

Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF050218\  
 Data File : BF105039.D  
 Acq On : 2 May 2018 18:56  
 Operator : JU/SJ  
 Sample : J2626-04  
 Misc :  
 ALS Vial : 21 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 EPE-MX-4(90-92)

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:\HPCHEM1\BNA\_F\METHODS\8270-BF040618.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         | 4.993       | 490           | 494         | 506          | rBV      | 46544          | 62343         | 3.36%           | 0.406%        |
| 2         | 5.404       | 560           | 564         | 589          | rBV      | 1626982        | 1596392       | 85.98%          | 10.408%       |
| 3         | 6.428       | 734           | 738         | 756          | rBV      | 1485552        | 1610149       | 86.72%          | 10.498%       |
| 4         | 6.563       | 756           | 761         | 764          | rBV      | 1746596        | 1684458       | 90.72%          | 10.982%       |
| 5         | 6.787       | 796           | 799         | 803          | rBV      | 571217         | 460466        | 24.80%          | 3.002%        |
| 6         | 6.945       | 822           | 826         | 829          | rBV      | 1520613        | 1298536       | 69.93%          | 8.466%        |
| 7         | 7.357       | 892           | 896         | 910          | rBV      | 1053783        | 976841        | 52.61%          | 6.369%        |
| 8         | 8.075       | 1014          | 1018        | 1040         | rBV      | 622859         | 608653        | 32.78%          | 3.968%        |
| 9         | 9.151       | 1197          | 1201        | 1211         | rBV      | 2093938        | 1856799       | 100.00%         | 12.106%       |
| 10        | 9.545       | 1265          | 1268        | 1276         | rBV      | 133160         | 126243        | 6.80%           | 0.823%        |
| 11        | 9.828       | 1313          | 1316        | 1331         | rVB      | 654402         | 662031        | 35.65%          | 4.316%        |
| 12        | 10.251      | 1385          | 1388        | 1391         | rVB2     | 39848          | 29076         | 1.57%           | 0.190%        |
| 13        | 10.628      | 1448          | 1452        | 1461         | rBV      | 1012353        | 1049653       | 56.53%          | 6.844%        |
| 14        | 10.727      | 1466          | 1469        | 1473         | rVV      | 31425          | 31983         | 1.72%           | 0.209%        |
| 15        | 11.322      | 1566          | 1570        | 1579         | rBV      | 644030         | 597878        | 32.20%          | 3.898%        |
| 16        | 12.921      | 1837          | 1842        | 1845         | rBV      | 1746210        | 1532407       | 82.53%          | 9.991%        |
| 17        | 13.868      | 2000          | 2003        | 2010         | rBV      | 51851          | 70634         | 3.80%           | 0.461%        |
| 18        | 14.057      | 2031          | 2035        | 2041         | rVB      | 549502         | 563819        | 30.37%          | 3.676%        |
| 19        | 15.021      | 2196          | 2199        | 2205         | rVB2     | 38242          | 51310         | 2.76%           | 0.335%        |
| 20        | 15.662      | 2304          | 2308        | 2318         | rVB2     | 328808         | 468207        | 25.22%          | 3.053%        |

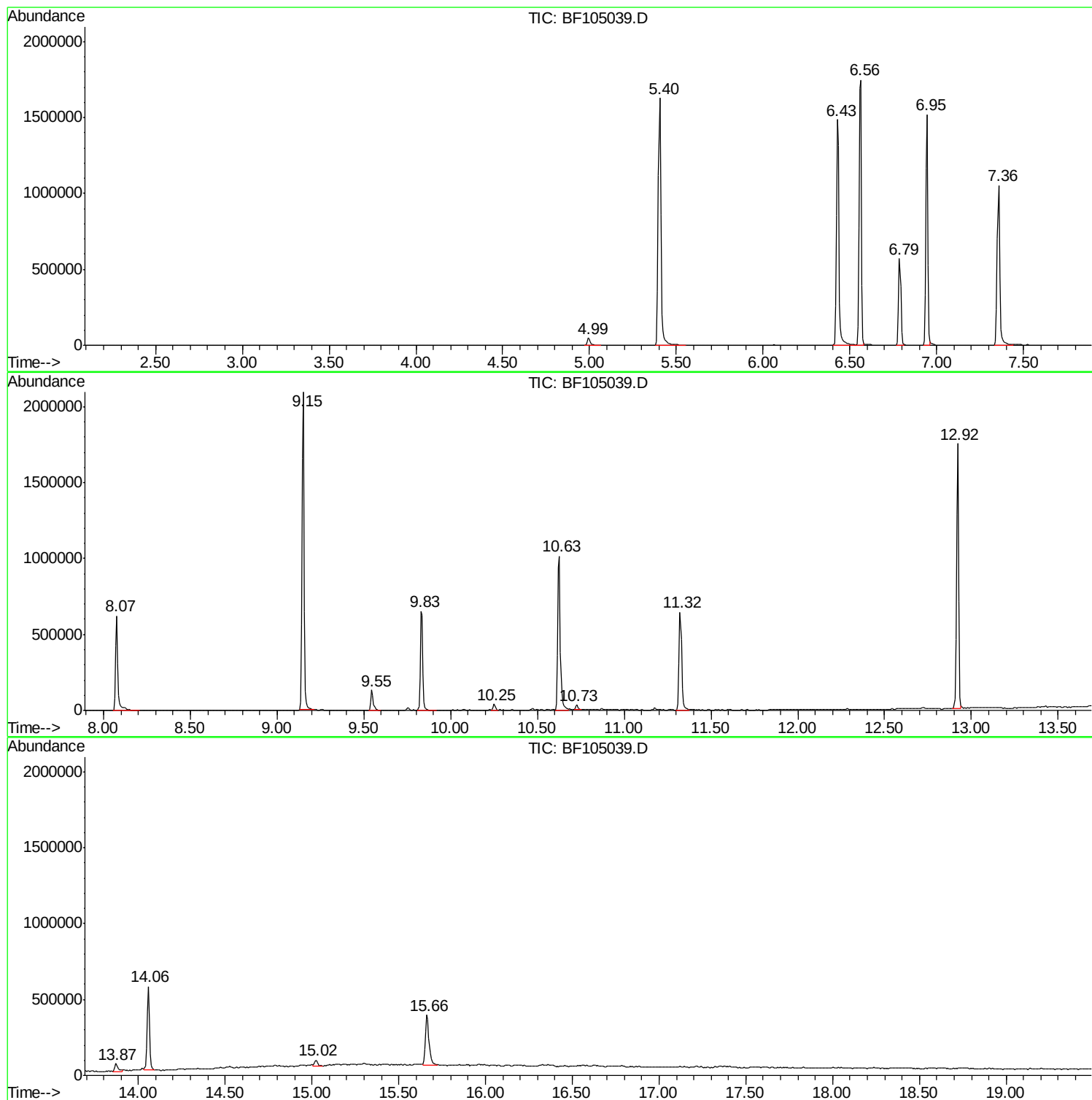
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ClientSampleId :  
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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF040618.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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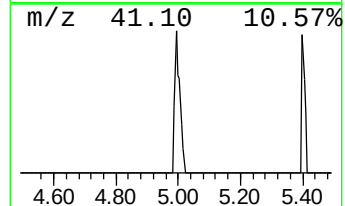
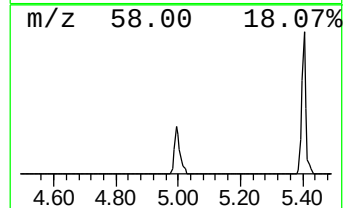
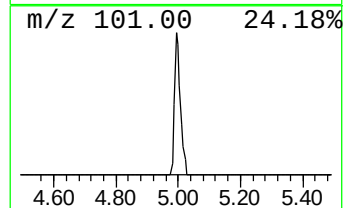
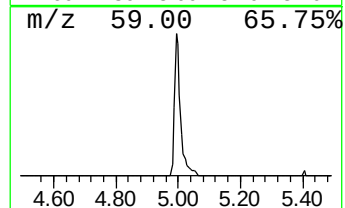
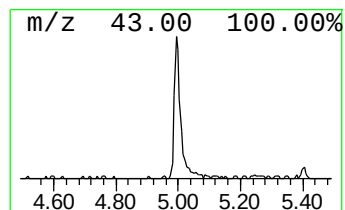
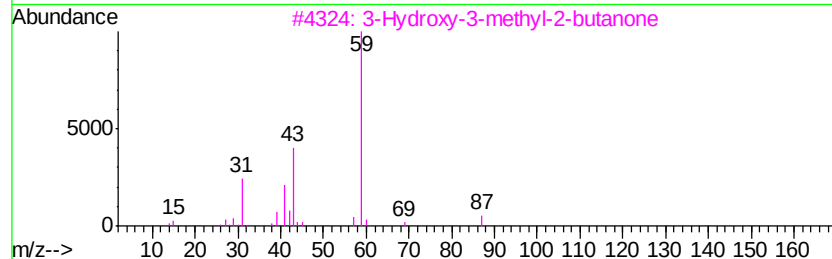
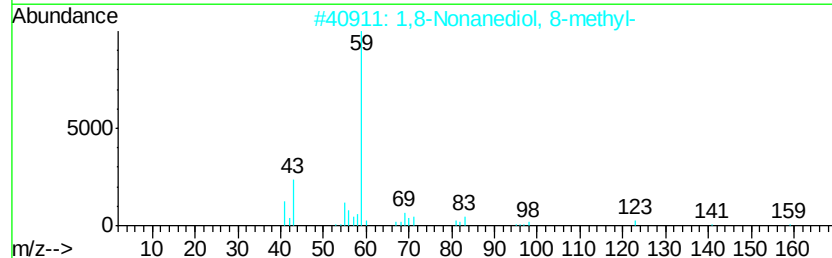
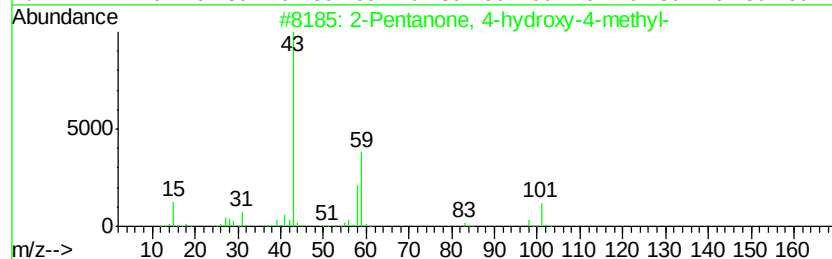
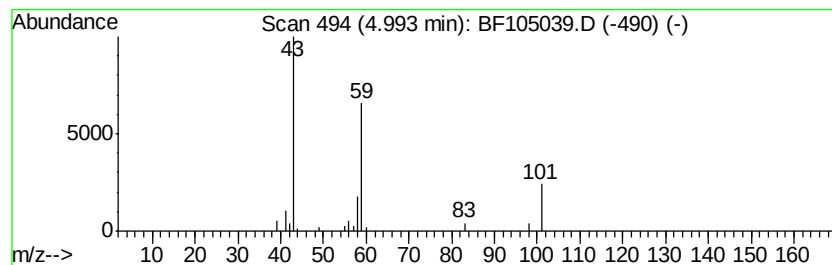
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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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. |
|------|---------|-------|------------------------|------|
| 4.99 | 2.71 ng | 62343 | 1,4-Dichlorobenzene-d4 | 6.79 |

| Hit# | of | 5 | Tentative ID                     | MW  | MolForm  | CAS#        | Qual |
|------|----|---|----------------------------------|-----|----------|-------------|------|
| 1    |    |   | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2  | 000123-42-2 | 38   |
| 2    |    |   | 1,8-Nonanediol, 8-methyl-        | 174 | C10H22O2 | 054725-73-4 | 25   |
| 3    |    |   | 3-Hydroxy-3-methyl-2-butanone    | 102 | C5H10O2  | 000115-22-0 | 17   |
| 4    |    |   | 5-Hexen-2-one                    | 98  | C6H10O   | 000109-49-9 | 9    |
| 5    |    |   | 1-Propen-2-ol, acetate           | 100 | C5H8O2   | 000108-22-5 | 9    |



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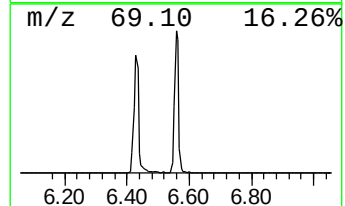
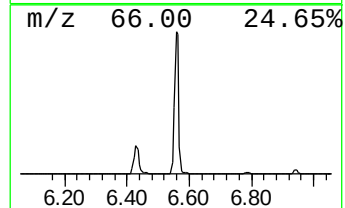
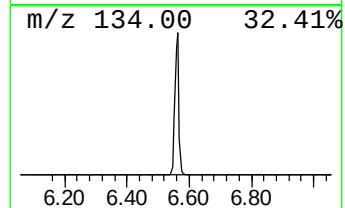
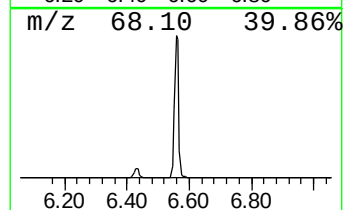
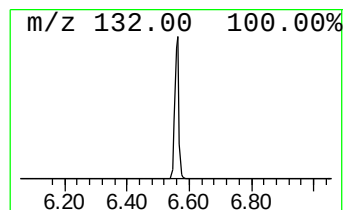
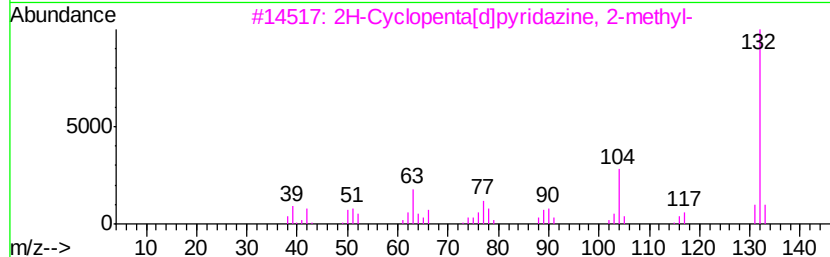
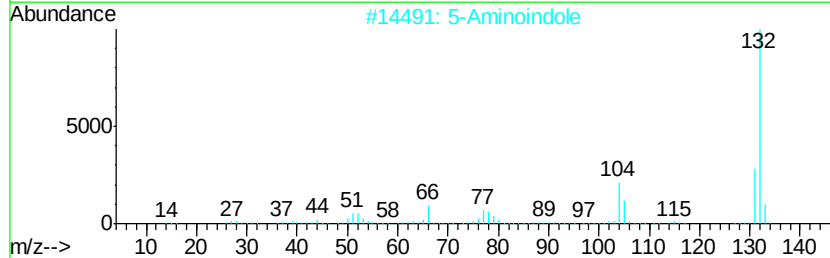
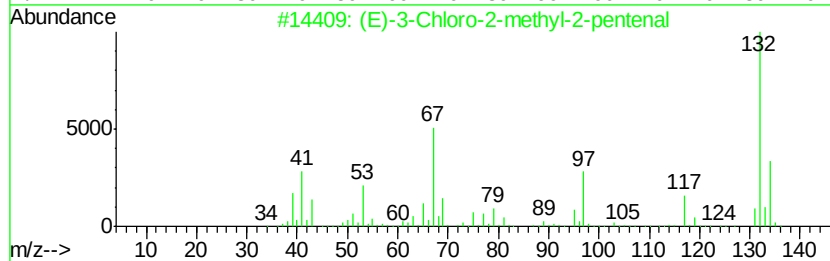
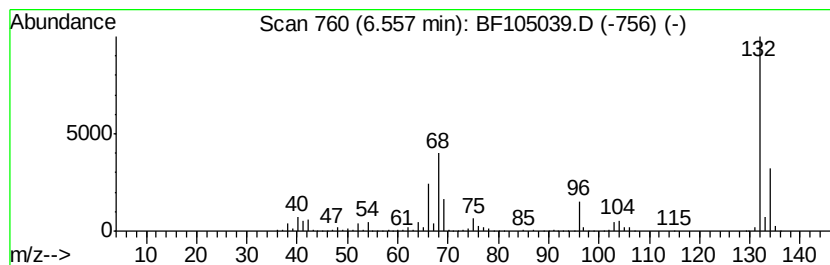
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Peak Number 2 unknown6.56 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.56 | 73.16 ng | 1684460 | 1,4-Dichlorobenzene-d4 | 6.79 |

| Hit# | of | Tentative ID                          | MW  | MolForm   | CAS#        | Qual |
|------|----|---------------------------------------|-----|-----------|-------------|------|
| 1    | 5  | (E)-3-Chloro-2-methyl-2-pentenal      | 132 | C6H9ClO   | 031357-76-3 | 17   |
| 2    |    | 5-Aminoindole                         | 132 | C8H8N2    | 005192-03-0 | 12   |
| 3    |    | 2H-Cyclopenta[d]pyridazine, 2-methyl- | 132 | C8H8N2    | 022291-85-6 | 9    |
| 4    |    | 4-Chloro-2-fluoro-pyrimidine          | 132 | C4H2ClFN2 | 051422-00-5 | 9    |
| 5    |    | 1H-Benzimidazole, 2-methyl-           | 132 | C8H8N2    | 000615-15-6 | 9    |



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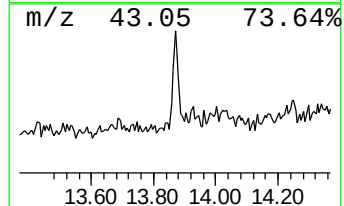
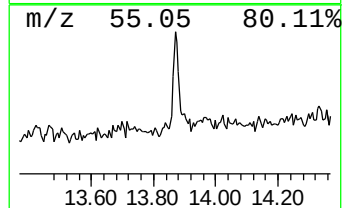
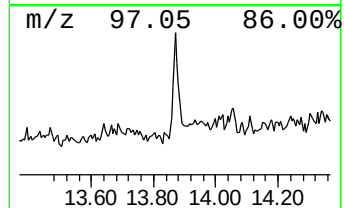
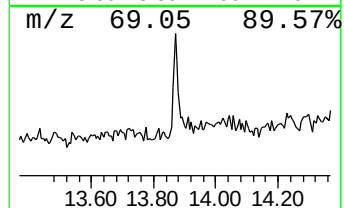
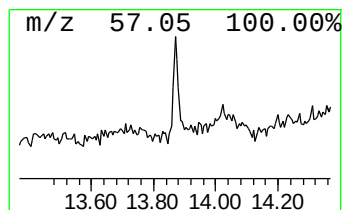
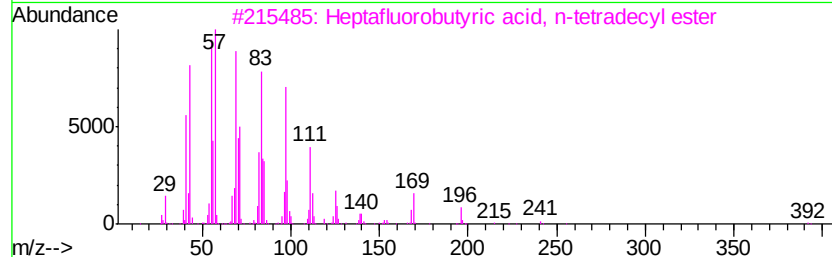
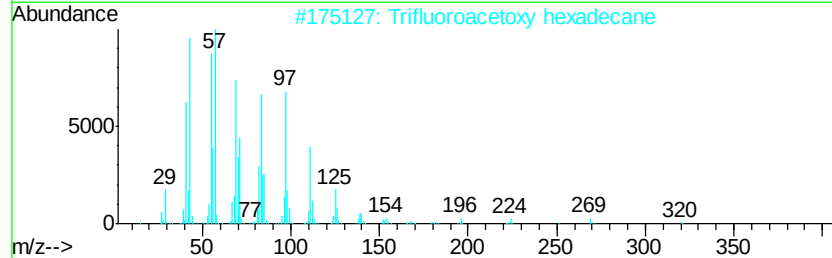
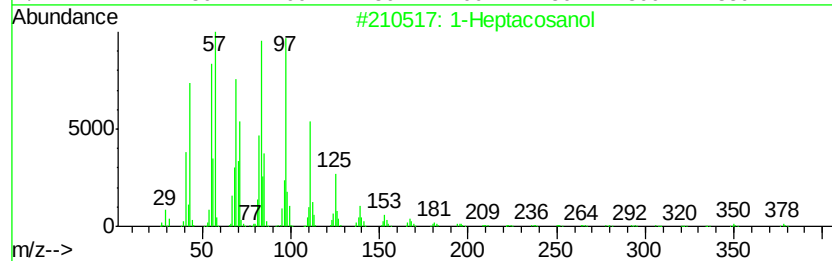
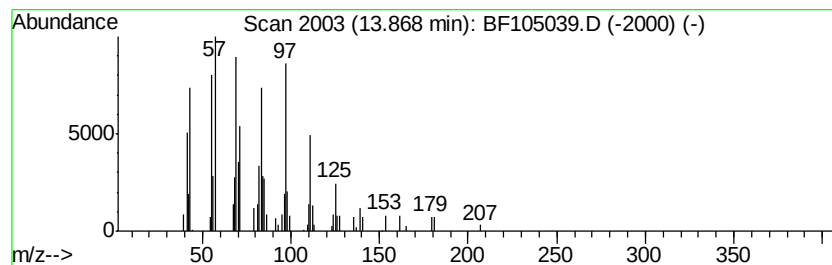
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Peak Number 4 1-Heptacosanol Concentration Rank 4

| R.T.  | EstConc | Area  | Relative to ISTD | R.T.  |
|-------|---------|-------|------------------|-------|
| 13.87 | 2.51 ng | 70634 | Chrysene-d12     | 14.06 |

| Hit# | of | Tentative ID                        | MW  | MolForm    | CAS#         | Qual |
|------|----|-------------------------------------|-----|------------|--------------|------|
| 1    | 5  | 1-Heptacosanol                      | 396 | C27H56O    | 002004-39-9  | 93   |
| 2    |    | Trifluoroacetoxy hexadecane         | 338 | C18H33F3O2 | 006222-03-3  | 91   |
| 3    |    | Heptafluorobutyric acid, n-tetra... | 410 | C18H29F7O2 | 007365-36-8  | 91   |
| 4    |    | Heptadecyl trifluoroacetate         | 352 | C19H35F3O2 | 1000351-87-0 | 90   |
| 5    |    | Octadecyl trifluoroacetate          | 366 | C20H37F3O2 | 079392-43-1  | 81   |



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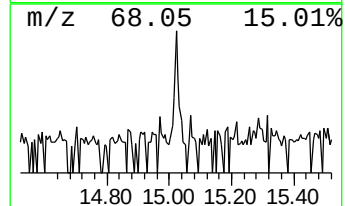
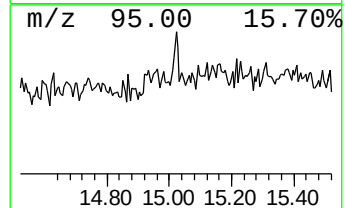
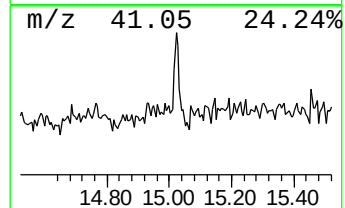
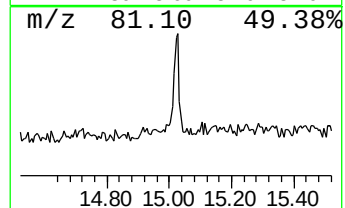
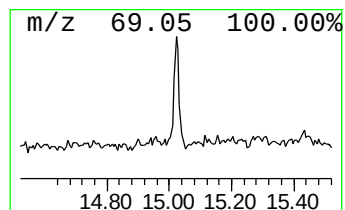
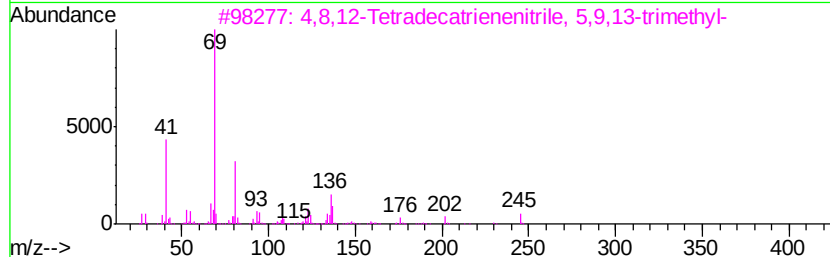
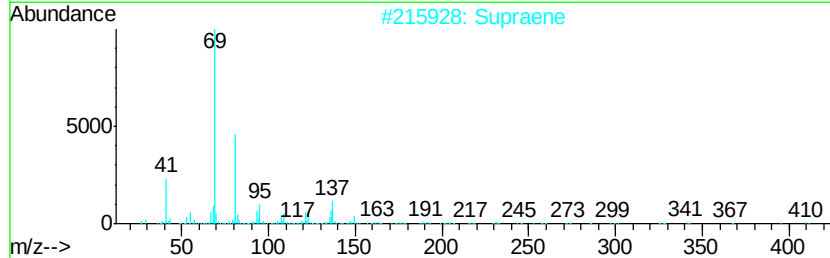
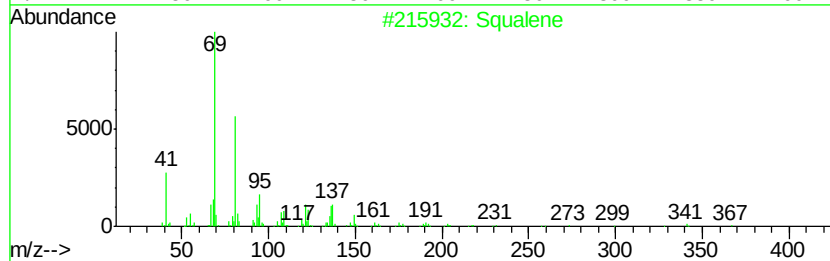
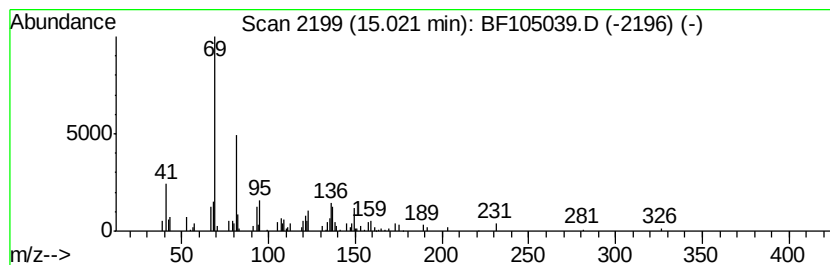
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\*\*\*\*\*  
Peak Number 5 Squalene Concentration Rank 5

| R.T.      | EstConc                             | Area  | Relative to ISTD | R.T.        |      |
|-----------|-------------------------------------|-------|------------------|-------------|------|
| 15.02     | 2.19 ng                             | 51310 | Perylene-d12     | 15.66       |      |
| Hit# of 5 | Tentative ID                        | MW    | MolForm          | CAS#        | Qual |
| 1         | Squalene                            | 410   | C30H50           | 000111-02-4 | 83   |
| 2         | Supraene                            | 410   | C30H50           | 007683-64-9 | 80   |
| 3         | 4,8,12-Tetradecatrienenitrile, 5... | 245   | C17H27N          | 005981-31-7 | 64   |
| 4         | 3,7,11-Tridecatrienenitrile, 4,8... | 231   | C16H25N          | 006006-01-5 | 64   |
| 5         | 3,7,11-Tridecatrienoic acid, 4,8... | 264   | C17H28O2         | 036237-69-1 | 59   |



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| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                      |       |         |       |          | #                     | RT    | Resp   | Conc |
| 2-Pentanone, 4-hy... | 4.99  | 2.7     | ng    | 62343    | 1                     | 6.79  | 460466 | 20.0 |
| unknown6.56          | 6.56  | 73.2    | ng    | 1684460  | 1                     | 6.79  | 460466 | 20.0 |
| 1-Heptacosanol       | 13.87 | 2.5     | ng    | 70634    | 5                     | 14.06 | 563819 | 20.0 |
| Squalene             | 15.02 | 2.2     | ng    | 51310    | 6                     | 15.66 | 468207 | 20.0 |