

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF083023\  
 Data File : BF135027.D  
 Acq On : 31 Aug 2023 03:28  
 Operator : CG\JU  
 Sample : 04198-01  
 Misc :  
 ALS Vial : 15 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 OR-309-OK-370-COMP-24

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-BF083023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135027.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         | 2.146       | 5             | 10          | 17           | rVB2     | 40666          | 65558         | 2.34%           | 0.339%        |
| 2         | 5.004       | 492           | 496         | 503          | rVB      | 83574          | 102495        | 3.66%           | 0.530%        |
| 3         | 5.404       | 559           | 564         | 567          | rBV      | 2804432        | 2632589       | 94.04%          | 13.603%       |
| 4         | 6.410       | 730           | 735         | 738          | rBV      | 2596242        | 2636475       | 94.18%          | 13.623%       |
| 5         | 6.604       | 764           | 768         | 778          | rBV      | 67044          | 71122         | 2.54%           | 0.368%        |
| 6         | 6.769       | 793           | 796         | 800          | rBV      | 997243         | 830464        | 29.67%          | 4.291%        |
| 7         | 7.334       | 887           | 892         | 895          | rBV      | 1860735        | 1654972       | 59.12%          | 8.552%        |
| 8         | 8.051       | 1009          | 1014        | 1017         | rBV      | 1302388        | 1083347       | 38.70%          | 5.598%        |
| 9         | 9.128       | 1192          | 1197        | 1201         | rBV      | 2978389        | 2799423       | 100.00%         | 14.465%       |
| 10        | 9.245       | 1214          | 1217        | 1222         | rVB      | 52352          | 50562         | 1.81%           | 0.261%        |
| 11        | 9.810       | 1309          | 1313        | 1316         | rBV      | 1197863        | 1076451       | 38.45%          | 5.562%        |
| 12        | 10.598      | 1443          | 1447        | 1451         | rBV      | 1674870        | 1440063       | 51.44%          | 7.441%        |
| 13        | 11.298      | 1562          | 1566        | 1569         | rBV      | 1030206        | 853477        | 30.49%          | 4.410%        |
| 14        | 11.839      | 1654          | 1658        | 1669         | rBV      | 364992         | 354287        | 12.66%          | 1.831%        |
| 15        | 12.516      | 1768          | 1773        | 1778         | rBV      | 40584          | 49900         | 1.78%           | 0.258%        |
| 16        | 12.627      | 1789          | 1792        | 1806         | rVB      | 80582          | 93865         | 3.35%           | 0.485%        |
| 17        | 12.898      | 1834          | 1838        | 1841         | rBV      | 2193417        | 1863994       | 66.58%          | 9.632%        |
| 18        | 13.810      | 1989          | 1993        | 2004         | rBV      | 162661         | 243073        | 8.68%           | 1.256%        |
| 19        | 13.957      | 2013          | 2018        | 2021         | rBV      | 765657         | 735195        | 26.26%          | 3.799%        |
| 20        | 14.445      | 2097          | 2101        | 2104         | rBV4     | 20838          | 37249         | 1.33%           | 0.192%        |
| 21        | 15.427      | 2262          | 2268        | 2273         | rBV      | 507224         | 678230        | 24.23%          | 3.505%        |

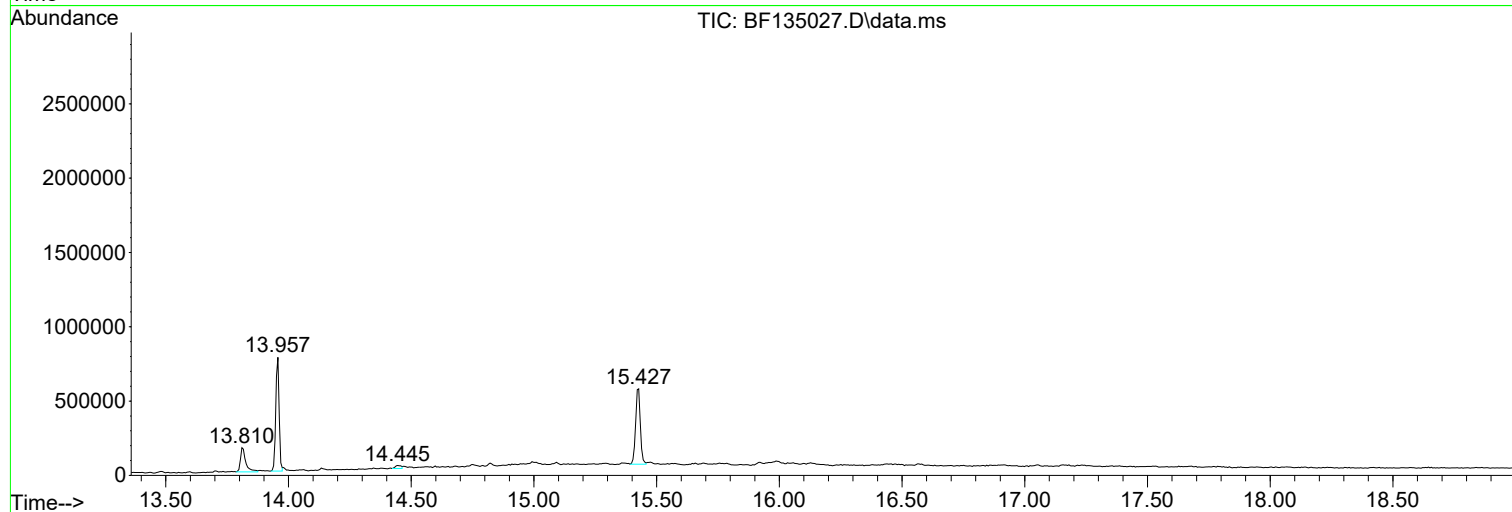
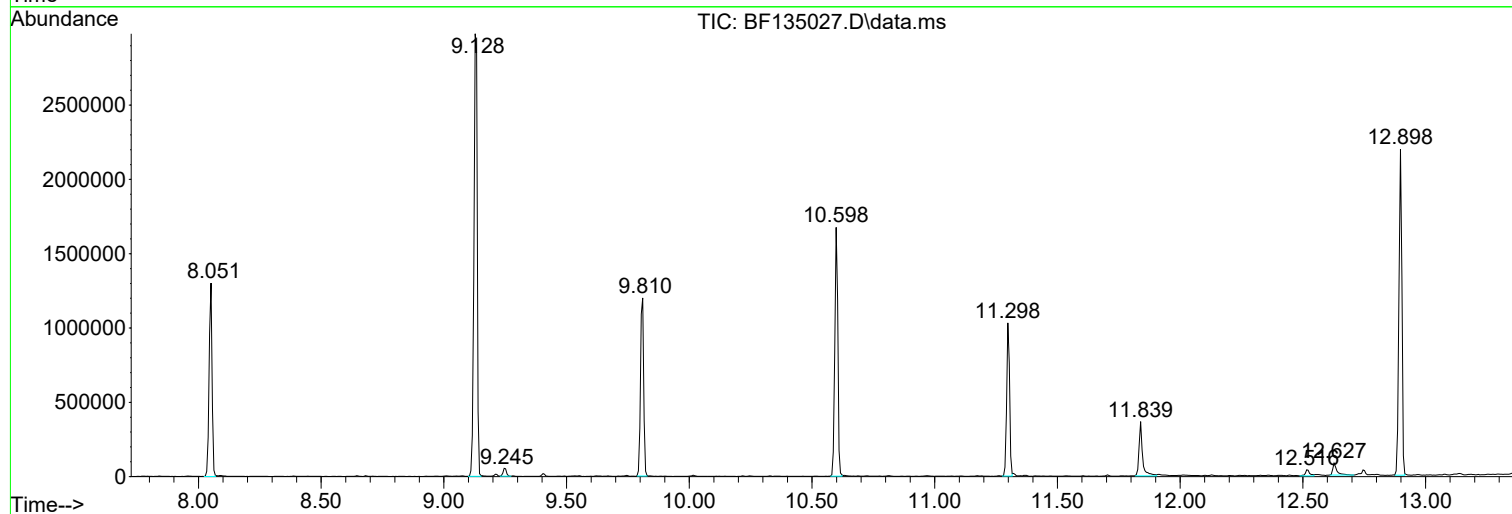
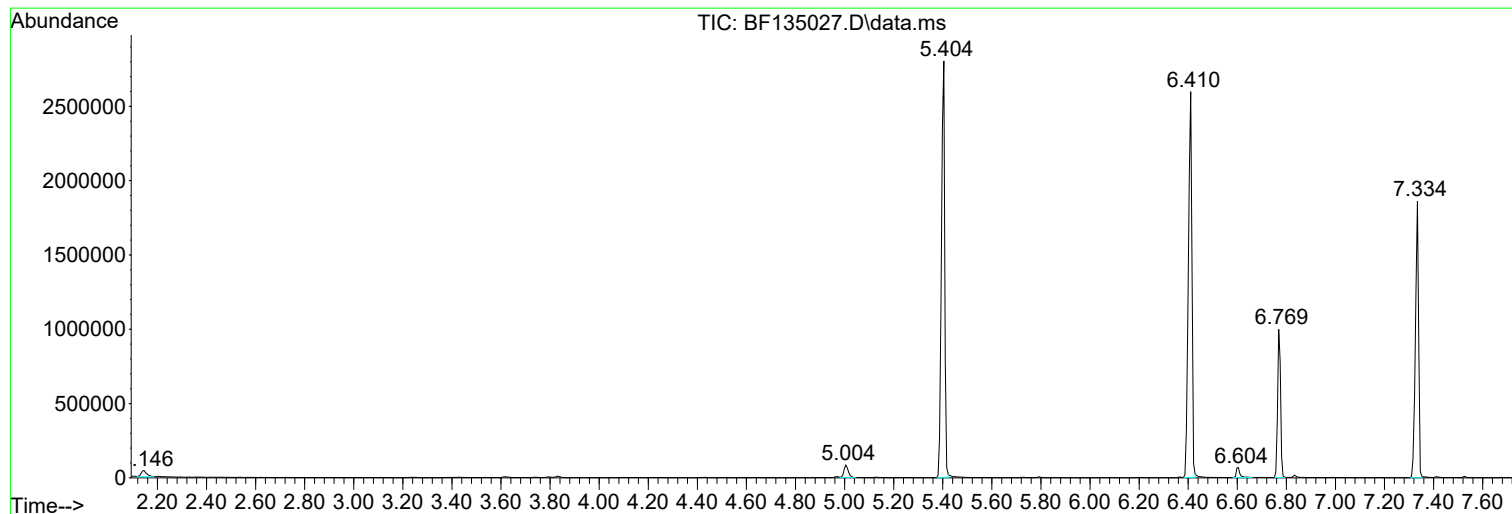
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ALS Vial : 15 Sample Multiplier: 1

Instrument :  
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ClientSampleId :  
OR-309-OK-370-COMP-24

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF083023.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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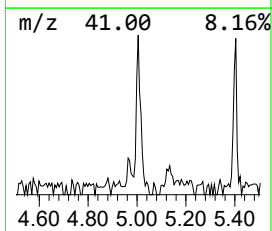
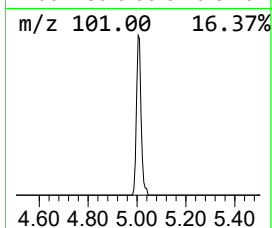
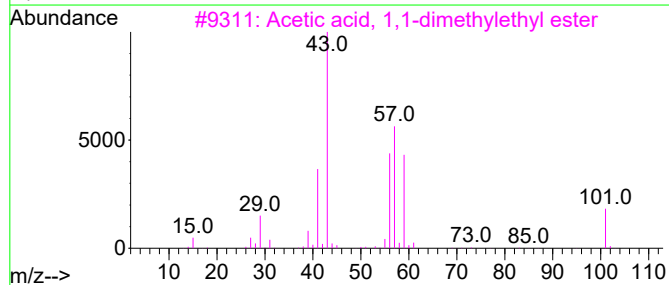
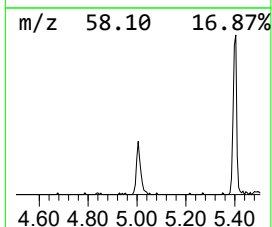
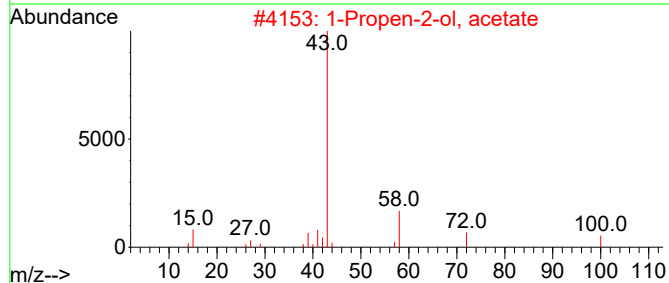
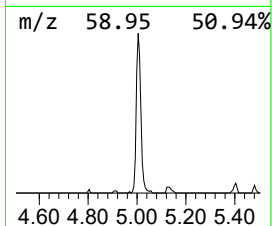
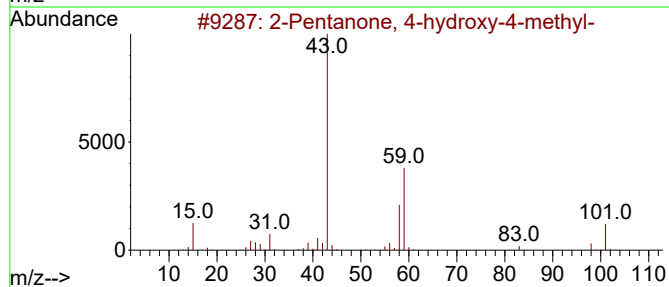
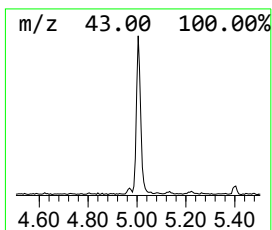
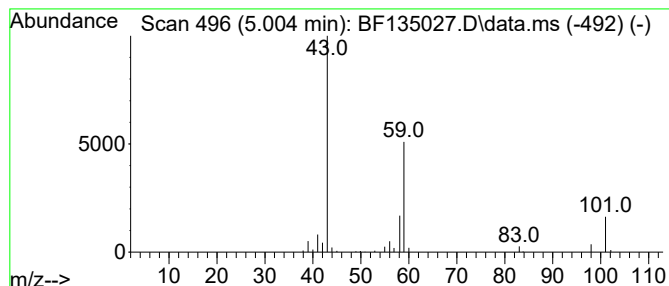
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T.  | EstConc | Area   | Relative to ISTD       | R.T.  |
|-------|---------|--------|------------------------|-------|
| 5.004 | 2.47 ng | 102495 | 1,4-Dichlorobenzene-d4 | 6.769 |

| Hit# | of                                  | 5   | Tentative ID | MW          | MolForm | CAS# | Qual |
|------|-------------------------------------|-----|--------------|-------------|---------|------|------|
| 1    | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2      | 000123-42-2 | 59      |      |      |
| 2    | 1-Propen-2-ol, acetate              | 100 | C5H8O2       | 000108-22-5 | 10      |      |      |
| 3    | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2      | 000540-88-5 | 9       |      |      |
| 4    | 2-Hexanol, 2-methyl-                | 116 | C7H16O       | 000625-23-0 | 9       |      |      |
| 5    | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2     | 001116-98-9 | 9       |      |      |



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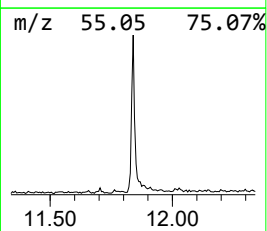
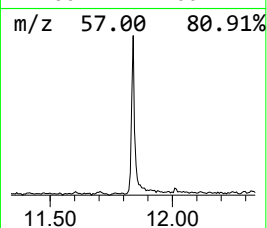
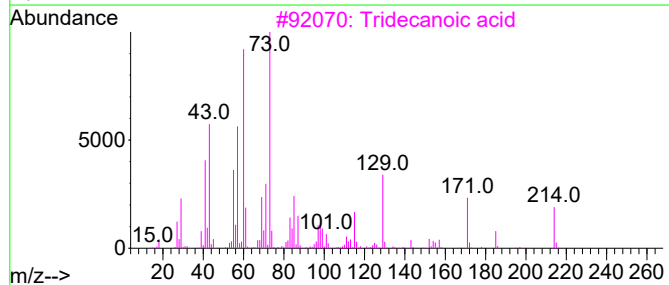
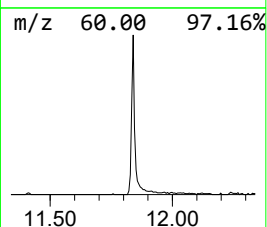
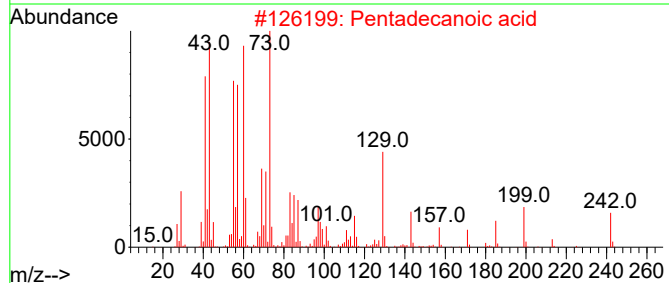
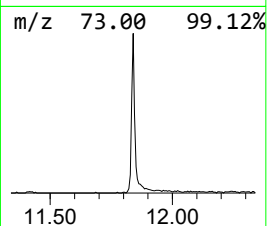
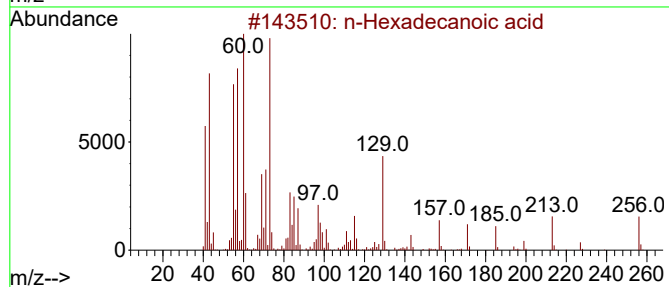
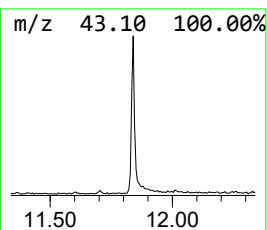
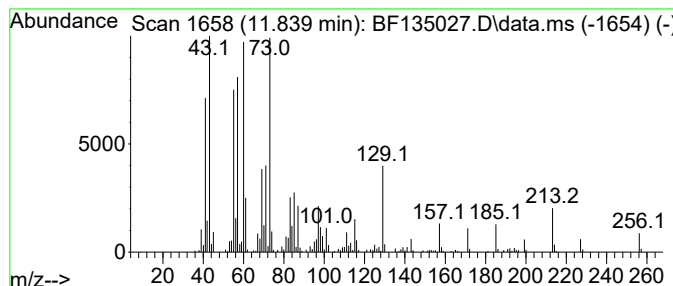
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF083023.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 11.839 | 8.30 ng | 354287 | Phenanthrene-d10 | 11.298 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 99   |
| 2    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 93   |
| 3    |    |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 86   |
| 4    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 80   |
| 5    |    |   | n-Decanoic acid     | 172 | C10H20O2 | 000334-48-5 | 76   |



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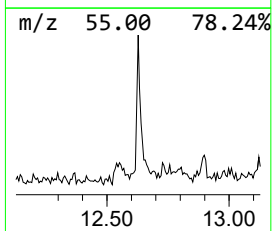
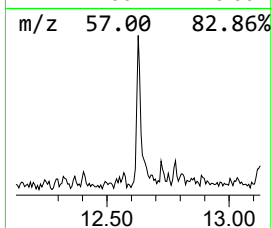
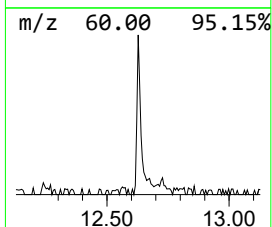
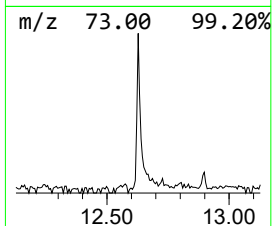
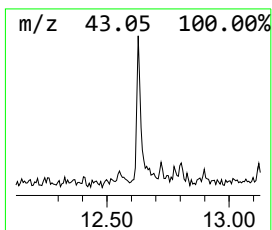
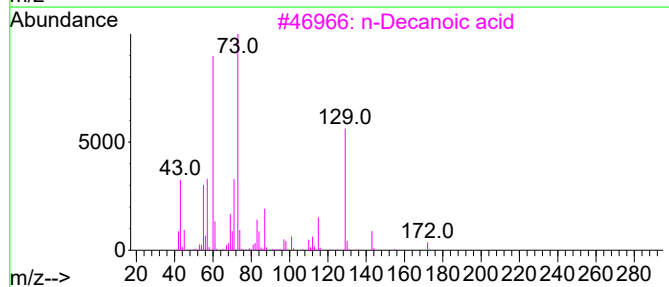
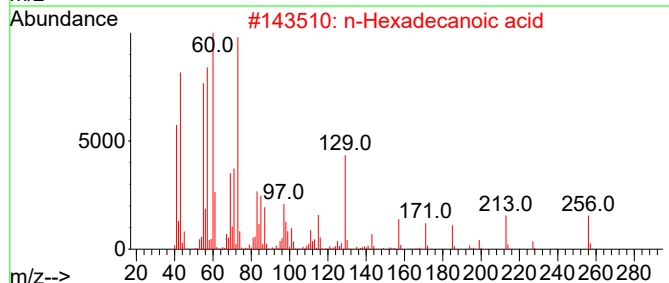
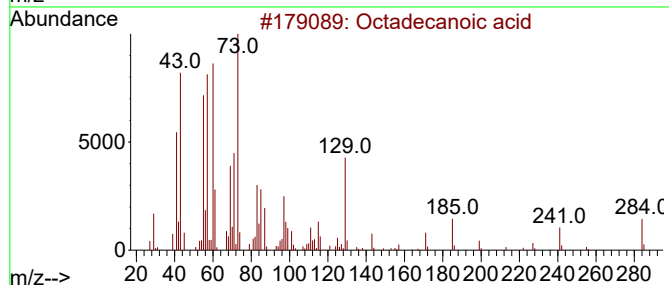
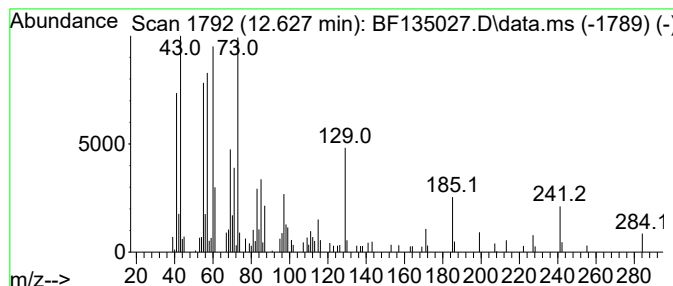
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TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 Octadecanoic acid Concentration Rank 4

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 12.627 | 2.20 ng | 93865 | Phenanthrene-d10 | 11.298 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | Octadecanoic acid   | 284 | C18H36O2 | 000057-11-4 | 93   |
| 2    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 90   |
| 3    |    |   | n-Decanoic acid     | 172 | C10H20O2 | 000334-48-5 | 86   |
| 4    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 83   |
| 5    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 83   |



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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF083023.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

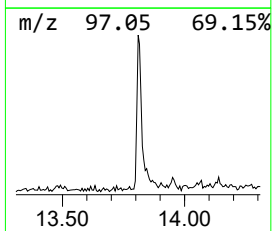
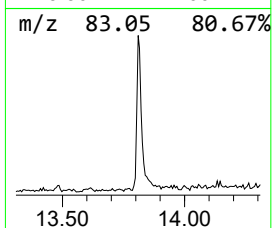
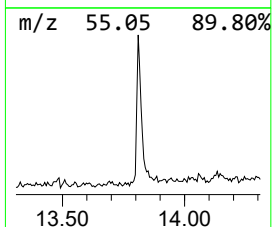
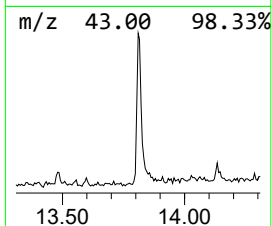
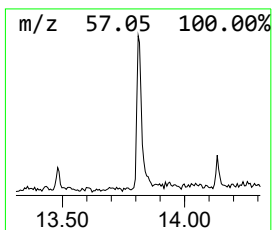
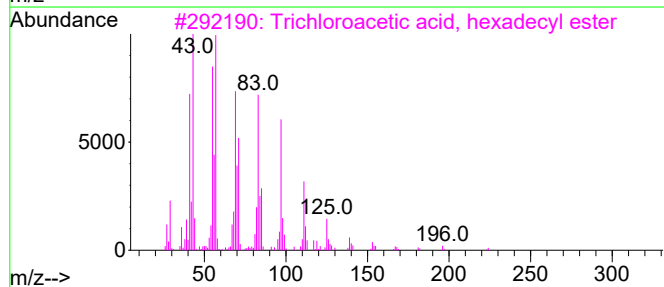
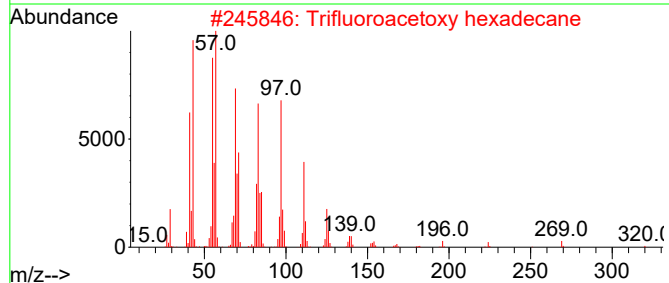
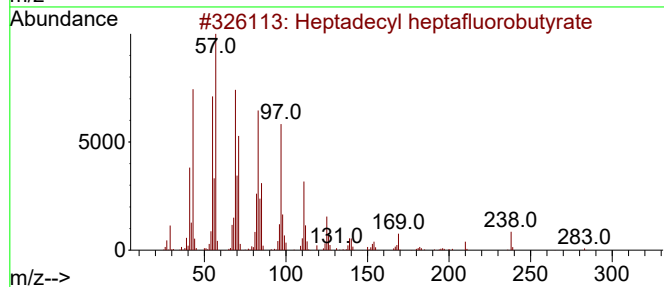
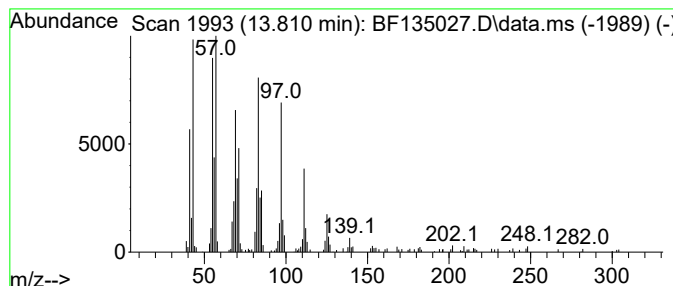
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 Heptadecyl heptafluorobutyrate Concentration Rank 2

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 13.810 | 6.61 ng | 243073 | Chrysene-d12     | 13.957 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm     | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|-------------|--------------|------|
| 1    |    |   | Heptadecyl heptafluorobutyrate      | 452 | C21H35F7O2  | 959085-66-6  | 94   |
| 2    |    |   | Trifluoroacetoxy hexadecane         | 338 | C18H33F3O2  | 006222-03-3  | 94   |
| 3    |    |   | Trichloroacetic acid, hexadecyl ... | 386 | C18H33Cl3O2 | 074339-54-1  | 94   |
| 4    |    |   | Heptadecyl trifluoroacetate         | 352 | C19H35F3O2  | 1010351-87-0 | 94   |
| 5    |    |   | 1-Docosene                          | 308 | C22H44      | 001599-67-3  | 94   |



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TIC Integration Parameters: LSCINT.P

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| 2-Pentanone, 4-... | 5.004  | 2.5     | ng    | 102495   | 1                     | 6.769  | 830464 | 20.0 |
| n-Hexadecanoic ... | 11.839 | 8.3     | ng    | 354287   | 4                     | 11.298 | 853477 | 20.0 |
| Octadecanoic acid  | 12.627 | 2.2     | ng    | 93865    | 4                     | 11.298 | 853477 | 20.0 |
| Heptadecyl hept... | 13.810 | 6.6     | ng    | 243073   | 5                     | 13.957 | 735195 | 20.0 |