

Data Path : Z:\HPCHEM1\BNA M\DATA\BM121217\  
 Data File : BM013350.D  
 Acq On : 12 Dec 2017 21:48  
 Operator : SJ/JU  
 Sample : I6776-16  
 Misc :  
 ALS Vial : 18 Sample Multiplier: 1

Instrument :  
 BNA\_M  
 ClientSampleId :  
 F9A45

## Integration Parameters: LSCINT.P

Integrator: RTE  
 Smoothing : OFF  
 Sampling : 1  
 Start Thrs: 0.2  
 Stop Thrs : 0

Filtering: 5  
 Min Area: 1 % 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\_M\METHODS\SOM-EPA-BM113017.M  
 Title : SVOA 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         | 6.863       | 636           | 642         | 656          | rVB2     | 686459         | 1260239       | 23.49%          | 2.178%        |
| 2         | 7.028       | 664           | 670         | 683          | rBV      | 541826         | 840457        | 15.67%          | 1.452%        |
| 3         | 7.222       | 695           | 703         | 713          | rBV      | 743928         | 1154760       | 21.53%          | 1.996%        |
| 4         | 7.687       | 775           | 782         | 790          | rBV      | 805870         | 1285228       | 23.96%          | 2.221%        |
| 5         | 8.393       | 895           | 902         | 911          | rBV      | 866608         | 1381912       | 25.76%          | 2.388%        |
| 6         | 8.840       | 971           | 978         | 988          | rVB      | 762256         | 1247058       | 23.25%          | 2.155%        |
| 7         | 9.557       | 1093          | 1100        | 1113         | rVB      | 623626         | 1063090       | 19.82%          | 1.837%        |
| 8         | 10.092      | 1184          | 1191        | 1205         | rBV      | 934748         | 1606402       | 29.95%          | 2.776%        |
| 9         | 10.463      | 1246          | 1254        | 1259         | rBV      | 1137358        | 1899208       | 35.40%          | 3.282%        |
| 10        | 10.516      | 1259          | 1263        | 1269         | rVB      | 153282         | 251392        | 4.69%           | 0.434%        |
| 11        | 10.610      | 1272          | 1279        | 1287         | rBV      | 426441         | 778948        | 14.52%          | 1.346%        |
| 12        | 12.133      | 1531          | 1538        | 1545         | rVB2     | 42312          | 71312         | 1.33%           | 0.123%        |
| 13        | 12.351      | 1569          | 1575        | 1586         | rVB2     | 32606          | 54781         | 1.02%           | 0.095%        |
| 14        | 13.151      | 1707          | 1711        | 1719         | rVB5     | 39044          | 62293         | 1.16%           | 0.108%        |
| 15        | 13.745      | 1805          | 1812        | 1816         | rBV      | 1821385        | 2545008       | 47.44%          | 4.398%        |
| 16        | 13.792      | 1816          | 1820        | 1828         | rVB      | 390625         | 549333        | 10.24%          | 0.949%        |
| 17        | 14.016      | 1849          | 1858        | 1870         | rBV      | 1988339        | 3055226       | 56.96%          | 5.280%        |
| 18        | 14.233      | 1890          | 1895        | 1901         | rVB      | 76209          | 94298         | 1.76%           | 0.163%        |
| 19        | 14.327      | 1904          | 1911        | 1918         | rBV2     | 1756443        | 2612496       | 48.70%          | 4.515%        |
| 20        | 14.392      | 1918          | 1922        | 1927         | rVB      | 66378          | 100938        | 1.88%           | 0.174%        |
| 21        | 14.539      | 1941          | 1947        | 1963         | rBV      | 673840         | 1120502       | 20.89%          | 1.936%        |
| 22        | 15.192      | 2053          | 2058        | 2063         | rVB      | 88483          | 114328        | 2.13%           | 0.198%        |
| 23        | 15.327      | 2072          | 2081        | 2086         | rBV      | 2538186        | 3657216       | 68.18%          | 6.320%        |
| 24        | 15.380      | 2086          | 2090        | 2096         | rVB      | 41606          | 59775         | 1.11%           | 0.103%        |
| 25        | 15.451      | 2096          | 2102        | 2114         | rBV      | 699351         | 980869        | 18.29%          | 1.695%        |
| 26        | 15.563      | 2114          | 2121        | 2124         | rBV5     | 32595          | 55594         | 1.04%           | 0.096%        |
| 27        | 16.051      | 2200          | 2204        | 2211         | rBV3     | 89885          | 141368        | 2.64%           | 0.244%        |
| 28        | 16.733      | 2316          | 2320        | 2326         | rBV4     | 44296          | 63673         | 1.19%           | 0.110%        |
| 29        | 16.845      | 2335          | 2339        | 2344         | rBV2     | 55467          | 72435         | 1.35%           | 0.125%        |
| 30        | 17.080      | 2371          | 2379        | 2383         | rBV2     | 2221350        | 3266160       | 60.89%          | 5.644%        |
| 31        | 17.115      | 2383          | 2385        | 2389         | rVV      | 159810         | 204280        | 3.81%           | 0.353%        |
| 32        | 17.174      | 2389          | 2395        | 2407         | rVB      | 2829813        | 4184102       | 78.00%          | 7.231%        |
| 33        | 17.486      | 2444          | 2448        | 2456         | rVB      | 39371          | 61844         | 1.15%           | 0.107%        |
| 34        | 17.980      | 2524          | 2532        | 2542         | rBV3     | 401525         | 642438        | 11.98%          | 1.110%        |

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

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 Title : SVOA CALIBRATION

|    |        |      |      |      |      |         |         |         |        |
|----|--------|------|------|------|------|---------|---------|---------|--------|
| 35 | 18.051 | 2542 | 2544 | 2552 | rVV9 | 27948   | 65955   | 1.23%   | 0.114% |
| 36 | 19.015 | 2703 | 2708 | 2714 | rBV8 | 27973   | 54286   | 1.01%   | 0.094% |
| 37 | 19.139 | 2720 | 2729 | 2734 | rBV2 | 267550  | 421526  | 7.86%   | 0.728% |
| 38 | 19.268 | 2746 | 2751 | 2759 | rBV3 | 243773  | 372453  | 6.94%   | 0.644% |
| 39 | 19.474 | 2780 | 2786 | 2799 | rBV  | 3533198 | 5364268 | 100.00% | 9.270% |
| 40 | 19.921 | 2858 | 2862 | 2865 | rBV2 | 89232   | 101919  | 1.90%   | 0.176% |
| 41 | 19.998 | 2872 | 2875 | 2879 | rVB3 | 75567   | 100169  | 1.87%   | 0.173% |
| 42 | 20.156 | 2897 | 2902 | 2907 | rBV4 | 58578   | 102033  | 1.90%   | 0.176% |
| 43 | 20.298 | 2923 | 2926 | 2930 | rBV2 | 52806   | 80923   | 1.51%   | 0.140% |
| 44 | 20.456 | 2950 | 2953 | 2959 | rVB  | 142192  | 203883  | 3.80%   | 0.352% |
| 45 | 20.745 | 2999 | 3002 | 3008 | rBV  | 58655   | 87206   | 1.63%   | 0.151% |
| 46 | 20.986 | 3039 | 3043 | 3051 | rBV2 | 1060476 | 1222511 | 22.79%  | 2.113% |
| 47 | 21.268 | 3084 | 3091 | 3095 | rBV  | 2898539 | 3966684 | 73.95%  | 6.855% |
| 48 | 21.303 | 3095 | 3097 | 3106 | rVB  | 378083  | 419923  | 7.83%   | 0.726% |
| 49 | 21.427 | 3116 | 3118 | 3122 | rVV5 | 52291   | 61950   | 1.15%   | 0.107% |
| 50 | 21.874 | 3192 | 3194 | 3199 | rVB4 | 170852  | 209117  | 3.90%   | 0.361% |
| 51 | 22.827 | 3351 | 3356 | 3360 | rBV2 | 419000  | 771925  | 14.39%  | 1.334% |
| 52 | 23.303 | 3433 | 3437 | 3440 | rBV  | 144112  | 257690  | 4.80%   | 0.445% |
| 53 | 23.356 | 3440 | 3446 | 3460 | rVB2 | 2149548 | 4308162 | 80.31%  | 7.445% |
| 54 | 23.497 | 3463 | 3470 | 3479 | rBV  | 1482803 | 2793235 | 52.07%  | 4.827% |
| 55 | 24.109 | 3570 | 3574 | 3584 | rVB7 | 167233  | 360612  | 6.72%   | 0.623% |

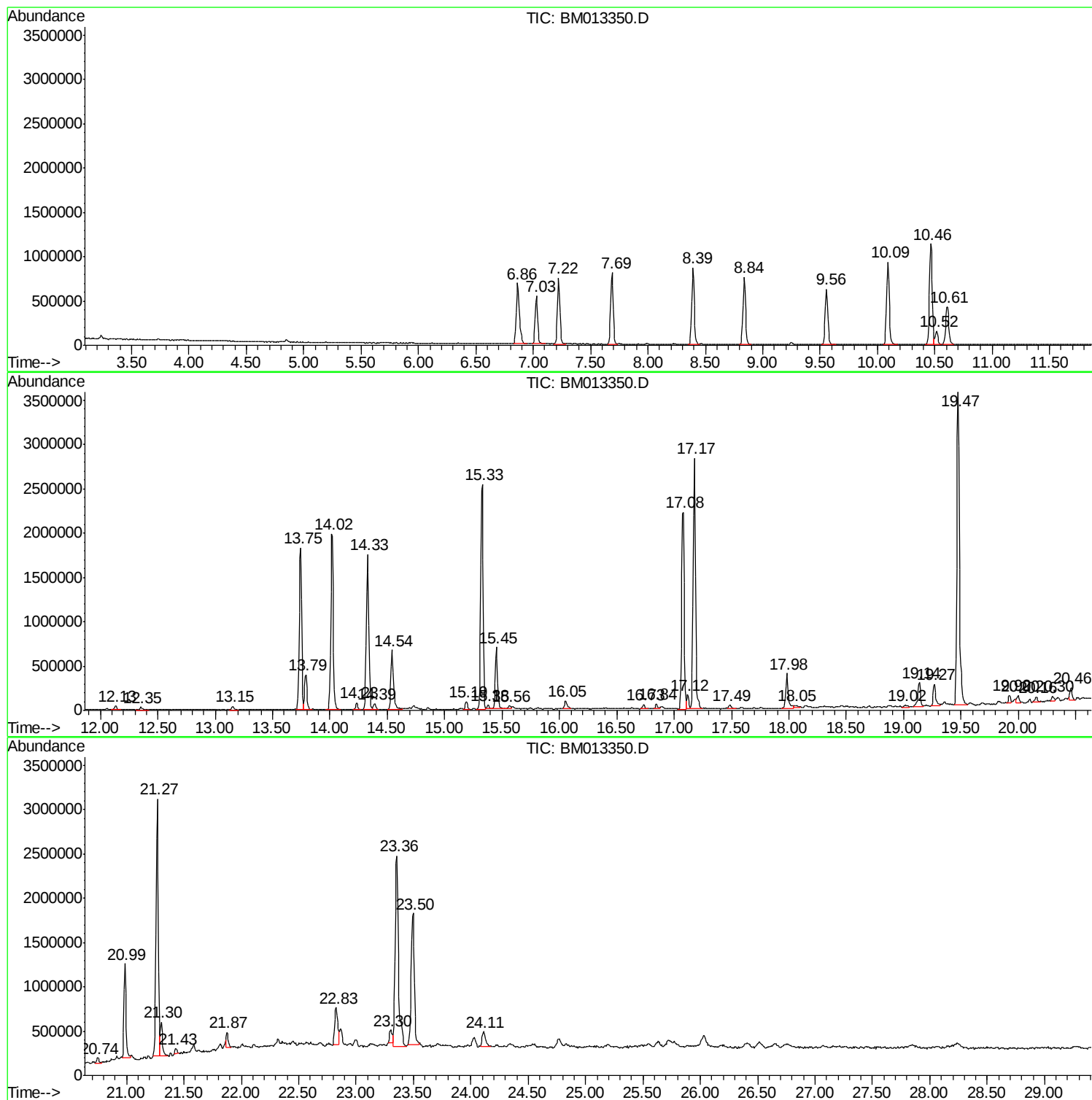
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Quant Method : Z:\HPCHEM1\BNA M\METHODS\SOM-EPA-BM113017.M  
Quant Title : SVOA CALIBRATION

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



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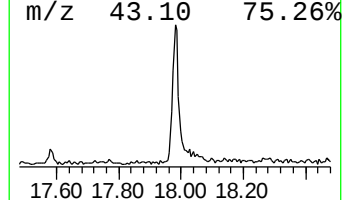
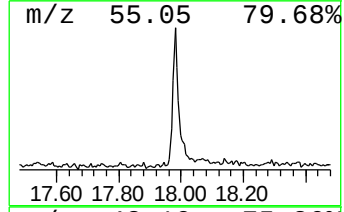
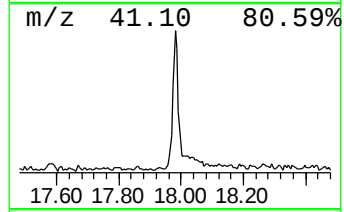
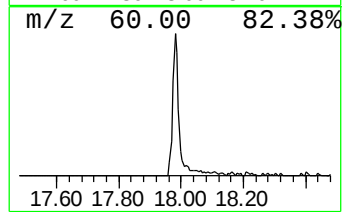
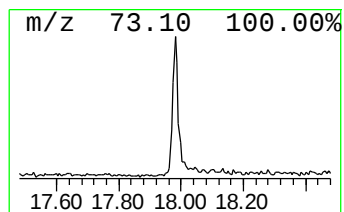
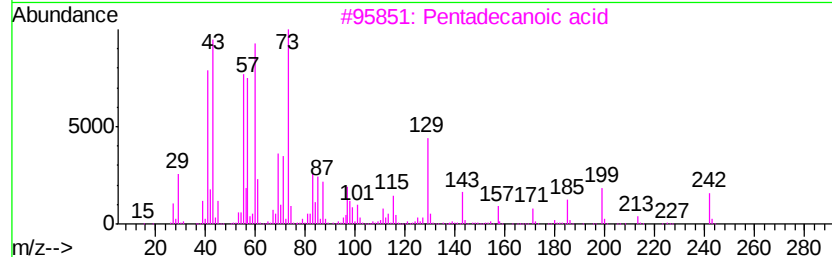
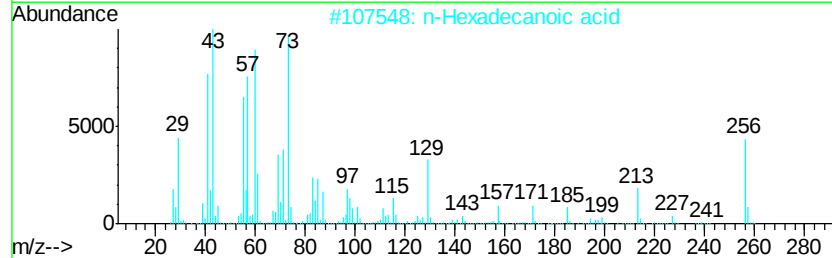
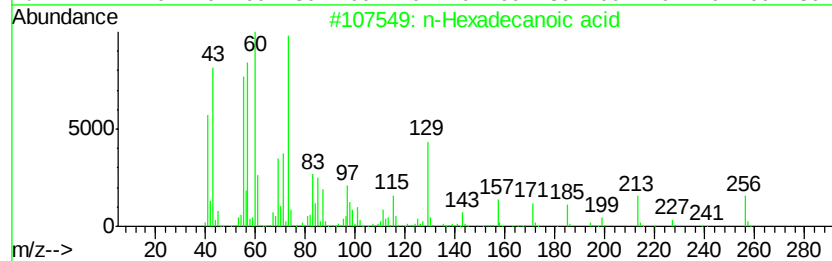
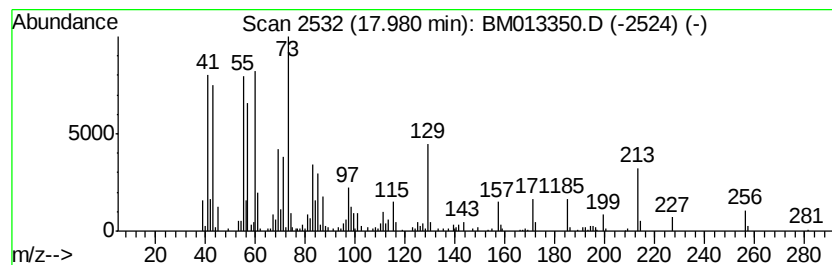
Instrument :  
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Quant Method : Z:\HPCHEM1\BNA M\METHODS\SOM-EPA-BM113017.M  
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TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

| R.T.      | EstConc             | Area   | Relative to ISTD |             | R.T.  |
|-----------|---------------------|--------|------------------|-------------|-------|
| 17.98     | 3.93 ng/ul          | 642438 | Phenanthrene-d10 |             | 17.07 |
| Hit# of 5 | Tentative ID        | MW     | MolForm          | CAS#        | Qual  |
| 1         | n-Hexadecanoic acid | 256    | C16H32O2         | 000057-10-3 | 98    |
| 2         | n-Hexadecanoic acid | 256    | C16H32O2         | 000057-10-3 | 96    |
| 3         | Pentadecanoic acid  | 242    | C15H30O2         | 001002-84-2 | 87    |
| 4         | n-Decanoic acid     | 172    | C10H20O2         | 000334-48-5 | 76    |
| 5         | n-Decanoic acid     | 172    | C10H20O2         | 000334-48-5 | 76    |



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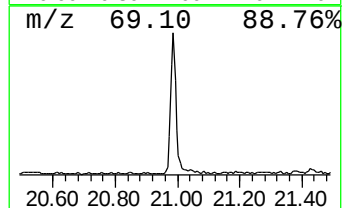
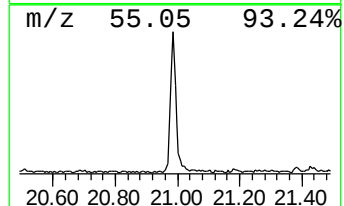
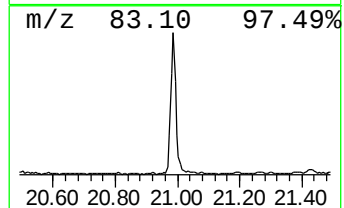
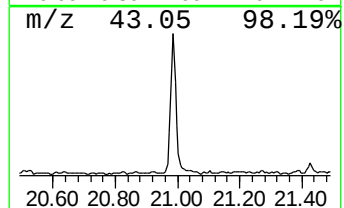
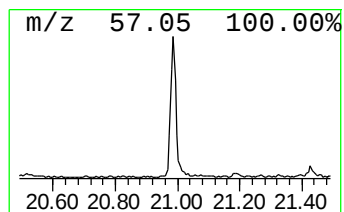
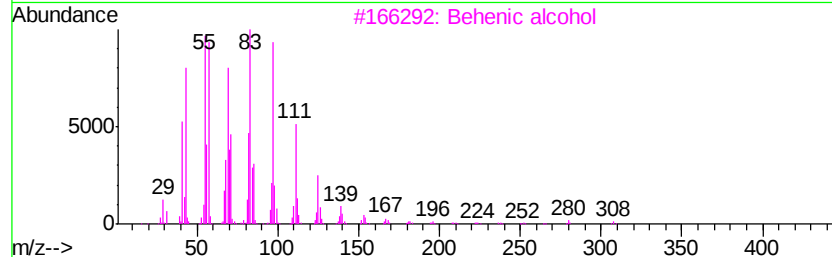
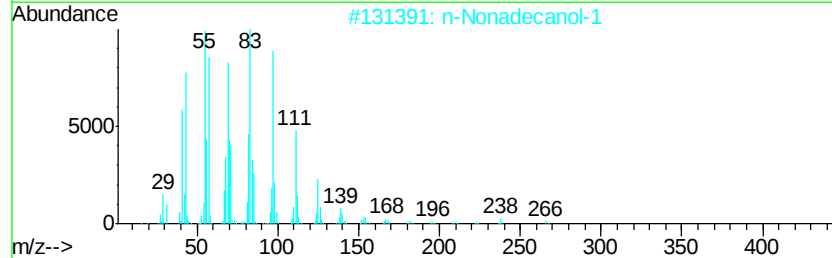
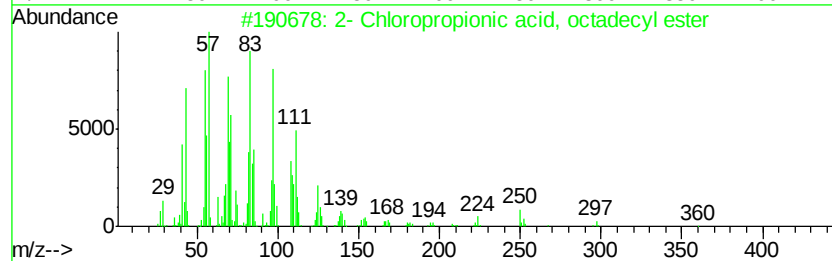
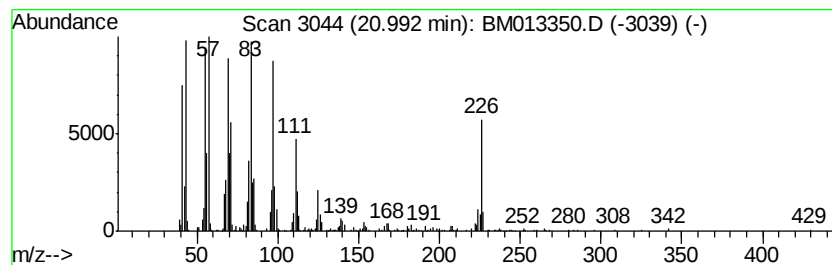
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 2- Chloropropionic acid, oc... Concentration Rank 1

| R.T.  | EstConc    | Area    | Relative to ISTD | R.T.  |
|-------|------------|---------|------------------|-------|
| 20.99 | 6.16 ng/ul | 1222510 | Chrysene-d12     | 21.27 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|------------|-------------|------|
| 1    |    |   | 2- Chloropropionic acid, octadec... | 360 | C21H41ClO2 | 088104-31-8 | 93   |
| 2    |    |   | n-Nonadecanol-1                     | 284 | C19H40O    | 001454-84-8 | 93   |
| 3    |    |   | Behenic alcohol                     | 326 | C22H46O    | 000661-19-8 | 93   |
| 4    |    |   | 1-Heptacosanol                      | 396 | C27H56O    | 002004-39-9 | 93   |
| 5    |    |   | 1-Heneicosanol                      | 312 | C21H44O    | 015594-90-8 | 93   |



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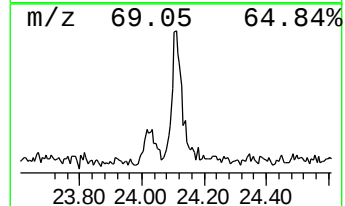
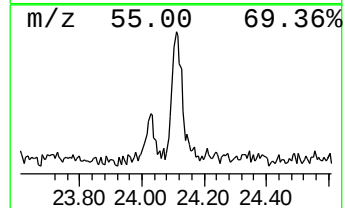
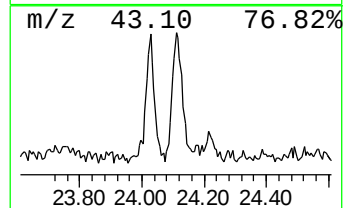
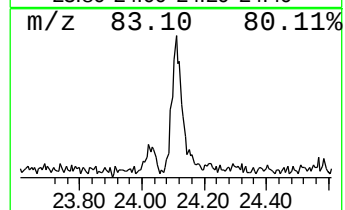
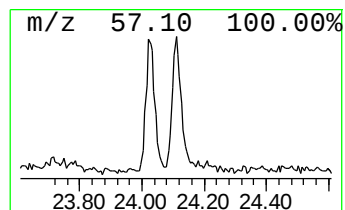
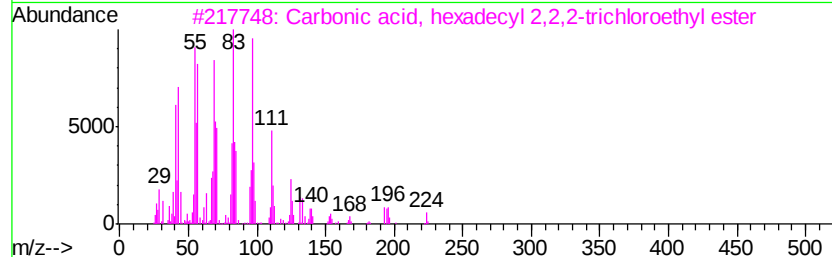
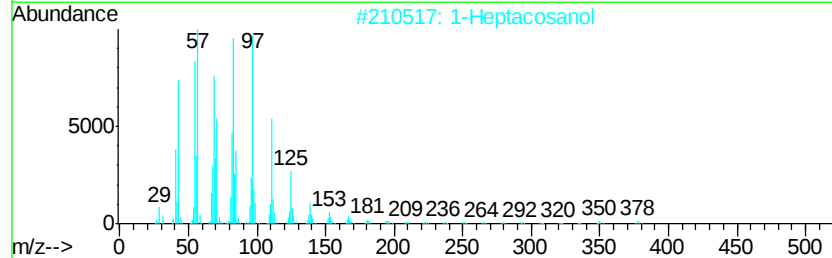
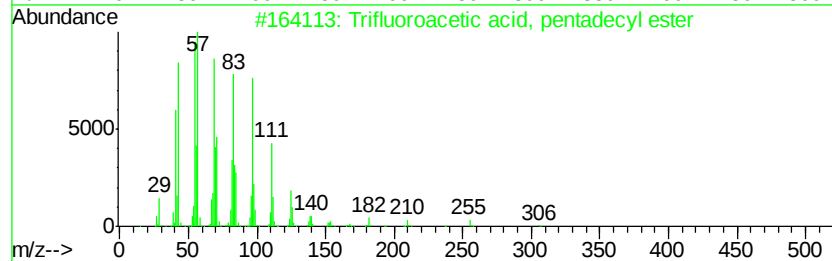
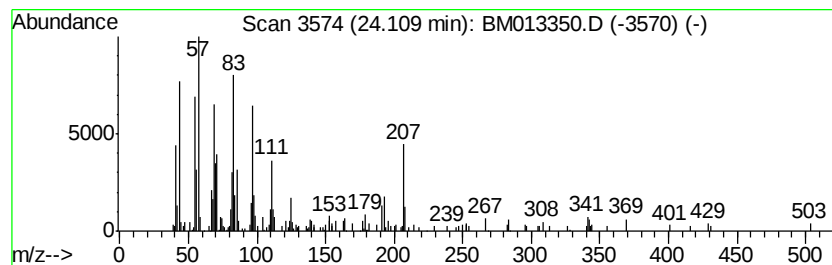
TIC Library : C:\DATABASE\NIST11.L  
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Peak Number 3 Trifluoroacetic acid, penta... Concentration Rank 3

| R.T.  | EstConc    | Area   | Relative to ISTD | R.T.  |
|-------|------------|--------|------------------|-------|
| 24.11 | 2.58 ng/ul | 360612 | Perylene-d12     | 23.50 |

| Hit# | of | Tentative ID                        | MW  | MolForm     | CAS#         | Qual |
|------|----|-------------------------------------|-----|-------------|--------------|------|
| 1    | 5  | Trifluoroacetic acid, pentadecyl... | 324 | C17H31F3O2  | 959010-23-2  | 89   |
| 2    |    | 1-Heptacosanol                      | 396 | C27H56O     | 002004-39-9  | 76   |
| 3    |    | Carbonic acid, hexadecyl 2,2,2-t... | 416 | C19H35Cl3O3 | 1000314-56-2 | 76   |
| 4    |    | 9-Octadecene, (E)-                  | 252 | C18H36      | 007206-25-9  | 70   |
| 5    |    | 1-Tricosene                         | 322 | C23H46      | 018835-32-0  | 68   |



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| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |         |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|---------|------|
|                      |       |         |       |          | #                     | RT    | Resp    | Conc |
| n-Hexadecanoic acid  | 17.98 | 3.9     | ng/ul | 642438   | 4                     | 17.07 | 3266160 | 20.0 |
| 2- Chloropropioni... | 20.99 | 6.2     | ng/ul | 1222510  | 5                     | 21.27 | 3966680 | 20.0 |
| Trifluoroacetic a... | 24.11 | 2.6     | ng/ul | 360612   | 6                     | 23.50 | 2793240 | 20.0 |