

Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF070117\  
 Data File : BF096384.D  
 Acq On : 1 Jul 2017 17:43  
 Operator : SJ/MA  
 Sample : I3996-01  
 Misc :  
 ALS Vial : 7 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 I-5-(A-H)-COMP

Integration Parameters: rteint.p  
 Integrator: RTE  
 Smoothing : ON  
 Sampling : 1  
 Start Thrs: 0.2  
 Stop Thrs : 0  
 Filtering: 5  
 Min Area: 3 % of largest Peak  
 Max Peaks: 100  
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >  
 Peak separation: 5

Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF070117.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         | 4.922       | 477           | 482         | 491          | rBV      | 361324         | 454908        | 16.65%          | 1.848%        |
| 2         | 5.345       | 549           | 554         | 557          | rBV      | 2507520        | 2273269       | 83.18%          | 9.233%        |
| 3         | 6.363       | 722           | 727         | 730          | rBV      | 2591593        | 2717738       | 99.44%          | 11.038%       |
| 4         | 6.498       | 746           | 750         | 754          | rBV      | 2735452        | 2654229       | 97.12%          | 10.780%       |
| 5         | 6.734       | 786           | 790         | 793          | rBV      | 1017984        | 848872        | 31.06%          | 3.448%        |
| 6         | 6.886       | 812           | 816         | 820          | rBV      | 2169183        | 2048029       | 74.94%          | 8.318%        |
| 7         | 7.292       | 879           | 885         | 888          | rBV      | 1664433        | 1719418       | 62.91%          | 6.983%        |
| 8         | 7.710       | 950           | 956         | 959          | rBV      | 34773          | 38132         | 1.40%           | 0.155%        |
| 9         | 8.016       | 1003          | 1008        | 1011         | rBV      | 1242113        | 1155326       | 42.27%          | 4.692%        |
| 10        | 9.092       | 1186          | 1191        | 1194         | rBV      | 2896214        | 2732958       | 100.00%         | 11.100%       |
| 11        | 9.480       | 1253          | 1257        | 1260         | rBV      | 995568         | 804062        | 29.42%          | 3.266%        |
| 12        | 9.710       | 1293          | 1296        | 1299         | rVB      | 56136          | 46336         | 1.70%           | 0.188%        |
| 13        | 9.763       | 1300          | 1305        | 1309         | rBV2     | 1218211        | 1130763       | 41.38%          | 4.593%        |
| 14        | 10.039      | 1348          | 1352        | 1355         | rBV2     | 26267          | 30548         | 1.12%           | 0.124%        |
| 15        | 10.210      | 1378          | 1381        | 1384         | rVB      | 78224          | 60260         | 2.20%           | 0.245%        |
| 16        | 10.545      | 1434          | 1438        | 1442         | rBV      | 1306174        | 1227774       | 44.92%          | 4.987%        |
| 17        | 10.680      | 1458          | 1461        | 1468         | rBV      | 88593          | 90817         | 3.32%           | 0.369%        |
| 18        | 11.127      | 1534          | 1537        | 1540         | rVB2     | 52519          | 43729         | 1.60%           | 0.178%        |
| 19        | 11.245      | 1553          | 1557        | 1559         | rBV      | 959884         | 904025        | 33.08%          | 3.672%        |
| 20        | 11.263      | 1559          | 1560        | 1563         | rVB      | 64250          | 44004         | 1.61%           | 0.179%        |
| 21        | 11.774      | 1644          | 1647        | 1650         | rBV3     | 29262          | 28814         | 1.05%           | 0.117%        |
| 22        | 12.445      | 1758          | 1761        | 1767         | rVB      | 76724          | 77869         | 2.85%           | 0.316%        |
| 23        | 12.574      | 1776          | 1783        | 1784         | rBV6     | 18632          | 29427         | 1.08%           | 0.120%        |
| 24        | 12.674      | 1796          | 1800        | 1804         | rVB      | 73743          | 79959         | 2.93%           | 0.325%        |
| 25        | 12.827      | 1820          | 1826        | 1829         | rBV      | 1825367        | 1687241       | 61.74%          | 6.853%        |
| 26        | 12.974      | 1847          | 1851        | 1854         | rBV6     | 18887          | 27593         | 1.01%           | 0.112%        |
| 27        | 13.727      | 1976          | 1979        | 1985         | rVB      | 145909         | 141070        | 5.16%           | 0.573%        |
| 28        | 13.868      | 1999          | 2003        | 2015         | rVB      | 808732         | 820783        | 30.03%          | 3.334%        |
| 29        | 15.280      | 2238          | 2243        | 2247         | rBV      | 601265         | 703207        | 25.73%          | 2.856%        |

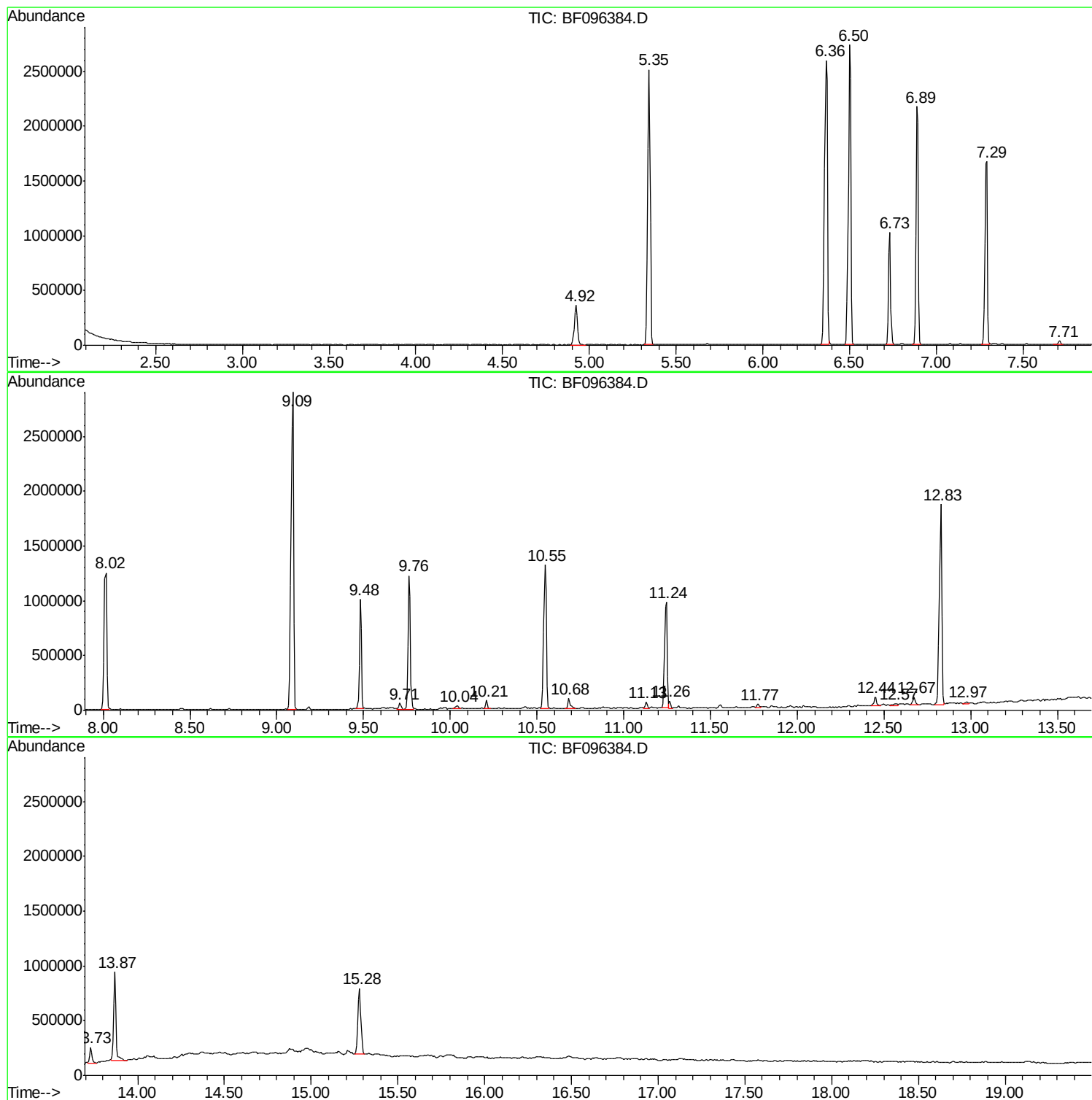
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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF070117.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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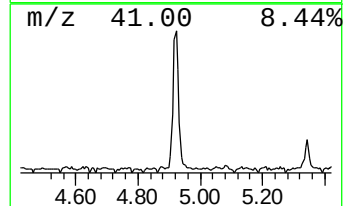
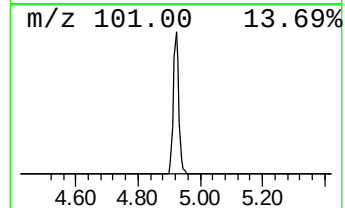
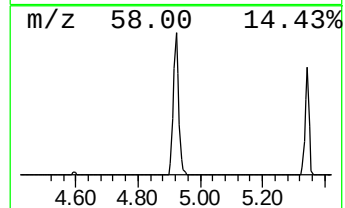
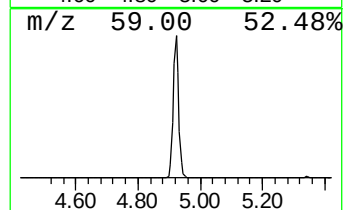
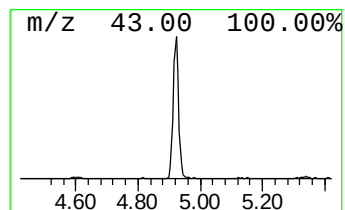
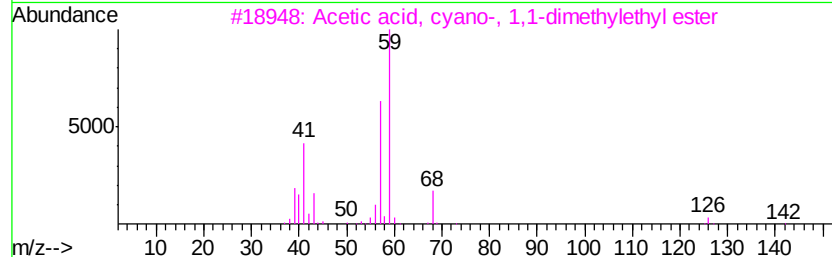
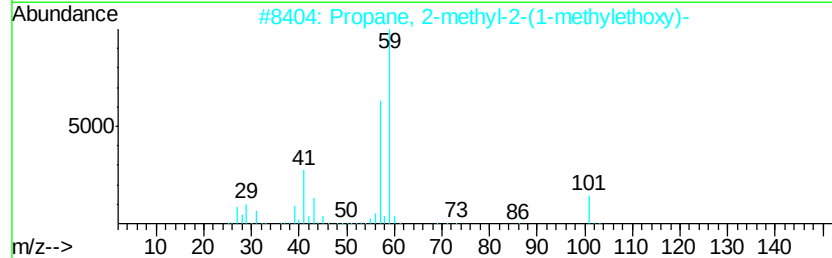
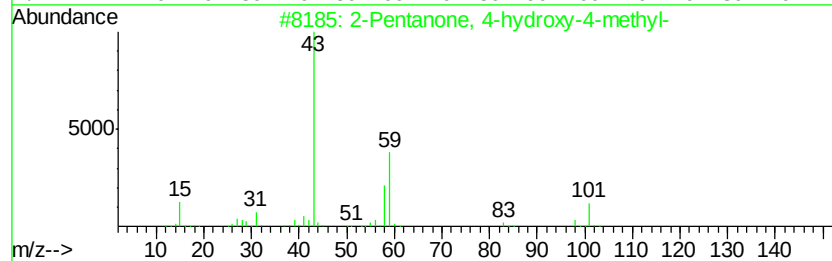
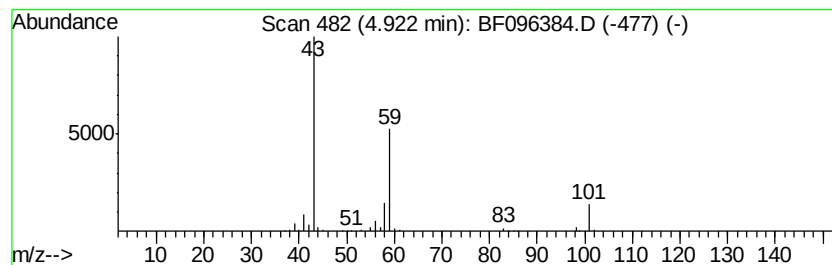
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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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. |
|------|----------|--------|------------------------|------|
| 4.92 | 10.72 ng | 454908 | 1,4-Dichlorobenzene-d4 | 6.73 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2  | 000123-42-2 | 50   |
| 2    |    |   | Propane, 2-methyl-2-(1-methyleth... | 116 | C7H16O   | 017348-59-3 | 36   |
| 3    |    |   | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 25   |
| 4    |    |   | 1-Propen-2-ol, acetate              | 100 | C5H8O2   | 000108-22-5 | 10   |
| 5    |    |   | 2,3-Butanedione, monooxime          | 101 | C4H7NO2  | 000057-71-6 | 9    |



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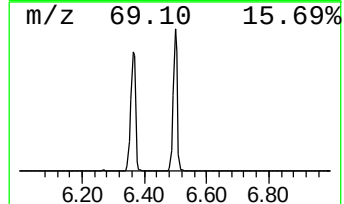
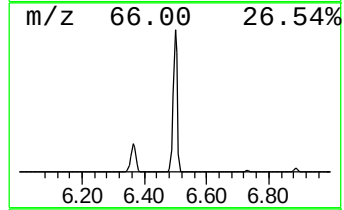
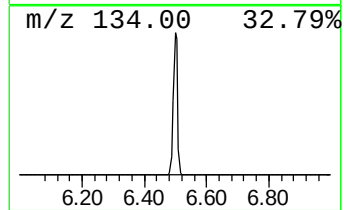
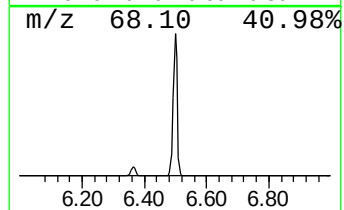
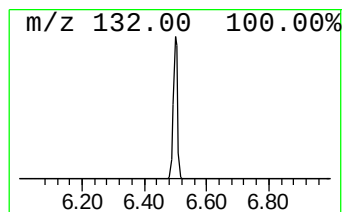
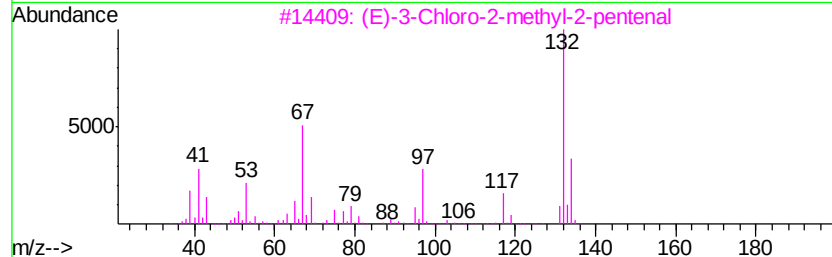
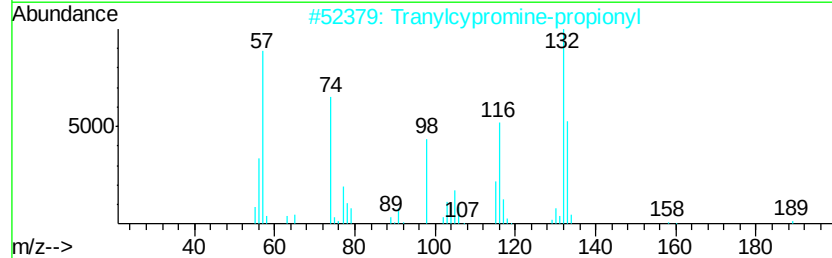
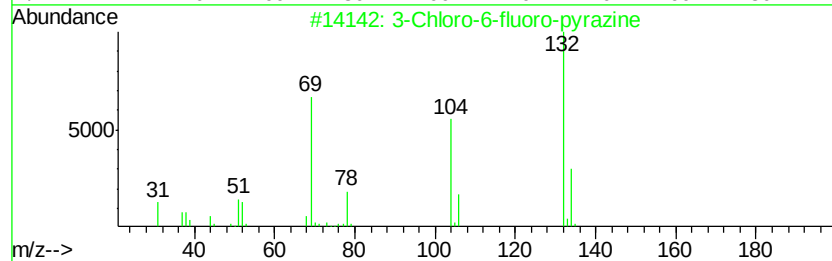
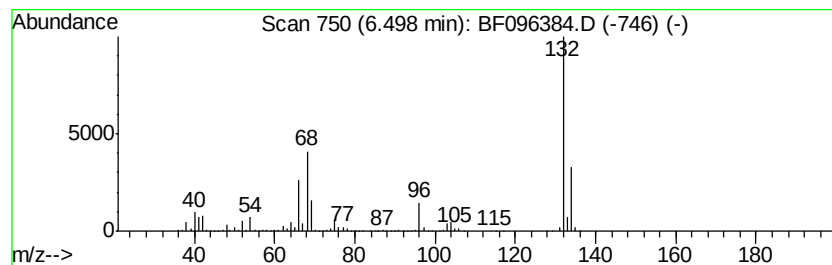
Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF070117.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 2 unknown6.50 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.50 | 62.54 ng | 2654230 | 1,4-Dichlorobenzene-d4 | 6.73 |

| Hit# | of | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|-------------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 3-Chloro-6-fluoro-pyrazine          | 132 | C4H2ClFN2 | 1000146-10-7 | 27   |
| 2    |    | Tranylcypromine-propionyl           | 189 | C12H15NO  | 1000123-86-3 | 10   |
| 3    |    | (E)-3-Chloro-2-methyl-2-pentenal    | 132 | C6H9ClO   | 031357-76-3  | 10   |
| 4    |    | 5-Fluoro-2-chloropyrimidine         | 132 | C4H2ClFN2 | 062802-42-0  | 9    |
| 5    |    | 2H-Cyclopenta[d]pyridazine, 2-me... | 132 | C8H8N2    | 022291-85-6  | 9    |



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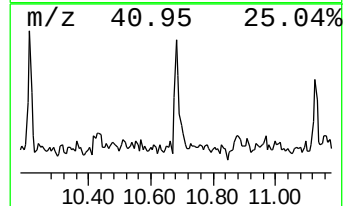
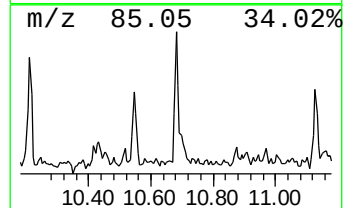
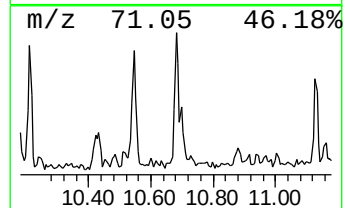
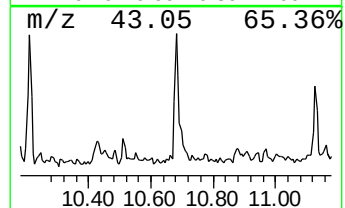
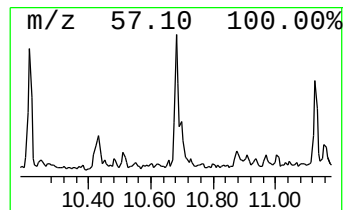
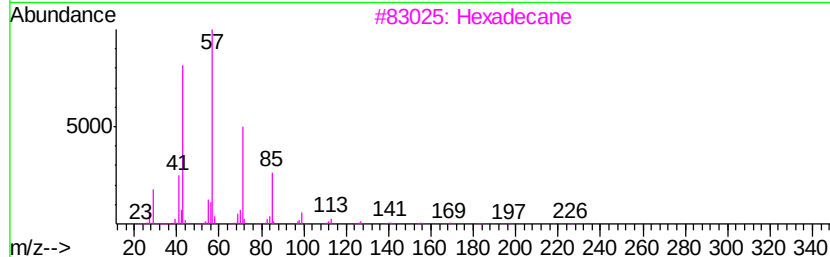
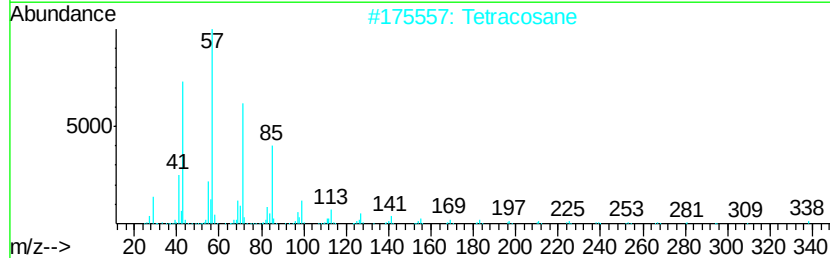
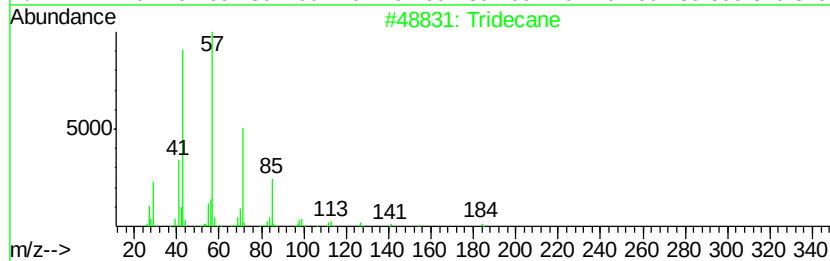
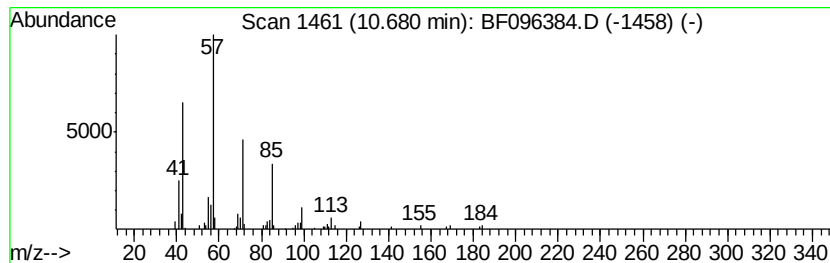
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I-5-(A-H)-COMP

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

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Peak Number 4 Tridecane Concentration Rank 5

| R.T.      | EstConc                      | Area  | Relative to ISTD | R.T.        |      |
|-----------|------------------------------|-------|------------------|-------------|------|
| 10.68     | 2.01 ng                      | 90817 | Phenanthrene-d10 | 11.24       |      |
| Hit# of 5 | Tentative ID                 | MW    | MolForm          | CAS#        | Qual |
| 1         | Tridecane                    | 184   | C13H28           | 000629-50-5 | 90   |
| 2         | Tetracosane                  | 338   | C24H50           | 000646-31-1 | 90   |
| 3         | Hexadecane                   | 226   | C16H34           | 000544-76-3 | 90   |
| 4         | Pentadecane                  | 212   | C15H32           | 000629-62-9 | 86   |
| 5         | Dodecane, 2-methyl-6-propyl- | 226   | C16H34           | 055045-08-4 | 86   |



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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF070117.M  
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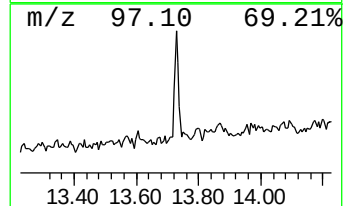
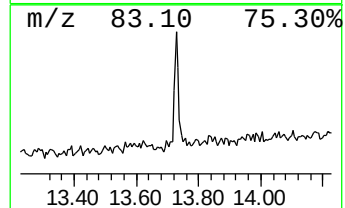
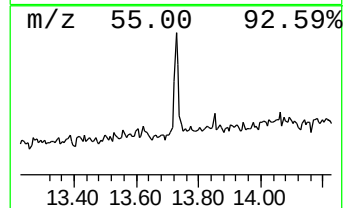
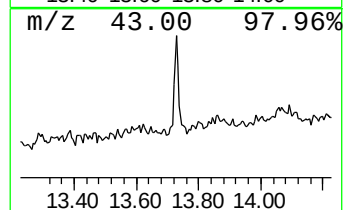
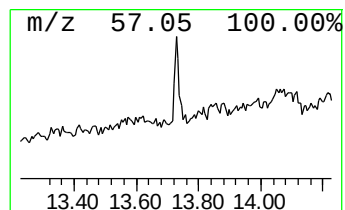
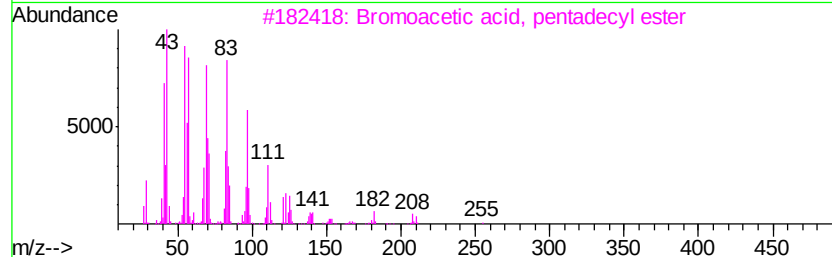
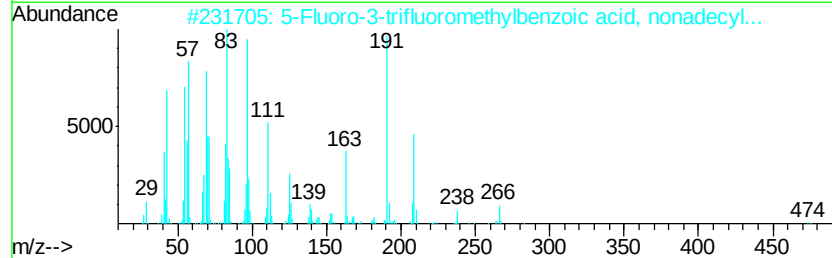
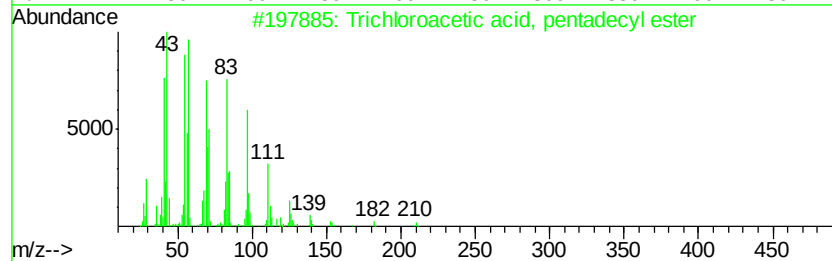
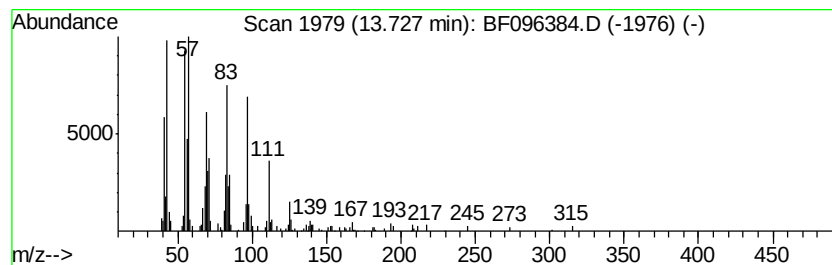
TIC Library : C:\DATABASE\NIST11.L  
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Peak Number 5 Trichloroacetic acid, penta... Concentration Rank 4

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 13.73 | 3.44 ng | 141070 | Chrysene-d12     | 13.87 |

| Hit# of | 5 | Tentative ID                        | MW  | MolForm     | CAS#         | Qual |
|---------|---|-------------------------------------|-----|-------------|--------------|------|
| 1       |   | Trichloroacetic acid, pentadecyl... | 372 | C17H31Cl3O2 | 074339-53-0  | 91   |
| 2       |   | 5-Fluoro-3-trifluoromethylbenzoi... | 474 | C27H42F4O2  | 1000338-91-1 | 91   |
| 3       |   | Bromoacetic acid, pentadecyl ester  | 348 | C17H33BrO2  | 131143-01-6  | 91   |
| 4       |   | 1-Heneicosyl formate                | 340 | C22H44O2    | 077899-03-7  | 91   |
| 5       |   | 1-Docosene                          | 308 | C22H44      | 001599-67-3  | 91   |



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| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                      |       |         |       |          | #                     | RT    | Resp   | Conc |
| 2-Pentanone, 4-hy... | 4.92  | 10.7    | ng    | 454908   | 1                     | 6.73  | 848872 | 20.0 |
| unknown6.50          | 6.50  | 62.5    | ng    | 2654230  | 1                     | 6.73  | 848872 | 20.0 |
| Tridecane            | 10.68 | 2.0     | ng    | 90817    | 4                     | 11.24 | 904025 | 20.0 |
| Trichloroacetic a... | 13.73 | 3.4     | ng    | 141070   | 5                     | 13.87 | 820783 | 20.0 |