

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF102624\  
 Data File : BF140059.D  
 Acq On : 26 Oct 2024 14:55  
 Operator : RC/JU  
 Sample : P4508-05  
 Misc :  
 ALS Vial : 11 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 BP-F23

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-BF101824.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140059.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         | 5.122       | 509           | 515         | 522          | rVB      | 23927          | 37040         | 1.15%           | 0.166%        |
| 2         | 5.504       | 574           | 580         | 586          | rBV      | 1878475        | 2553890       | 79.49%          | 11.422%       |
| 3         | 5.628       | 596           | 601         | 609          | rVB      | 33812          | 54080         | 1.68%           | 0.242%        |
| 4         | 5.993       | 658           | 663         | 672          | rVB      | 101580         | 153914        | 4.79%           | 0.688%        |
| 5         | 6.122       | 677           | 685         | 691          | rBV3     | 24407          | 51957         | 1.62%           | 0.232%        |
| 6         | 6.269       | 706           | 710         | 711          | rBV      | 45177          | 55312         | 1.72%           | 0.247%        |
| 7         | 6.287       | 711           | 713         | 718          | rVB      | 64494          | 75857         | 2.36%           | 0.339%        |
| 8         | 6.504       | 744           | 750         | 755          | rBV      | 1904288        | 2624005       | 81.68%          | 11.736%       |
| 9         | 6.887       | 810           | 815         | 820          | rBV      | 730365         | 889465        | 27.69%          | 3.978%        |
| 10        | 7.446       | 903           | 910         | 915          | rBV      | 1299412        | 1744072       | 54.29%          | 7.800%        |
| 11        | 8.169       | 1027          | 1033        | 1038         | rBV      | 955141         | 1212836       | 37.75%          | 5.424%        |
| 12        | 9.245       | 1209          | 1216        | 1227         | rBV      | 2331267        | 3212692       | 100.00%         | 14.368%       |
| 13        | 9.922       | 1325          | 1331        | 1345         | rBV      | 1088341        | 1423463       | 44.31%          | 6.366%        |
| 14        | 10.634      | 1446          | 1452        | 1459         | rBV      | 257215         | 326128        | 10.15%          | 1.459%        |
| 15        | 10.710      | 1459          | 1465        | 1480         | rVV      | 1467589        | 1926498       | 59.97%          | 8.616%        |
| 16        | 11.410      | 1578          | 1584        | 1589         | rBV      | 1127525        | 1401204       | 43.61%          | 6.267%        |
| 17        | 11.933      | 1665          | 1673        | 1687         | rBV2     | 152293         | 262325        | 8.17%           | 1.173%        |
| 18        | 12.716      | 1801          | 1806        | 1814         | rBV4     | 17226          | 33854         | 1.05%           | 0.151%        |
| 19        | 12.992      | 1848          | 1853        | 1859         | rBV      | 2003412        | 2625688       | 81.73%          | 11.743%       |
| 20        | 13.892      | 2000          | 2006        | 2023         | rBV      | 71473          | 172265        | 5.36%           | 0.770%        |
| 21        | 14.045      | 2025          | 2032        | 2047         | rVB      | 534226         | 739954        | 23.03%          | 3.309%        |
| 22        | 14.810      | 2157          | 2162        | 2169         | rBV3     | 19746          | 42658         | 1.33%           | 0.191%        |
| 23        | 15.527      | 2277          | 2284        | 2297         | rBV      | 443105         | 740295        | 23.04%          | 3.311%        |

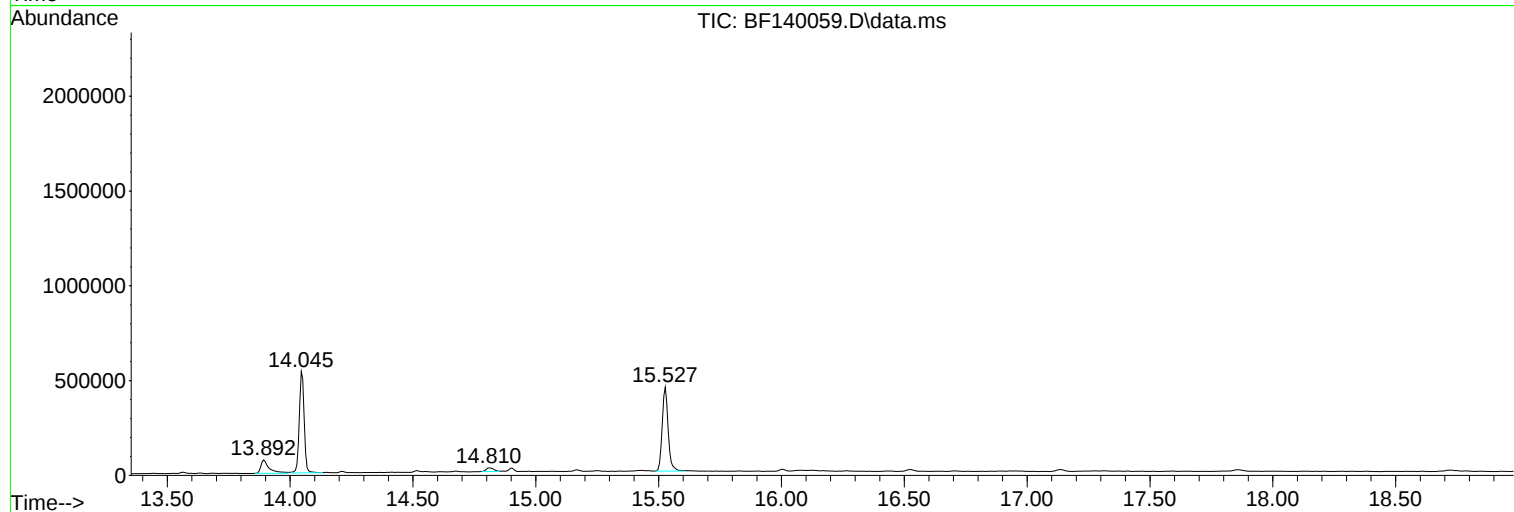
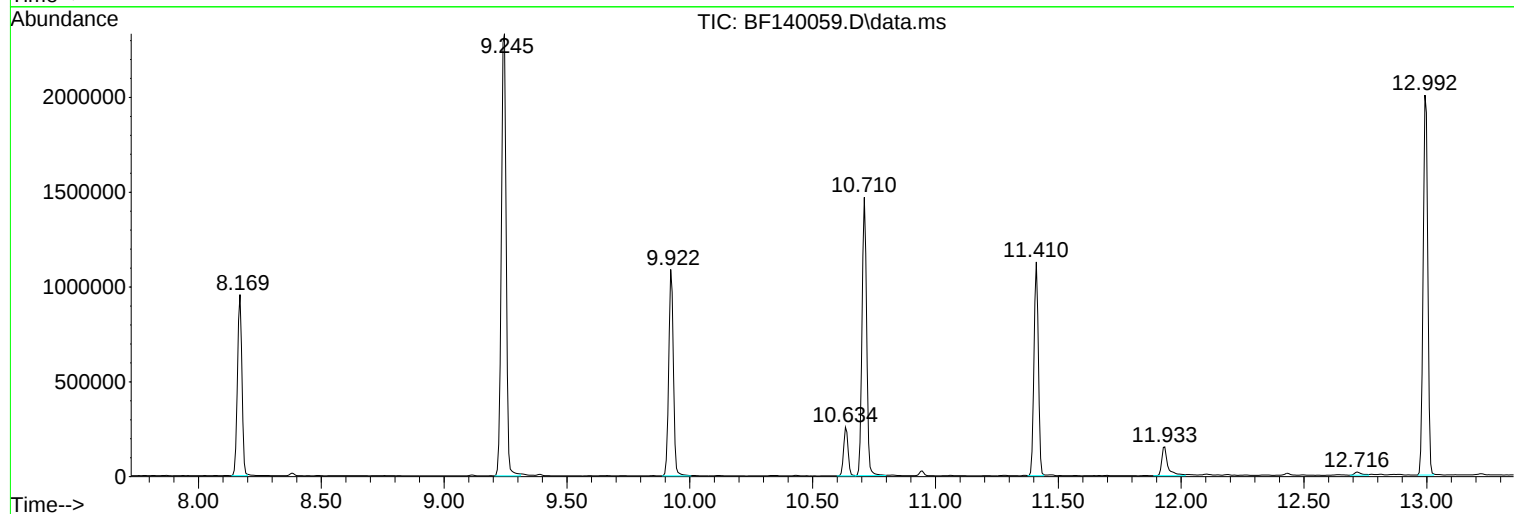
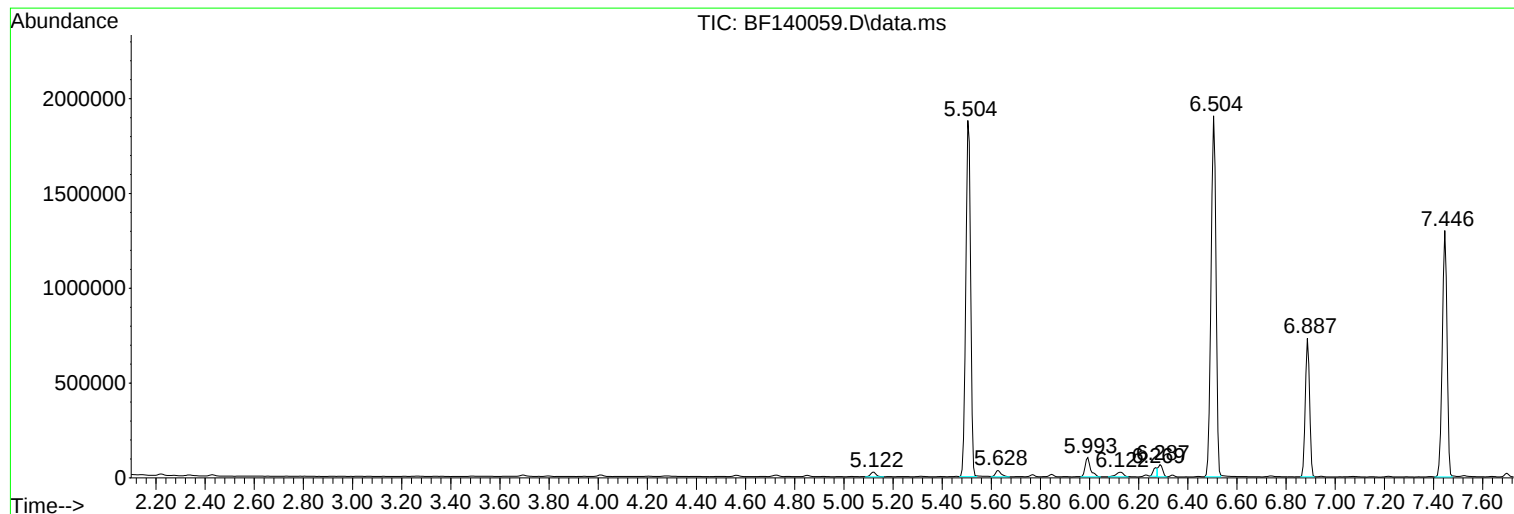
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ALS Vial : 11 Sample Multiplier: 1

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BNA\_F  
ClientSampleId :  
BP-F23

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF101824.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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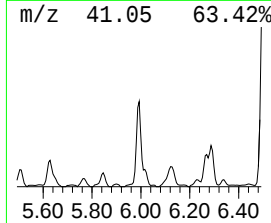
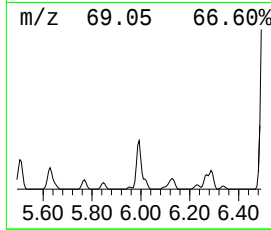
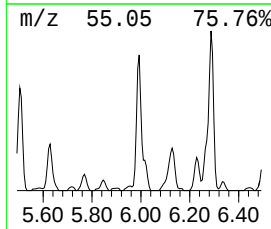
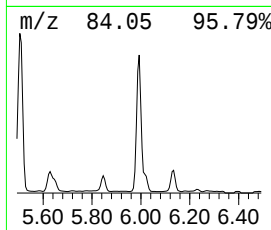
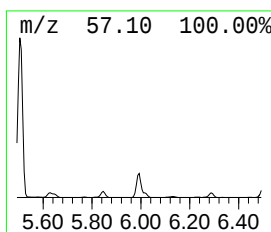
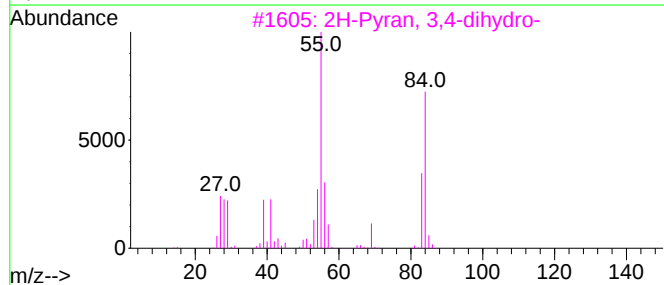
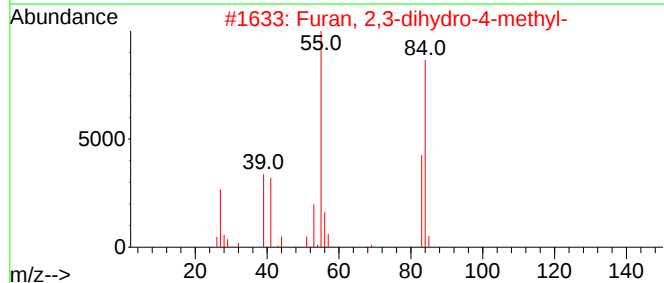
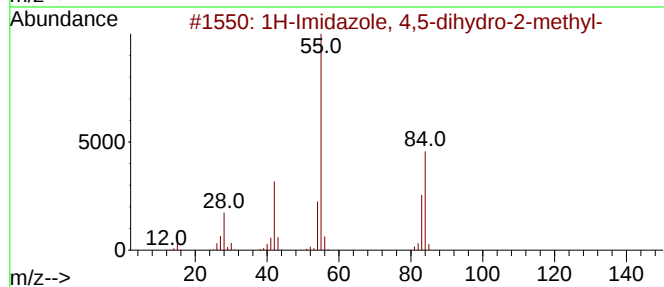
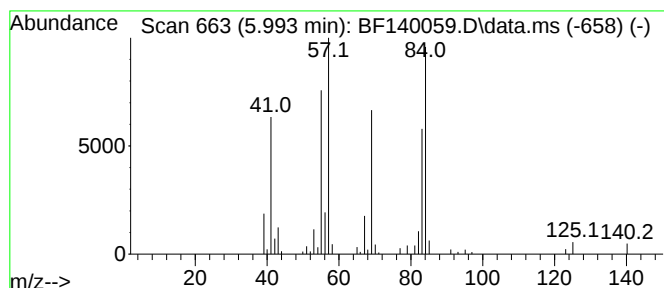
TIC Integration Parameters: LSCINT.P

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Peak Number 1 1H-Imidazole, 4,5-dihydro-2... Concentration Rank 4

| R.T.  | EstConc | Area   | Relative to ISTD       | R.T.  |
|-------|---------|--------|------------------------|-------|
| 5.993 | 3.46 ng | 153914 | 1,4-Dichlorobenzene-d4 | 6.887 |

| Hit# | of | 5 | Tentative ID                        | MW | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------------|----|---------|-------------|------|
| 1    |    |   | 1H-Imidazole, 4,5-dihydro-2-methyl- | 84 | C4H8N2  | 000534-26-9 | 59   |
| 2    |    |   | Furan, 2,3-dihydro-4-methyl-        | 84 | C5H8O   | 034314-83-5 | 59   |
| 3    |    |   | 2H-Pyran, 3,4-dihydro-              | 84 | C5H8O   | 000110-87-2 | 53   |
| 4    |    |   | 2-Butenal, 3-methyl-                | 84 | C5H8O   | 000107-86-8 | 53   |
| 5    |    |   | 2-Pentenal, (E)-                    | 84 | C5H8O   | 001576-87-0 | 50   |



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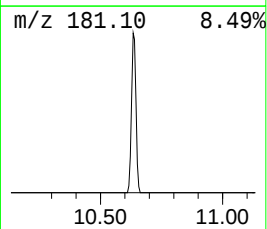
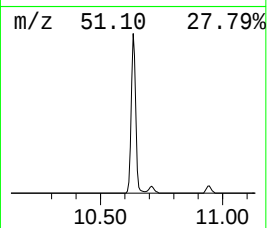
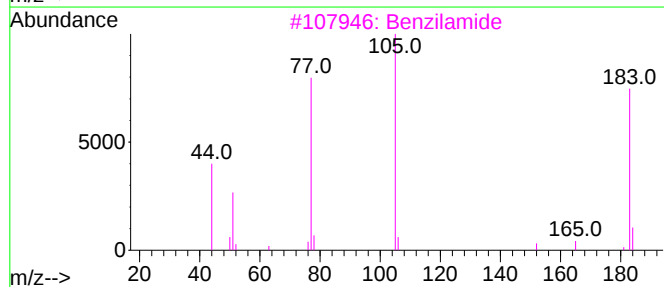
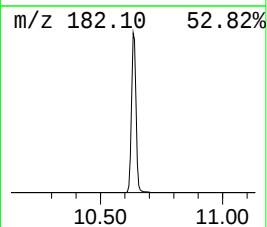
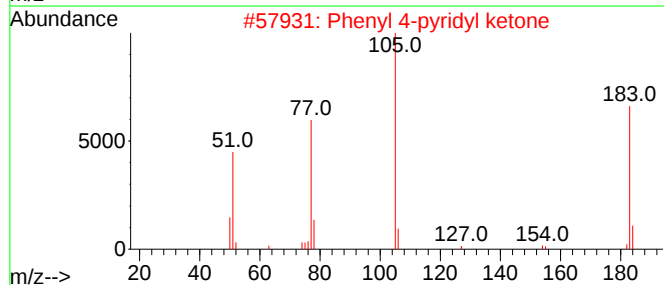
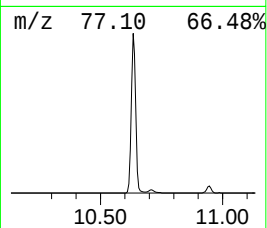
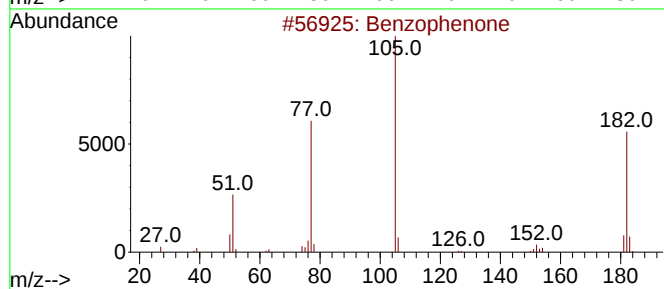
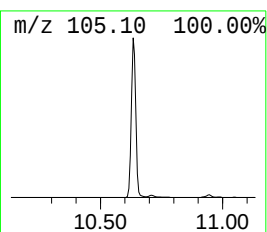
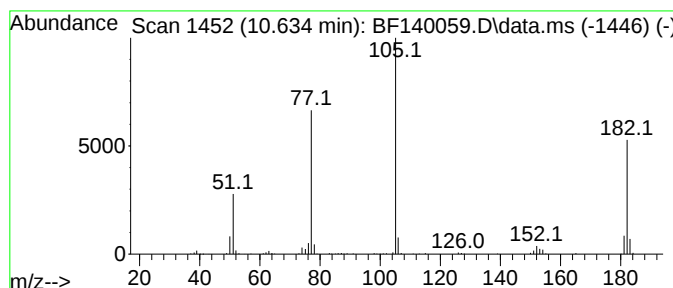
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF101824.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 2 Benzophenone Concentration Rank 2

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.  |
|--------|---------|--------|------------------|-------|
| 10.634 | 4.58 ng | 326128 | Acenaphthene-d10 | 9.922 |

| Hit# | of | 5 | Tentative ID                    | MW  | MolForm   | CAS#        | Qual |
|------|----|---|---------------------------------|-----|-----------|-------------|------|
| 1    |    |   | Benzophenone                    | 182 | C13H10O   | 000119-61-9 | 96   |
| 2    |    |   | Phenyl 4-pyridyl ketone         | 183 | C12H9NO   | 014548-46-0 | 50   |
| 3    |    |   | Benzilamide                     | 227 | C14H13NO2 | 004746-87-6 | 47   |
| 4    |    |   | Pentafluoroethyl phenyl ketone  | 224 | C9H5F5O   | 000394-52-5 | 47   |
| 5    |    |   | 1-Propanone, 3-chloro-1-phenyl- | 168 | C9H9ClO   | 000936-59-4 | 47   |



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Sample : P4508-05  
Misc :  
ALS Vial : 11 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
BP-F23

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF101824.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

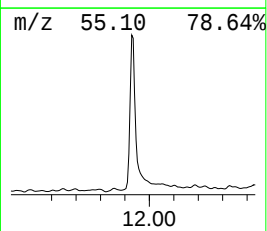
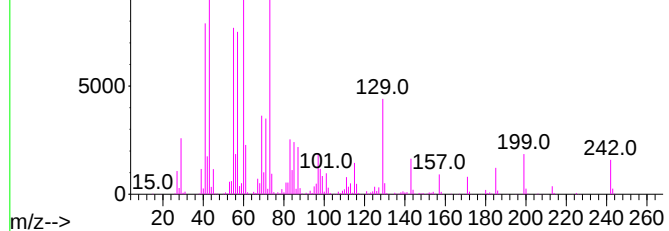
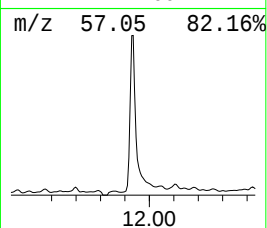
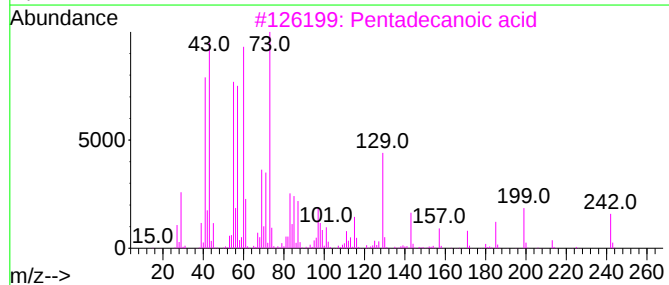
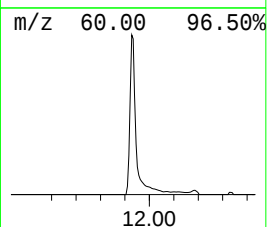
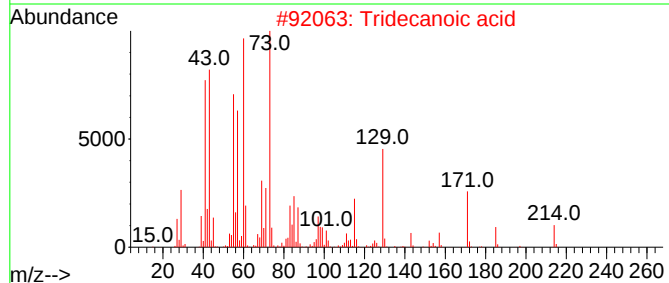
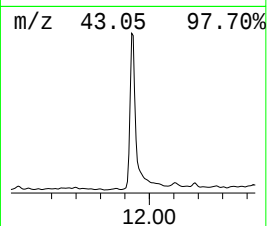
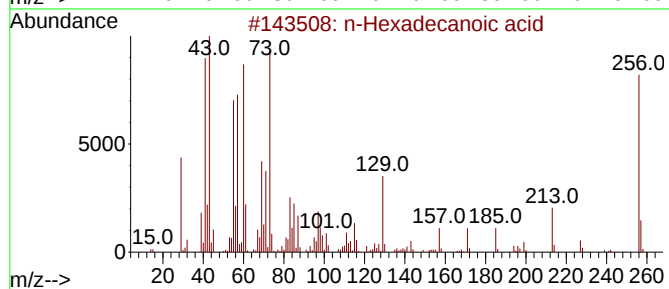
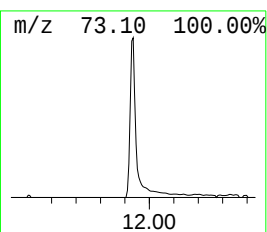
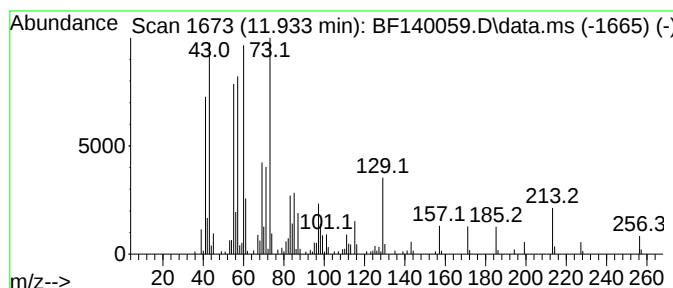
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 11.934 | 3.74 ng | 262325 | Phenanthrene-d10 | 11.410 |

| Hit# | of 5 | Tentative ID          | MW  | MolForm  | CAS#        | Qual |
|------|------|-----------------------|-----|----------|-------------|------|
| 1    |      | n-Hexadecanoic acid   | 256 | C16H32O2 | 000057-10-3 | 99   |
| 2    |      | Tridecanoic acid      | 214 | C13H26O2 | 000638-53-9 | 89   |
| 3    |      | Pentadecanoic acid    | 242 | C15H30O2 | 001002-84-2 | 87   |
| 4    |      | Tetradecanoic acid    | 228 | C14H28O2 | 000544-63-8 | 62   |
| 5    |      | 8-Methylnonanoic acid | 172 | C10H20O2 | 005963-14-4 | 55   |



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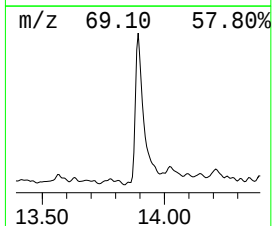
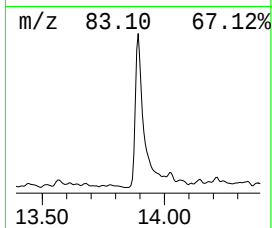
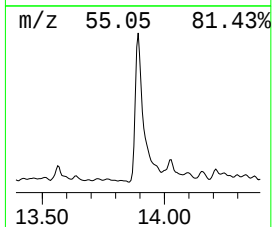
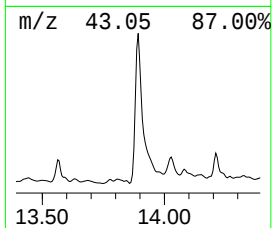
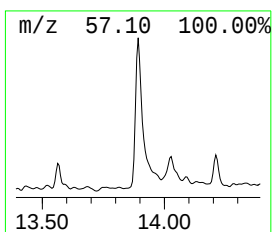
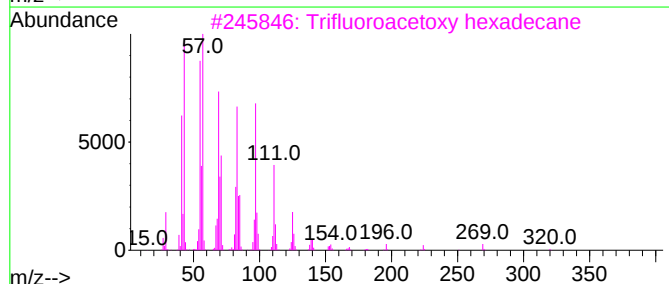
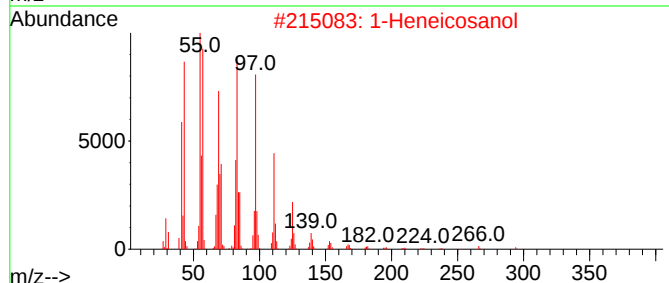
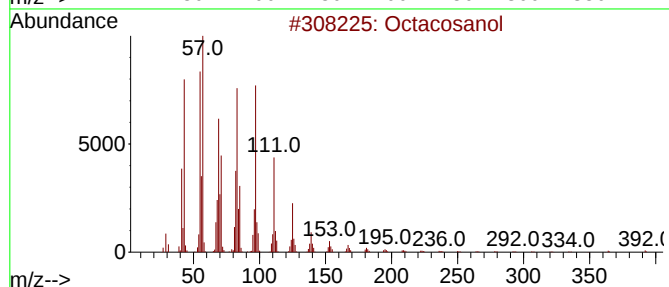
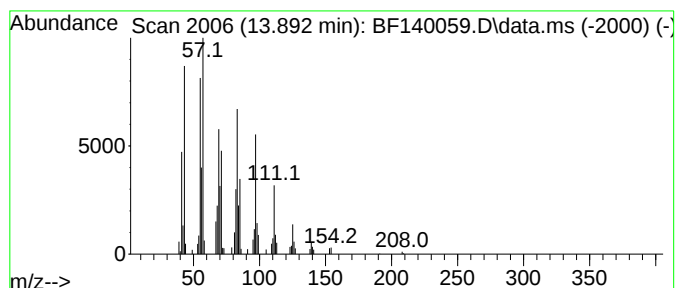
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Peak Number 4 Octacosanol Concentration Rank 1

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 13.892 | 4.66 ng | 172265 | Chrysene-d12     | 14.045 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|------------|-------------|------|
| 1    |    |   | Octacosanol                         | 410 | C28H58O    | 000557-61-9 | 94   |
| 2    |    |   | 1-Heneicosanol                      | 312 | C21H44O    | 015594-90-8 | 93   |
| 3    |    |   | Trifluoroacetoxy hexadecane         | 338 | C18H33F3O2 | 006222-03-3 | 91   |
| 4    |    |   | n-Tetracosanol-1                    | 354 | C24H50O    | 000506-51-4 | 91   |
| 5    |    |   | Pentafluoropropionic acid, tetra... | 360 | C17H29F5O2 | 006222-06-6 | 91   |



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TIC Library : C:\Database\NIST20.L  
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| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |         |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|---------|------|
|                    |        |         |       |          | #                     | RT     | Resp    | Conc |
| 1H-Imidazole, 4... | 5.993  | 3.5     | ng    | 153914   | 1                     | 6.887  | 889465  | 20.0 |
| Benzophenone       | 10.634 | 4.6     | ng    | 326128   | 3                     | 9.922  | 1423460 | 20.0 |
| n-Hexadecanoic ... | 11.934 | 3.7     | ng    | 262325   | 4                     | 11.410 | 1401200 | 20.0 |
| Octacosanol        | 13.892 | 4.7     | ng    | 172265   | 5                     | 14.045 | 739954  | 20.0 |