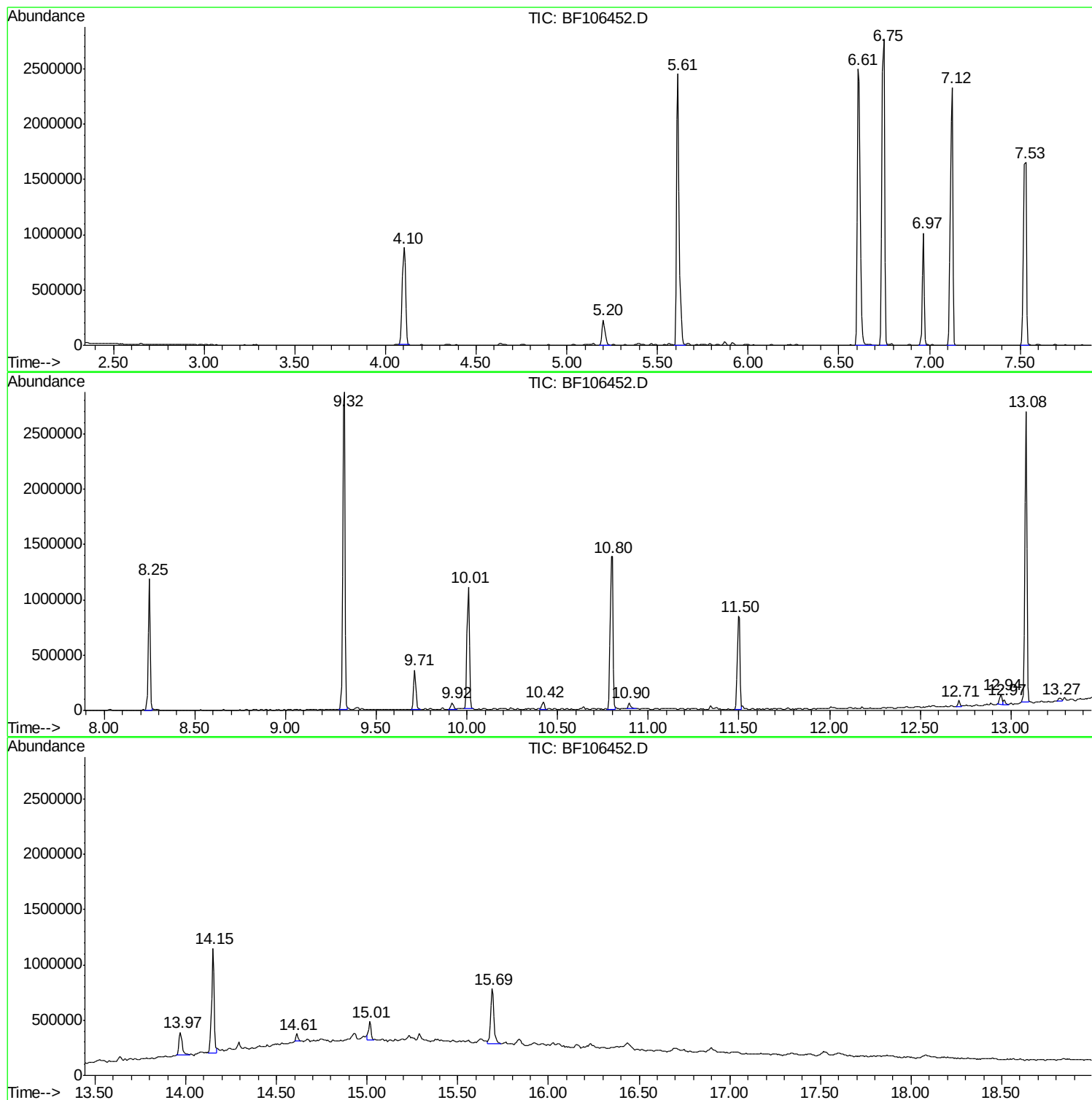
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ALS Vial : 18 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampled :  
TP-E-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061118.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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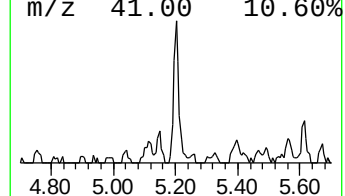
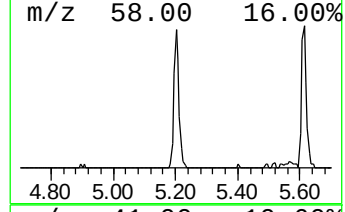
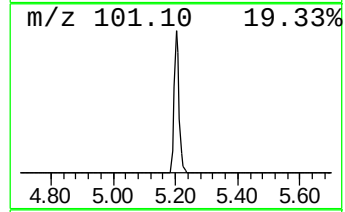
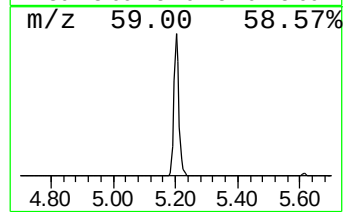
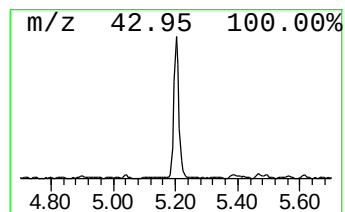
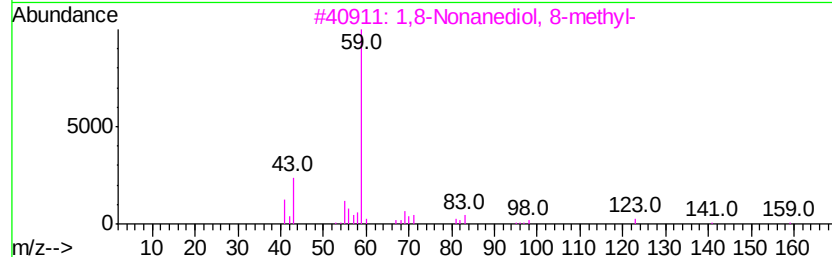
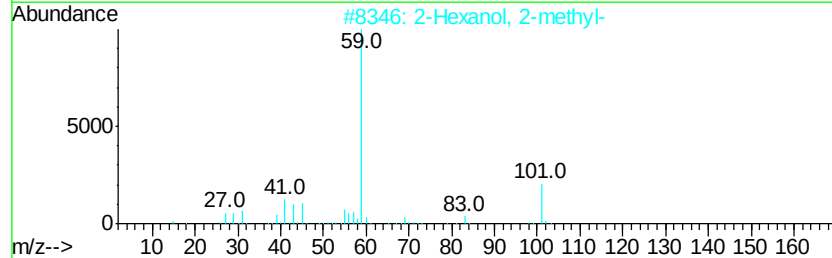
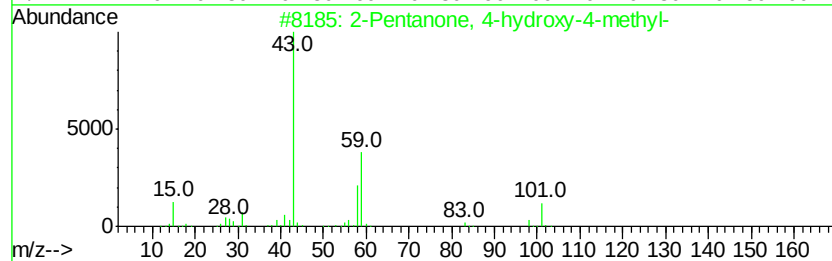
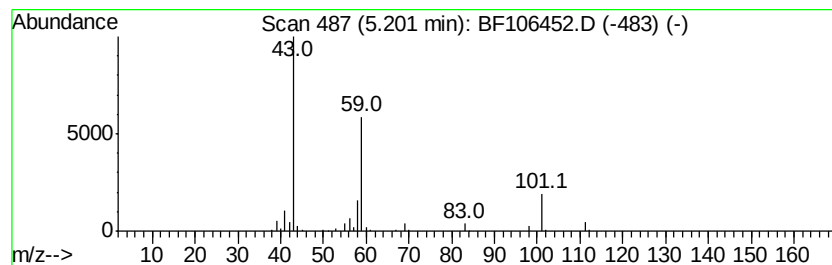
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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

| R.T. | EstConc | Area   | Relative to ISTD       | R.T. |
|------|---------|--------|------------------------|------|
| 5.20 | 6.54 ng | 257434 | 1,4-Dichlorobenzene-d4 | 6.97 |

| 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 | 38   |
| 3    |    |   | 1,8-Nonanediol, 8-methyl-            | 174 | C10H22O2 | 054725-73-4 | 17   |
| 4    |    |   | Acetic acid, cyano-, 1,1-dimethyl... | 141 | C7H11NO2 | 001116-98-9 | 12   |
| 5    |    |   | 4-Penten-2-one, 4-methyl-            | 98  | C6H10O   | 003744-02-3 | 9    |



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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061118.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

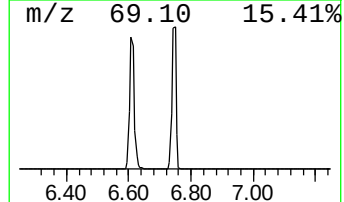
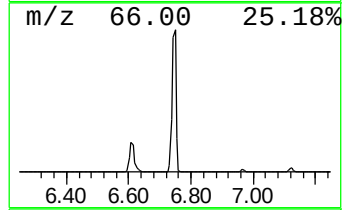
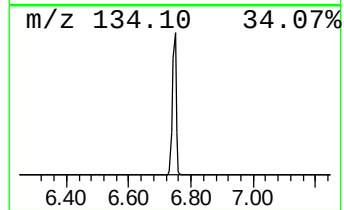
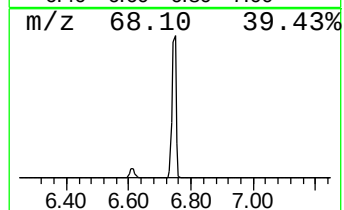
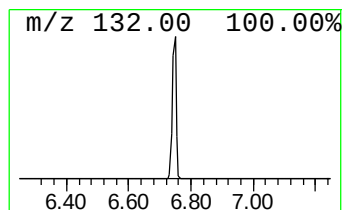
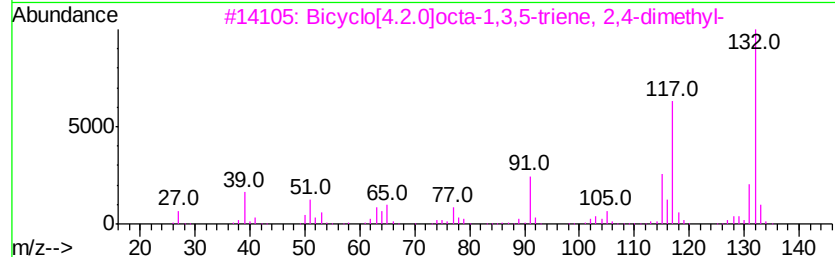
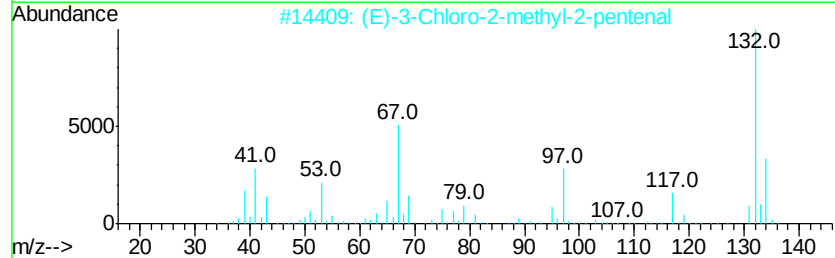
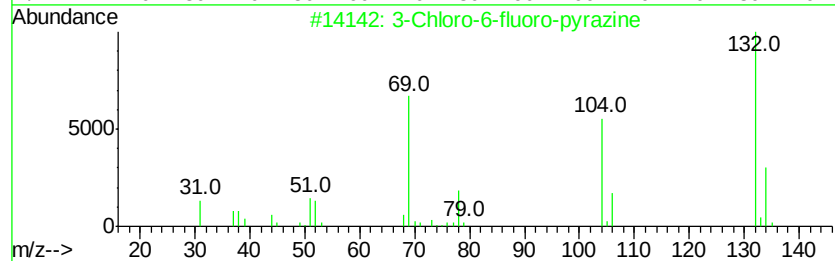
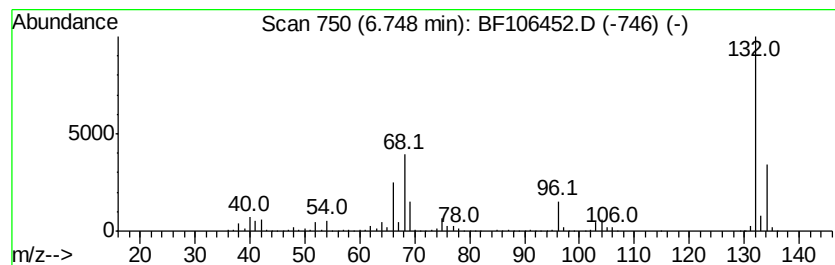
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 unknown6.75 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.75 | 63.50 ng | 2499770 | 1,4-Dichlorobenzene-d4 | 6.97 |

| 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  | 16   |
| 3    |    | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12    | 028749-81-7  | 9    |
| 4    |    | 4-Chloro-2-fluoro-pyrimidine        | 132 | C4H2ClFN2 | 051422-00-5  | 9    |
| 5    |    | 2H-Cyclopenta[d]pyridazine, 2-me... | 132 | C8H8N2    | 022291-85-6  | 9    |



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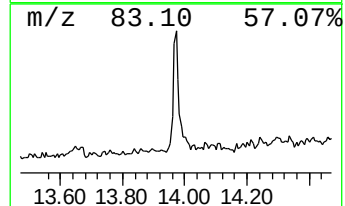
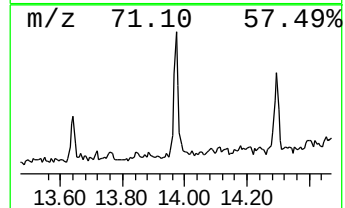
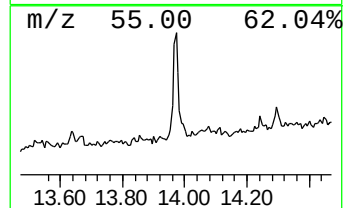
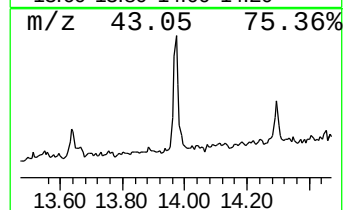
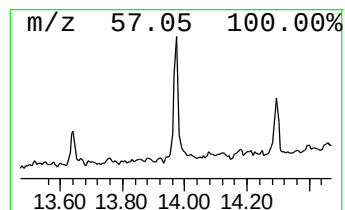
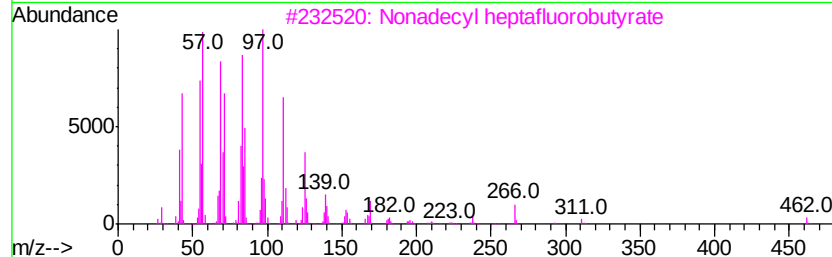
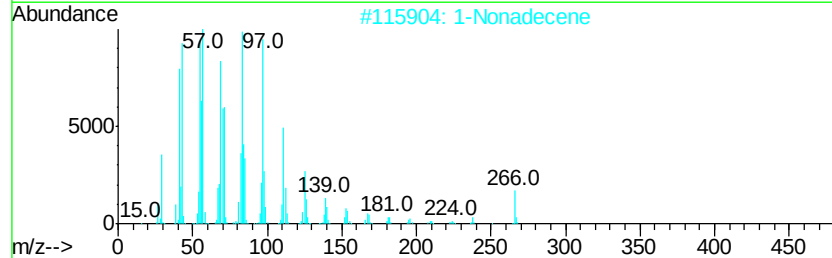
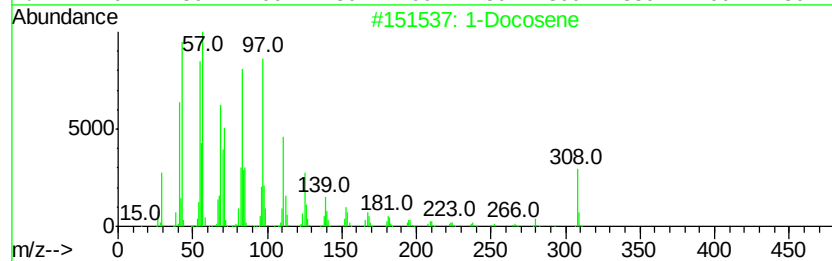
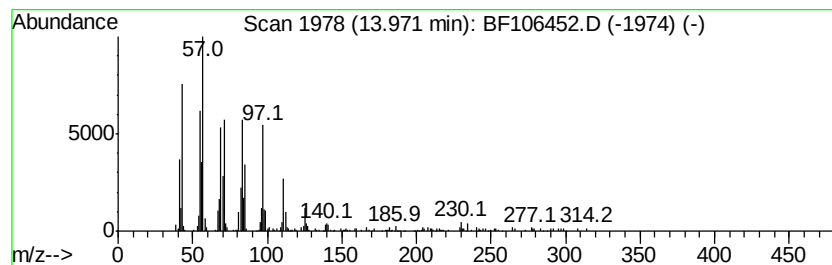
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 1-Docosene Concentration Rank 5

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 13.97 | 5.49 ng | 250594 | Chrysene-d12     | 14.15 |

| Hit# | of | Tentative ID                    | MW  | MolForm    | CAS#         | Qual |
|------|----|---------------------------------|-----|------------|--------------|------|
| 1    | 5  | 1-Docosene                      | 308 | C22H44     | 001599-67-3  | 93   |
| 2    |    | 1-Nonadecene                    | 266 | C19H38     | 018435-45-5  | 92   |
| 3    |    | Nonadecyl heptafluorobutvrate   | 480 | C23H39F7O2 | 1000351-83-9 | 91   |
| 4    |    | Nonadecyl pentafluoropropionate | 430 | C22H39F5O2 | 1000351-88-8 | 91   |
| 5    |    | E-7-Octadecene                  | 252 | C18H36     | 1000130-92-0 | 91   |



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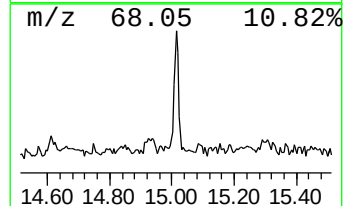
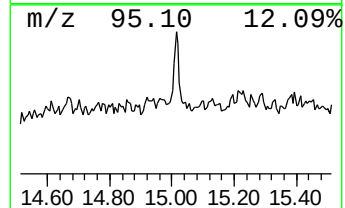
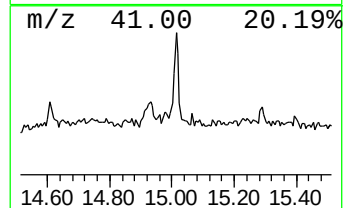
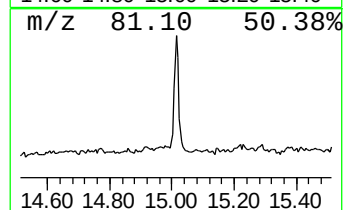
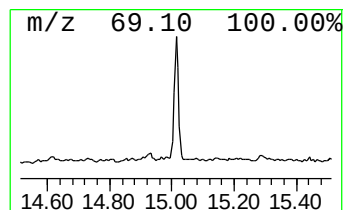
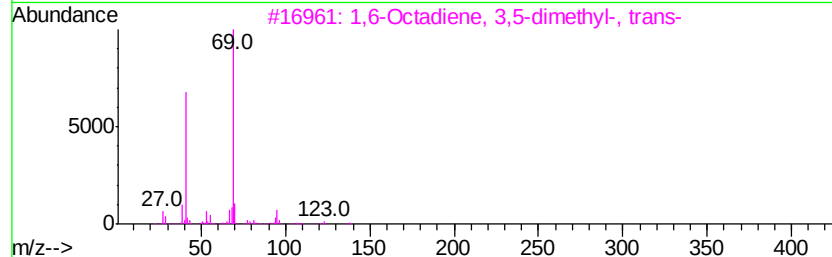
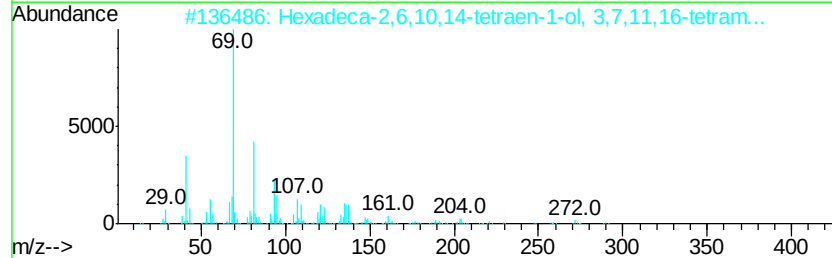
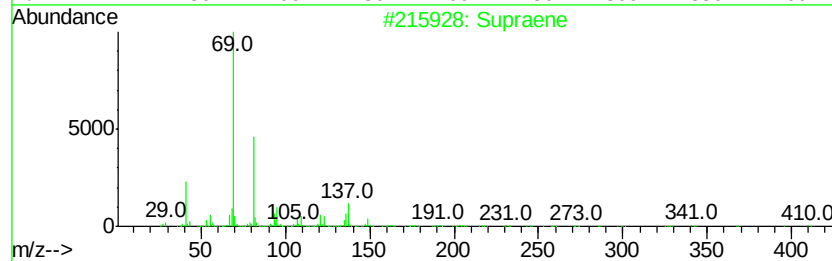
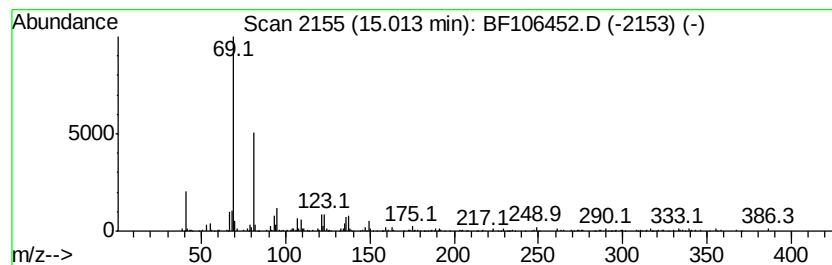
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Peak Number 6 Supraene Concentration Rank 6

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 15.01 | 4.70 ng | 158391 | Perylene-d12     | 15.69 |

| Hit# | of | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|-------------------------------------|-----|----------|-------------|------|
| 1    | 5  | Supraene                            | 410 | C30H50   | 007683-64-9 | 74   |
| 2    |    | Hexadeca-2,6,10,14-tetraen-1-ol,... | 290 | C20H34O  | 007614-21-3 | 72   |
| 3    |    | 1,6-Octadiene, 3,5-dimethyl-, tr... | 138 | C10H18   | 074630-87-8 | 64   |
| 4    |    | 2,6-Octadiene, 4-methyl-            | 124 | C9H16    | 074498-94-5 | 59   |
| 5    |    | 2,6,10-Dodecatrien-1-ol, 3,7,11-... | 264 | C17H28O2 | 004128-17-0 | 59   |



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

| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                      |       |         |       |          | #                     | RT    | Resp   | Conc |
| 2-Pentanone, 4-hy... | 5.20  | 6.5     | ng    | 257434   | 1                     | 6.97  | 787325 | 20.0 |
| unknown6.75          | 6.75  | 63.5    | ng    | 2499770  | 1                     | 6.97  | 787325 | 20.0 |
| 1-Docosene           | 13.97 | 5.5     | ng    | 250594   | 5                     | 14.15 | 913148 | 20.0 |
| Supraene             | 15.01 | 4.7     | ng    | 158391   | 6                     | 15.69 | 673409 | 20.0 |