

Data Path : Z:\SVOASRV\HPCHEM1\BNA\_F\DATA\BF061918\  
 Data File : BF106602.D  
 Acq On : 20 Jun 2018 00:16  
 Operator : JU/SJ  
 Sample : J3554-07  
 Misc :  
 ALS Vial : 23 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 A-6(3.0)

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-BF061918.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         | 5.213       | 484           | 489         | 498          | rVB      | 199499         | 263818        | 10.26%          | 1.205%        |
| 2         | 5.607       | 553           | 556         | 561          | rBV      | 2419806        | 2501257       | 97.30%          | 11.423%       |
| 3         | 6.607       | 721           | 726         | 729          | rBV      | 2439338        | 2556539       | 99.45%          | 11.676%       |
| 4         | 6.742       | 744           | 749         | 752          | rBV      | 2588377        | 2570698       | 100.00%         | 11.740%       |
| 5         | 6.960       | 783           | 786         | 790          | rVB      | 750437         | 615570        | 23.95%          | 2.811%        |
| 6         | 7.119       | 809           | 813         | 816          | rBV      | 2208505        | 2023447       | 78.71%          | 9.241%        |
| 7         | 7.525       | 877           | 882         | 885          | rBV      | 1563677        | 1746437       | 67.94%          | 7.976%        |
| 8         | 8.242       | 1000          | 1004        | 1008         | rBV      | 847839         | 714580        | 27.80%          | 3.263%        |
| 9         | 9.319       | 1182          | 1187        | 1190         | rBV      | 2670877        | 2454002       | 95.46%          | 11.207%       |
| 10        | 9.707       | 1250          | 1253        | 1261         | rVB      | 320846         | 269863        | 10.50%          | 1.232%        |
| 11        | 9.919       | 1284          | 1289        | 1293         | rBV      | 41350          | 39514         | 1.54%           | 0.180%        |
| 12        | 10.001      | 1299          | 1303        | 1307         | rBV      | 711480         | 674728        | 26.25%          | 3.081%        |
| 13        | 10.130      | 1321          | 1325        | 1331         | rBV3     | 23730          | 30847         | 1.20%           | 0.141%        |
| 14        | 10.419      | 1371          | 1374        | 1377         | rVB      | 61850          | 48813         | 1.90%           | 0.223%        |
| 15        | 10.507      | 1386          | 1389        | 1394         | rBV      | 47949          | 37593         | 1.46%           | 0.172%        |
| 16        | 10.795      | 1434          | 1438        | 1442         | rBV      | 1436450        | 1317593       | 51.25%          | 6.017%        |
| 17        | 10.889      | 1451          | 1454        | 1458         | rBV      | 58013          | 51609         | 2.01%           | 0.236%        |
| 18        | 11.495      | 1553          | 1557        | 1561         | rBV      | 662951         | 550000        | 21.39%          | 2.512%        |
| 19        | 13.083      | 1822          | 1827        | 1830         | rBV      | 2184887        | 1983789       | 77.17%          | 9.060%        |
| 20        | 13.966      | 1973          | 1977        | 1984         | rBV      | 68822          | 81280         | 3.16%           | 0.371%        |
| 21        | 14.148      | 2004          | 2008        | 2012         | rBV      | 765909         | 689923        | 26.84%          | 3.151%        |
| 22        | 14.607      | 2083          | 2086        | 2092         | rBV5     | 26159          | 41863         | 1.63%           | 0.191%        |
| 23        | 15.283      | 2198          | 2201        | 2204         | rBV2     | 25201          | 30109         | 1.17%           | 0.138%        |
| 24        | 15.689      | 2265          | 2270        | 2279         | rVB      | 421976         | 550301        | 21.41%          | 2.513%        |
| 25        | 16.148      | 2344          | 2348        | 2355         | rVB      | 33698          | 52123         | 2.03%           | 0.238%        |

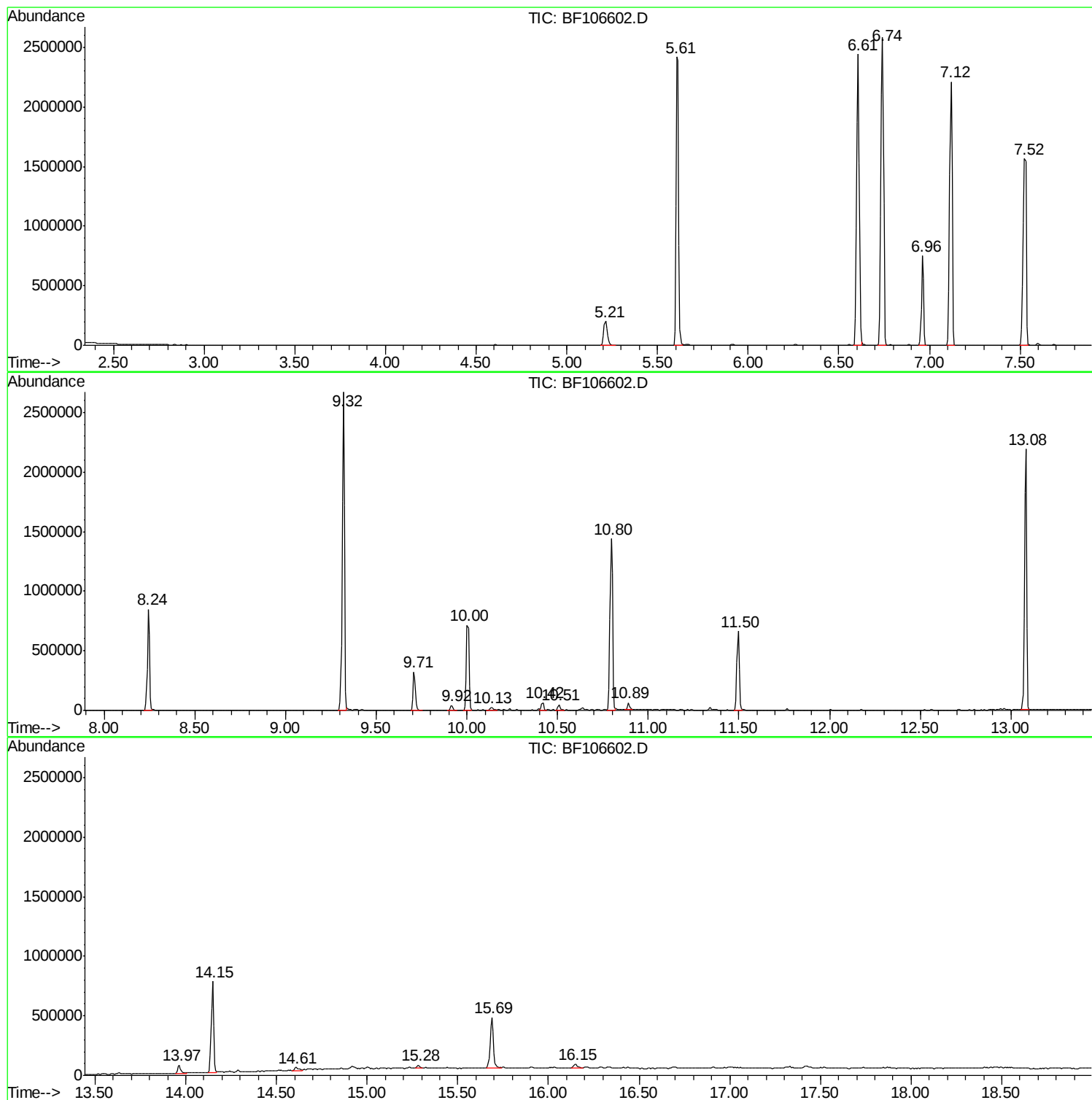
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF061918.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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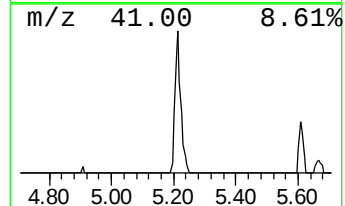
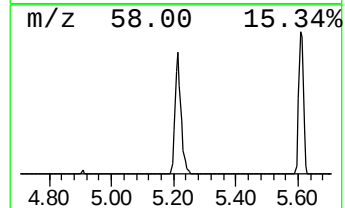
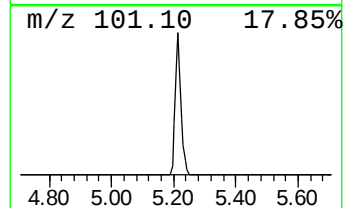
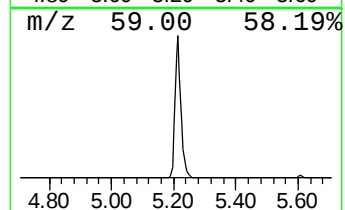
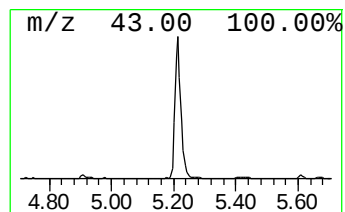
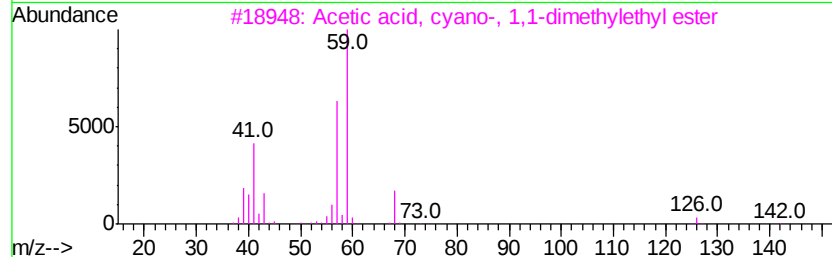
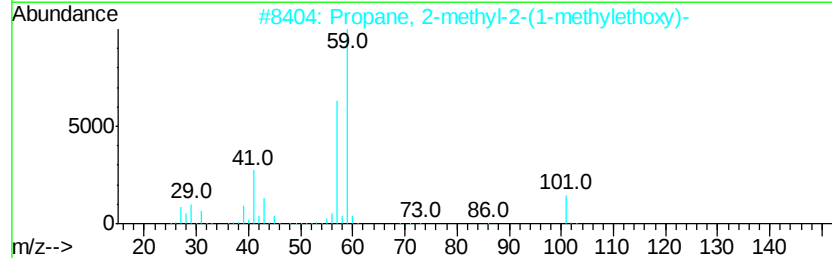
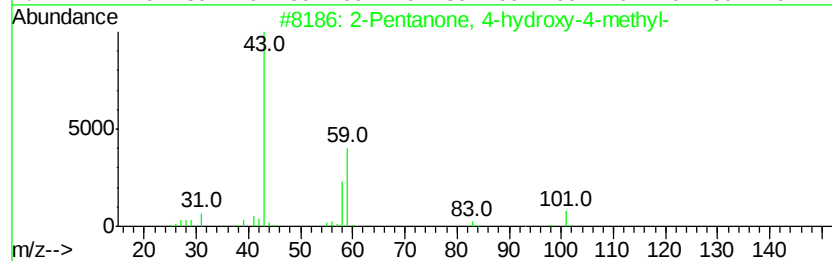
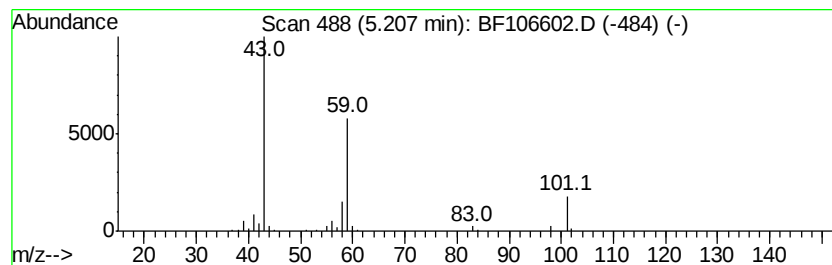
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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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. |
|------|---------|--------|------------------------|------|
| 5.21 | 8.57 ng | 263818 | 1,4-Dichlorobenzene-d4 | 6.96 |

| Hit# | of | 5 | Tentative ID                         | MW  | MolForm  | CAS#        | Qual |
|------|----|---|--------------------------------------|-----|----------|-------------|------|
| 1    |    |   | 2-Pentanone, 4-hydroxy-4-methyl-     | 116 | C6H12O2  | 000123-42-2 | 45   |
| 2    |    |   | Propane, 2-methyl-2-(1-methyleth...  | 116 | C7H16O   | 017348-59-3 | 33   |
| 3    |    |   | Acetic acid, cyano-, 1,1-dimethyl... | 141 | C7H11NO2 | 001116-98-9 | 25   |
| 4    |    |   | 1-Propen-2-ol, acetate               | 100 | C5H8O2   | 000108-22-5 | 10   |
| 5    |    |   | Morpholine, 4-methyl-                | 101 | C5H11NO  | 000109-02-4 | 9    |



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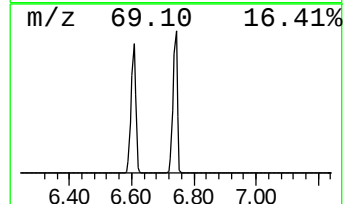
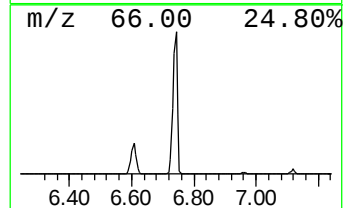
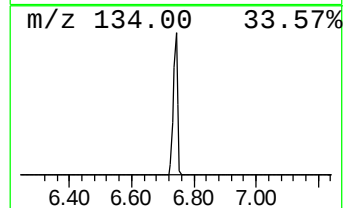
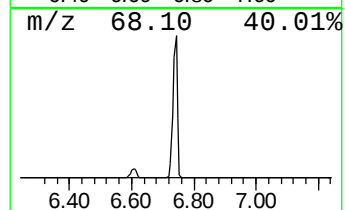
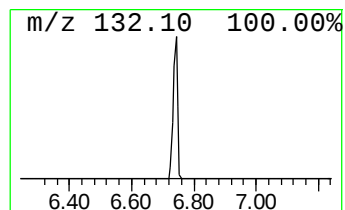
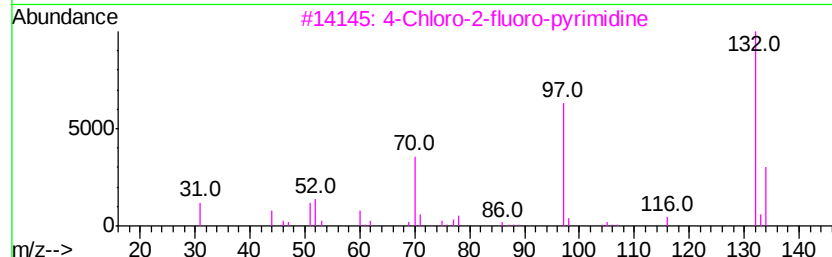
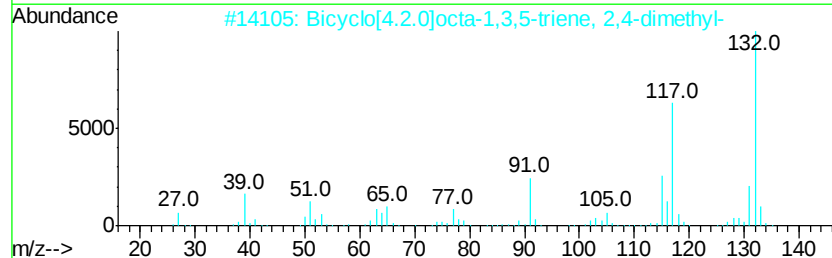
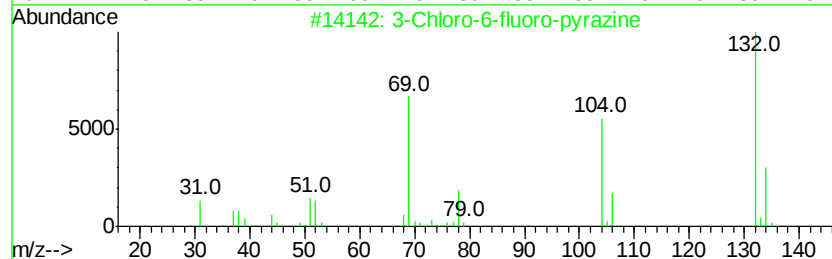
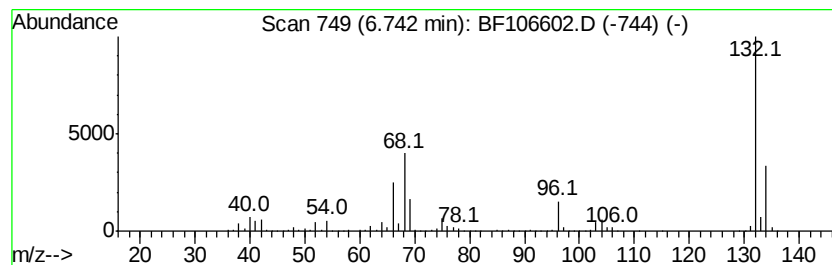
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Peak Number 2 unknown6.74 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.74 | 83.52 ng | 2570700 | 1,4-Dichlorobenzene-d4 | 6.96 |

| Hit# | of | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|-------------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 3-Chloro-6-fluoro-pyrazine          | 132 | C4H2ClFN2 | 1000146-10-7 | 16   |
| 2    |    | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12    | 028749-81-7  | 9    |
| 3    |    | 4-Chloro-2-fluoro-pyrimidine        | 132 | C4H2ClFN2 | 051422-00-5  | 9    |
| 4    |    | 1-Methylpyrrolo[1,2-a]pyrazine      | 132 | C8H8N2    | 064608-59-9  | 9    |
| 5    |    | Imidazole, 4,5-dicyano-1-methyl-    | 132 | C6H4N4    | 019485-35-9  | 9    |



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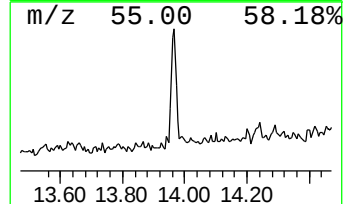
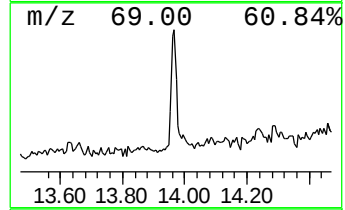
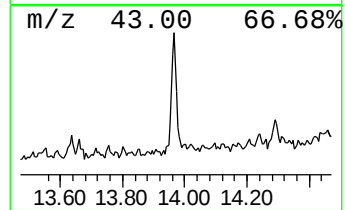
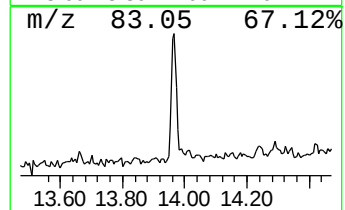
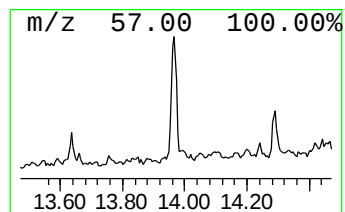
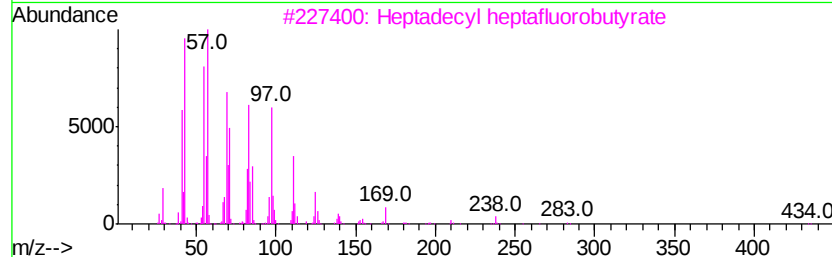
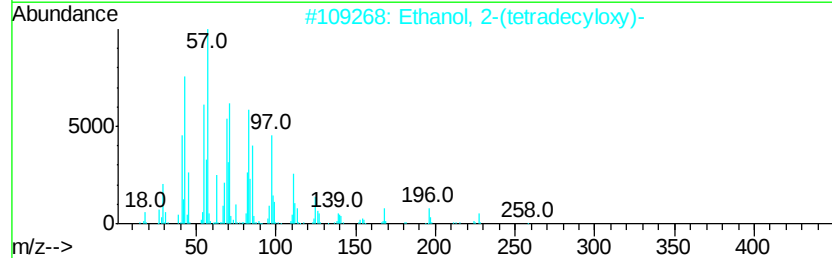
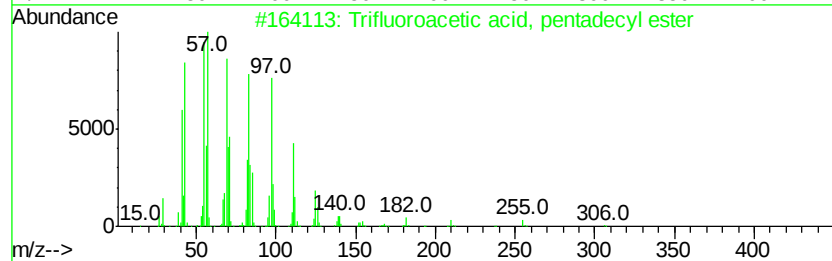
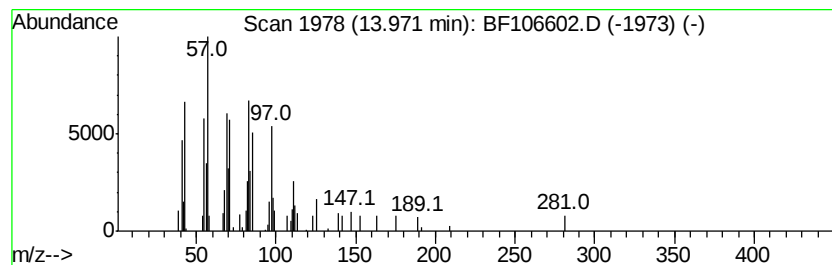
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Peak Number 4 Trifluoroacetic acid, penta... Concentration Rank 4

| R.T.  | EstConc | Area  | Relative to ISTD | R.T.  |
|-------|---------|-------|------------------|-------|
| 13.97 | 2.36 ng | 81280 | Chrysene-d12     | 14.15 |

| Hit# | of | Tentative ID                        | MW  | MolForm     | CAS#        | Qual |
|------|----|-------------------------------------|-----|-------------|-------------|------|
| 1    | 5  | Trifluoroacetic acid, pentadecyl... | 324 | C17H31F3O2  | 959010-23-2 | 93   |
| 2    |    | Ethanol, 2-(tetradecyloxy)-         | 258 | C16H34O2    | 002136-70-1 | 91   |
| 3    |    | Heptadecyl heptafluorobutyrate      | 452 | C21H35F7O2  | 959085-66-6 | 87   |
| 4    |    | Trifluoroacetoxv hexadecane         | 338 | C18H33F3O2  | 006222-03-3 | 87   |
| 5    |    | Trichloroacetic acid, pentadecyl... | 372 | C17H31Cl3O2 | 074339-53-0 | 87   |



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| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                      |       |         |       |          | #                     | RT    | Resp   | Conc |
| 2-Pentanone, 4-hy... | 5.21  | 8.6     | ng    | 263818   | 1                     | 6.96  | 615570 | 20.0 |
| unknown6.74          | 6.74  | 83.5    | ng    | 2570700  | 1                     | 6.96  | 615570 | 20.0 |
| Trifluoroacetic a... | 13.97 | 2.4     | ng    | 81280    | 5                     | 14.15 | 689923 | 20.0 |