

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF100722\  
 Data File : BF130586.D  
 Acq On : 07 Oct 2022 21:24  
 Operator : CG\JU  
 Sample : N5046-06  
 Misc :  
 ALS Vial : 13 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 R-6

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-BF091422.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130586.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         | 4.787       | 454           | 459         | 472          | rVB      | 402150         | 525209        | 29.99%          | 4.149%        |
| 2         | 5.216       | 528           | 532         | 552          | rBV      | 1783038        | 1664539       | 95.04%          | 13.149%       |
| 3         | 5.616       | 597           | 600         | 610          | rVB      | 33448          | 34457         | 1.97%           | 0.272%        |
| 4         | 6.257       | 705           | 709         | 712          | rBV      | 1736164        | 1522944       | 86.96%          | 12.030%       |
| 5         | 6.610       | 766           | 769         | 773          | rBV      | 526846         | 433246        | 24.74%          | 3.422%        |
| 6         | 7.181       | 862           | 866         | 869          | rBV      | 1272152        | 1014343       | 57.92%          | 8.013%        |
| 7         | 7.833       | 972           | 977         | 984          | rBV3     | 13658          | 43639         | 2.49%           | 0.345%        |
| 8         | 7.892       | 984           | 987         | 1004         | rVB      | 658303         | 534554        | 30.52%          | 4.223%        |
| 9         | 8.969       | 1166          | 1170        | 1173         | rBV      | 2188121        | 1751342       | 100.00%         | 13.835%       |
| 10        | 9.639       | 1281          | 1284        | 1288         | rBV      | 562184         | 478457        | 27.32%          | 3.780%        |
| 11        | 10.427      | 1414          | 1418        | 1430         | rVB      | 1103760        | 942893        | 53.84%          | 7.448%        |
| 12        | 10.621      | 1448          | 1451        | 1454         | rBV      | 18857          | 24264         | 1.39%           | 0.192%        |
| 13        | 11.121      | 1532          | 1536        | 1539         | rBV      | 561140         | 438237        | 25.02%          | 3.462%        |
| 14        | 11.663      | 1624          | 1628        | 1632         | rBV4     | 18858          | 25170         | 1.44%           | 0.199%        |
| 15        | 12.227      | 1718          | 1724        | 1727         | rBV6     | 22759          | 23626         | 1.35%           | 0.187%        |
| 16        | 12.327      | 1737          | 1741        | 1745         | rBV      | 37672          | 31636         | 1.81%           | 0.250%        |
| 17        | 12.557      | 1775          | 1780        | 1783         | rBV      | 41597          | 44206         | 2.52%           | 0.349%        |
| 18        | 12.704      | 1801          | 1805        | 1809         | rBV      | 1839667        | 1708169       | 97.53%          | 13.494%       |
| 19        | 13.751      | 1977          | 1983        | 1986         | rBV      | 621976         | 588961        | 33.63%          | 4.652%        |
| 20        | 13.774      | 1986          | 1987        | 1993         | rVB      | 41345          | 43993         | 2.51%           | 0.348%        |
| 21        | 13.927      | 2010          | 2013        | 2016         | rVB2     | 22541          | 21901         | 1.25%           | 0.173%        |
| 22        | 14.233      | 2062          | 2065        | 2068         | rBV      | 30845          | 26465         | 1.51%           | 0.209%        |
| 23        | 14.527      | 2112          | 2115        | 2124         | rBV2     | 32026          | 41105         | 2.35%           | 0.325%        |
| 24        | 14.751      | 2150          | 2153        | 2161         | rVB      | 29675          | 45494         | 2.60%           | 0.359%        |
| 25        | 14.827      | 2164          | 2166        | 2170         | rVB      | 37068          | 32987         | 1.88%           | 0.261%        |
| 26        | 15.080      | 2206          | 2209        | 2214         | rVB      | 24736          | 29350         | 1.68%           | 0.232%        |
| 27        | 15.133      | 2214          | 2218        | 2222         | rBV      | 427565         | 485414        | 27.72%          | 3.834%        |
| 28        | 15.551      | 2285          | 2289        | 2292         | rBV      | 38340          | 50833         | 2.90%           | 0.402%        |
| 29        | 15.992      | 2360          | 2364        | 2371         | rVB3     | 29926          | 51736         | 2.95%           | 0.409%        |

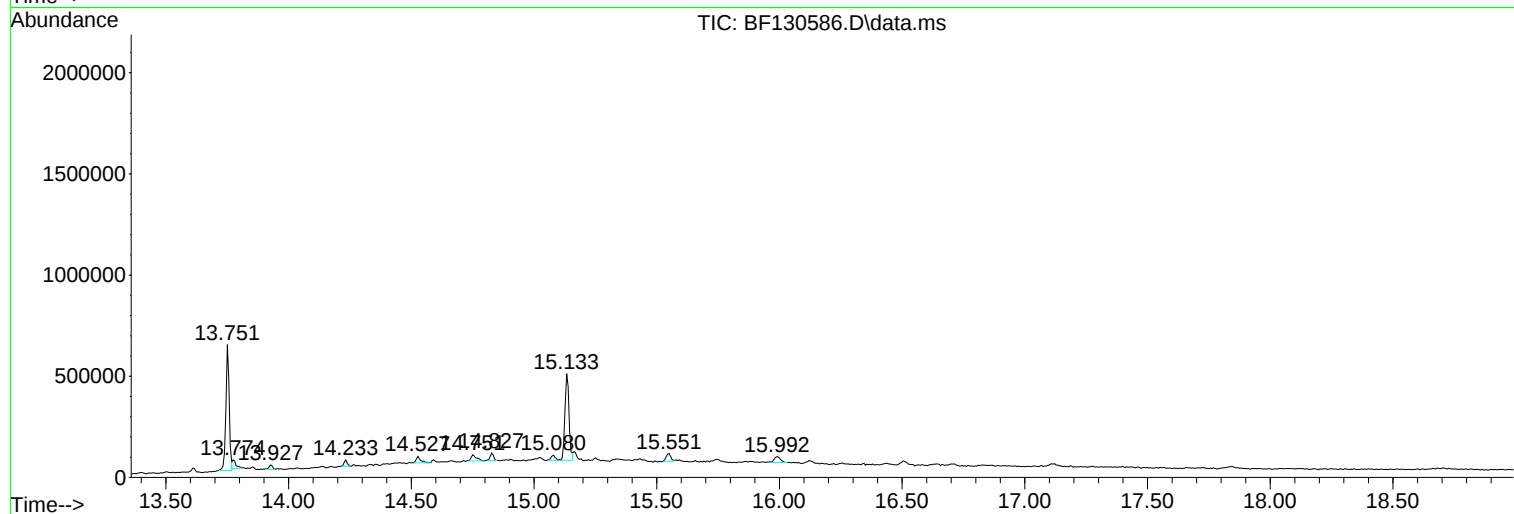
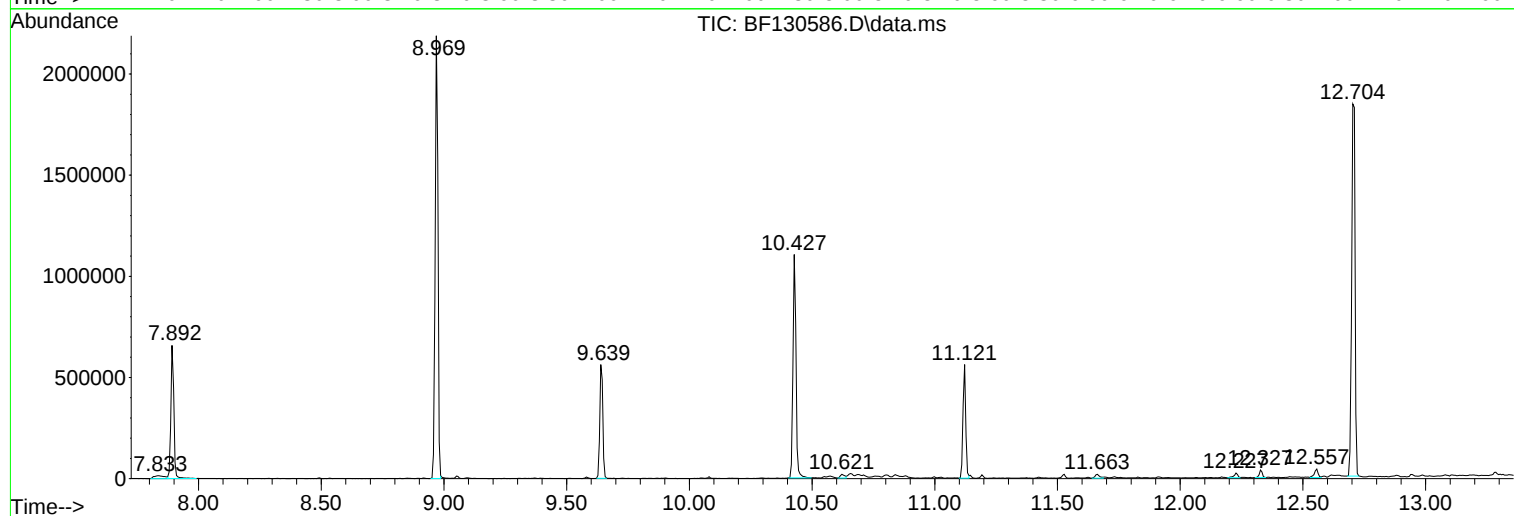
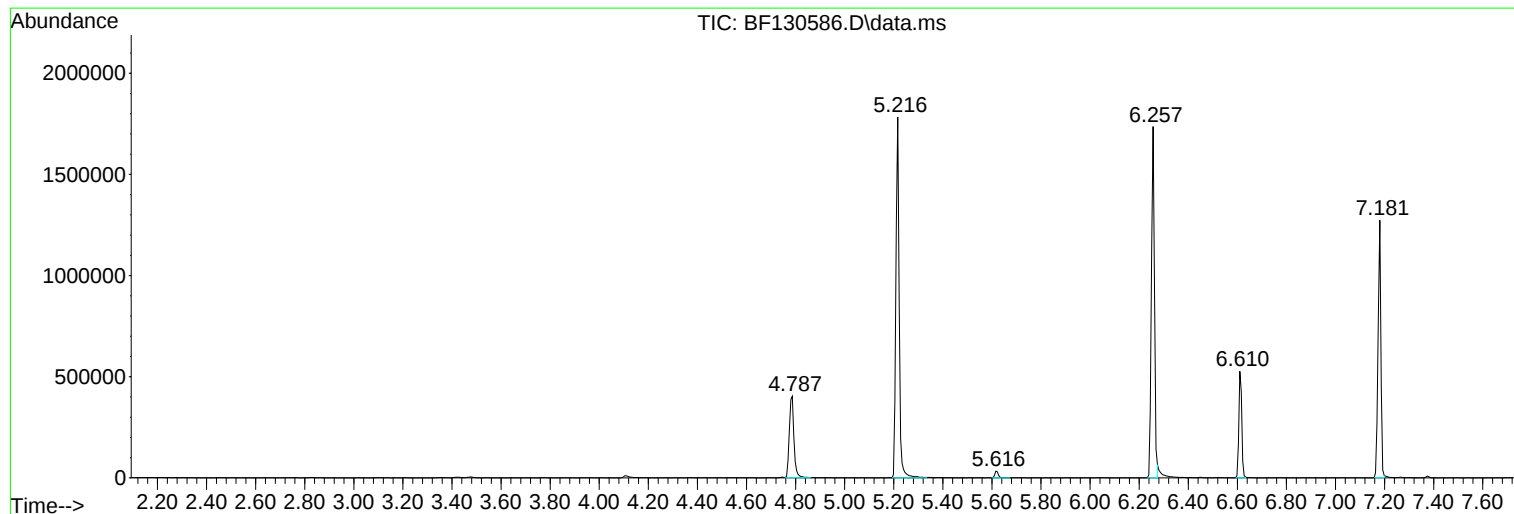
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ALS Vial : 13 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
R-6

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF091422.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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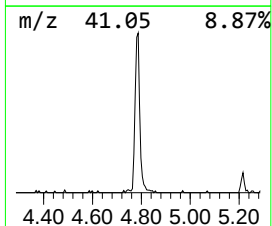
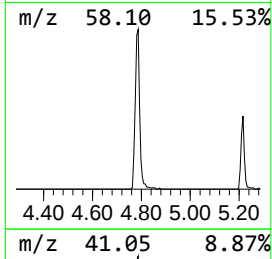
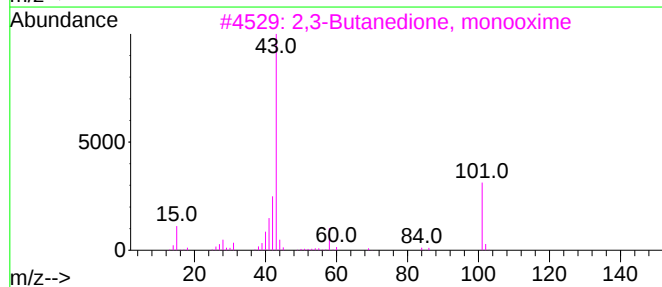
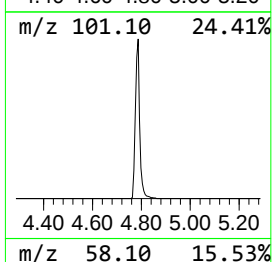
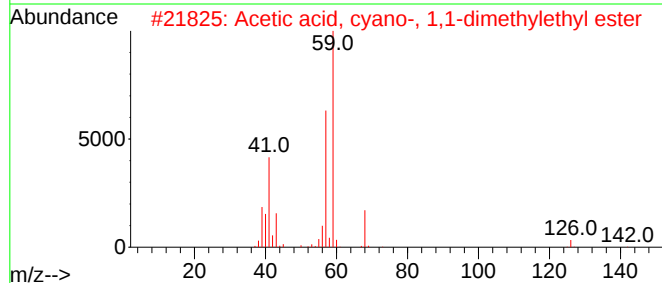
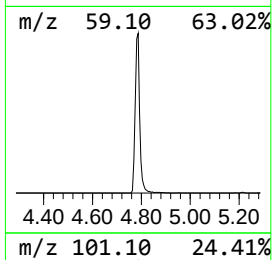
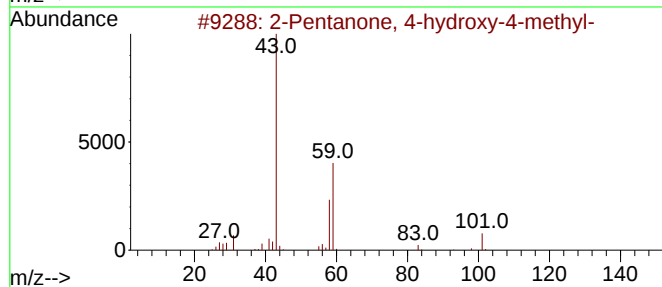
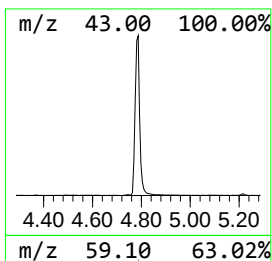
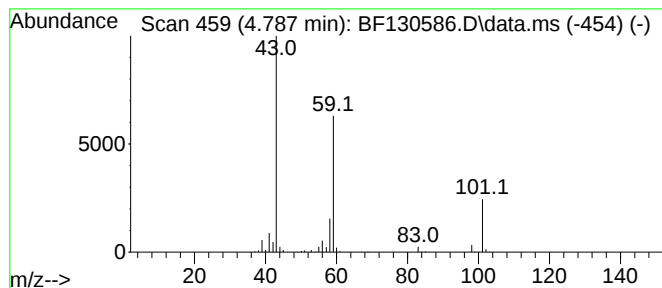
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

| R.T.  | EstConc  | Area   | Relative to ISTD       | R.T.  |
|-------|----------|--------|------------------------|-------|
| 4.787 | 24.25 ng | 525209 | 1,4-Dichlorobenzene-d4 | 6.610 |

| Hit# | of                                  | 5   | Tentative ID | MW          | MolForm | CAS# | Qual |
|------|-------------------------------------|-----|--------------|-------------|---------|------|------|
| 1    | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2      | 000123-42-2 | 56      |      |      |
| 2    | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2     | 001116-98-9 | 23      |      |      |
| 3    | 2,3-Butanedione, monooxime          | 101 | C4H7NO2      | 000057-71-6 | 17      |      |      |
| 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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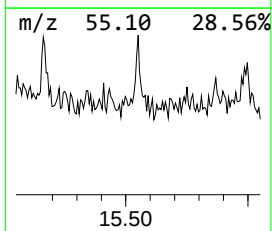
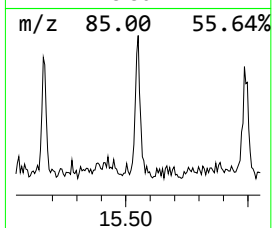
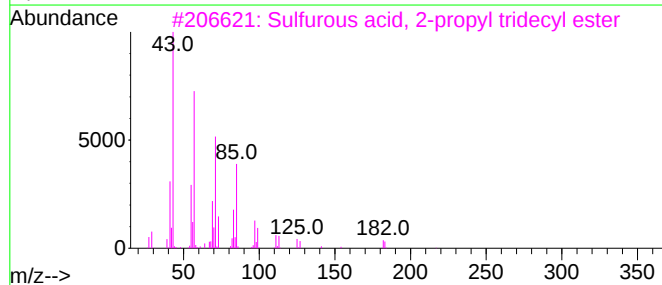
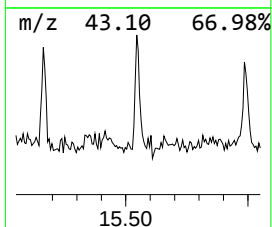
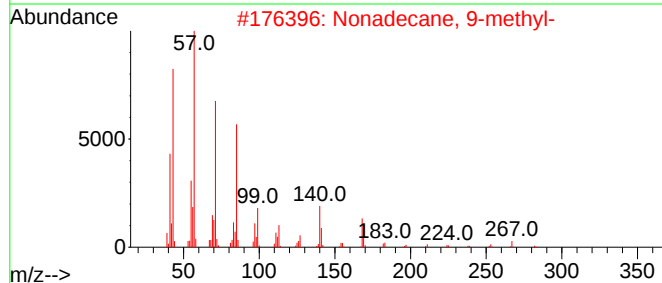
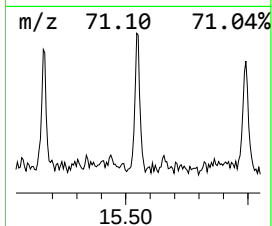
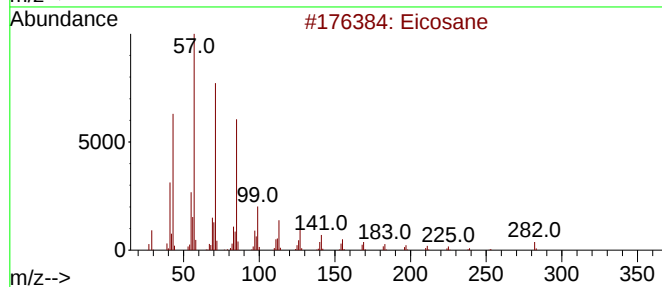
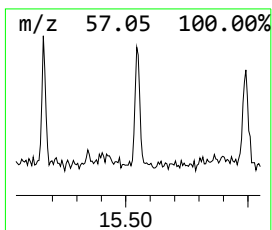
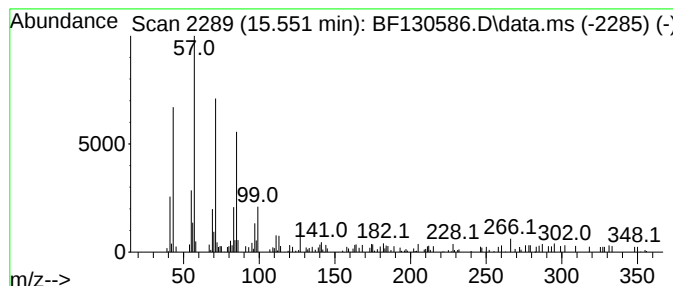
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TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 Eicosane Concentration Rank 3

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 15.551 | 2.09 ng | 50833 | Perylene-d12     | 15.133 |

| Hit# | of                                  | 5 | Tentative ID | MW  | MolForm   | CAS#         | Qual |
|------|-------------------------------------|---|--------------|-----|-----------|--------------|------|
| 1    | Eicosane                            |   |              | 282 | C20H42    | 000112-95-8  | 89   |
| 2    | Nonadecane, 9-methyl-               |   |              | 282 | C20H42    | 013287-24-6  | 72   |
| 3    | Sulfurous acid, 2-propyl tridecy... |   |              | 306 | C16H34O3S | 1000309-12-4 | 72   |
| 4    | Tetratetracontane                   |   |              | 619 | C44H90    | 007098-22-8  | 58   |
| 5    | 3,5-Dimethyldodecane                |   |              | 198 | C14H30    | 107770-99-0  | 53   |



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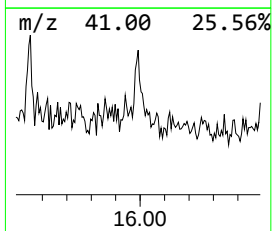
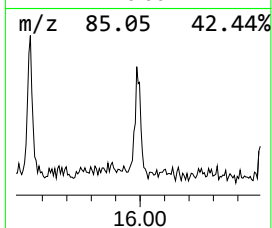
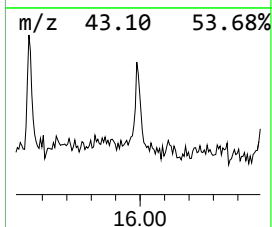
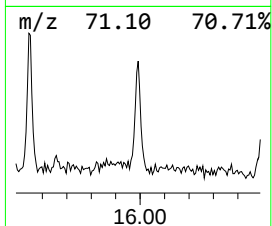
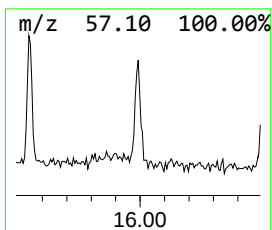
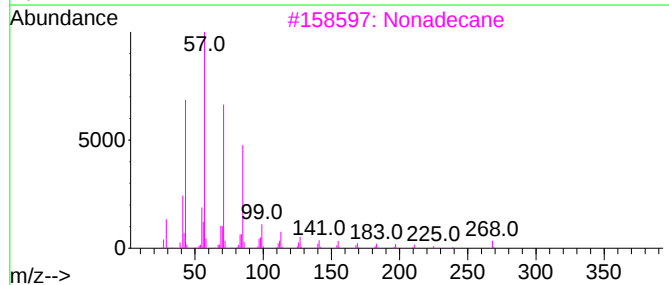
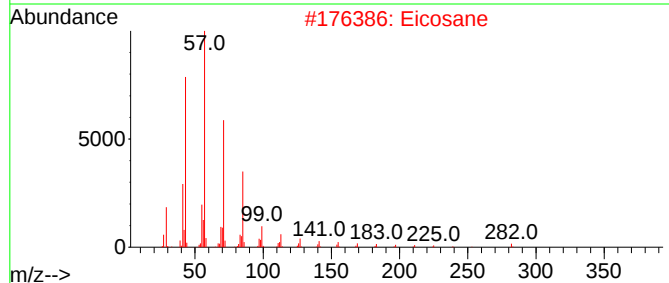
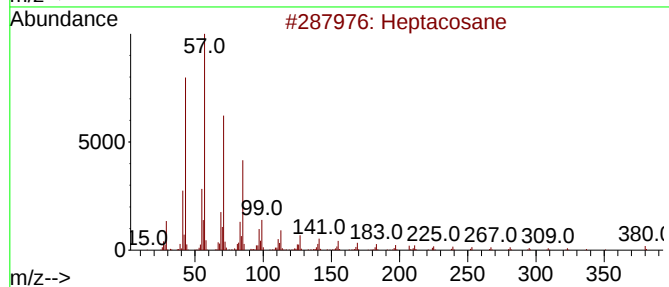
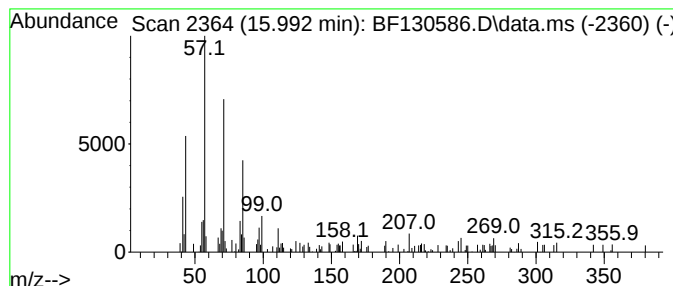
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 Heptacosane Concentration Rank 2

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 15.992 | 2.13 ng | 51736 | Perylene-d12     | 15.133 |

| Hit# | of | 5 | Tentative ID                      | MW  | MolForm   | CAS#         | Qual |
|------|----|---|-----------------------------------|-----|-----------|--------------|------|
| 1    |    |   | Heptacosane                       | 380 | C27H56    | 000593-49-7  | 86   |
| 2    |    |   | Eicosane                          | 282 | C20H42    | 000112-95-8  | 64   |
| 3    |    |   | Nonadecane                        | 268 | C19H40    | 000629-92-5  | 64   |
| 4    |    |   | Sulfurous acid, hexyl octyl ester | 278 | C14H30O3S | 1000309-13-0 | 52   |
| 5    |    |   | Nonadecane, 2-methyl-             | 282 | C20H42    | 001560-86-7  | 52   |



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| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| 2-Pentanone, 4-... | 4.787  | 24.3    | ng    | 525209   | 1                     | 6.610  | 433246 | 20.0 |
| Eicosane           | 15.551 | 2.1     | ng    | 50833    | 6                     | 15.133 | 485414 | 20.0 |
| Heptacosane        | 15.992 | 2.1     | ng    | 51736    | 6                     | 15.133 | 485414 | 20.0 |