

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF090523\  
 Data File : BF135094.D  
 Acq On : 05 Sep 2023 14:26  
 Operator : CG\JU  
 Sample : 04109-01  
 Misc :  
 ALS Vial : 8 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 TP-01(6-7)

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: BF135094.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         | 5.404       | 559           | 564         | 567          | rBV      | 2209717        | 2125820       | 88.25%          | 13.293%       |
| 2         | 6.410       | 730           | 735         | 738          | rBV      | 2070985        | 2143450       | 88.98%          | 13.403%       |
| 3         | 6.604       | 764           | 768         | 780          | rBV2     | 44551          | 62059         | 2.58%           | 0.388%        |
| 4         | 6.769       | 793           | 796         | 803          | rVB      | 721256         | 576511        | 23.93%          | 3.605%        |
| 5         | 7.333       | 888           | 892         | 895          | rVB      | 1551251        | 1340382       | 55.65%          | 8.382%        |
| 6         | 7.786       | 964           | 969         | 973          | rBV2     | 23656          | 27359         | 1.14%           | 0.171%        |
| 7         | 8.051       | 1009          | 1014        | 1017         | rBV      | 880592         | 780700        | 32.41%          | 4.882%        |
| 8         | 9.128       | 1193          | 1197        | 1200         | rBV      | 2772298        | 2408800       | 100.00%         | 15.063%       |
| 9         | 9.245       | 1214          | 1217        | 1220         | rVB      | 36292          | 31652         | 1.31%           | 0.198%        |
| 10        | 9.810       | 1309          | 1313        | 1316         | rBV      | 864342         | 805140        | 33.42%          | 5.035%        |
| 11        | 10.598      | 1443          | 1447        | 1451         | rBV      | 1565393        | 1430727       | 59.40%          | 8.947%        |
| 12        | 11.298      | 1562          | 1566        | 1569         | rBV      | 907567         | 749249        | 31.10%          | 4.685%        |
| 13        | 11.833      | 1653          | 1657        | 1667         | rBV      | 287385         | 332017        | 13.78%          | 2.076%        |
| 14        | 12.516      | 1770          | 1773        | 1776         | rBV      | 27508          | 28190         | 1.17%           | 0.176%        |
| 15        | 12.627      | 1788          | 1792        | 1803         | rBV      | 77977          | 103010        | 4.28%           | 0.644%        |
| 16        | 12.898      | 1834          | 1838        | 1841         | rBV      | 2013438        | 1729740       | 71.81%          | 10.816%       |
| 17        | 13.133      | 1875          | 1878        | 1884         | rBV4     | 17564          | 26544         | 1.10%           | 0.166%        |
| 18        | 13.815      | 1990          | 1994        | 2001         | rBV2     | 107880         | 149103        | 6.19%           | 0.932%        |
| 19        | 13.957      | 2013          | 2018        | 2021         | rBV      | 520463         | 515680        | 21.41%          | 3.225%        |
| 20        | 14.815      | 2161          | 2164        | 2169         | rBV      | 67644          | 66418         | 2.76%           | 0.415%        |
| 21        | 15.421      | 2262          | 2267        | 2273         | rBV      | 455128         | 559304        | 23.22%          | 3.497%        |

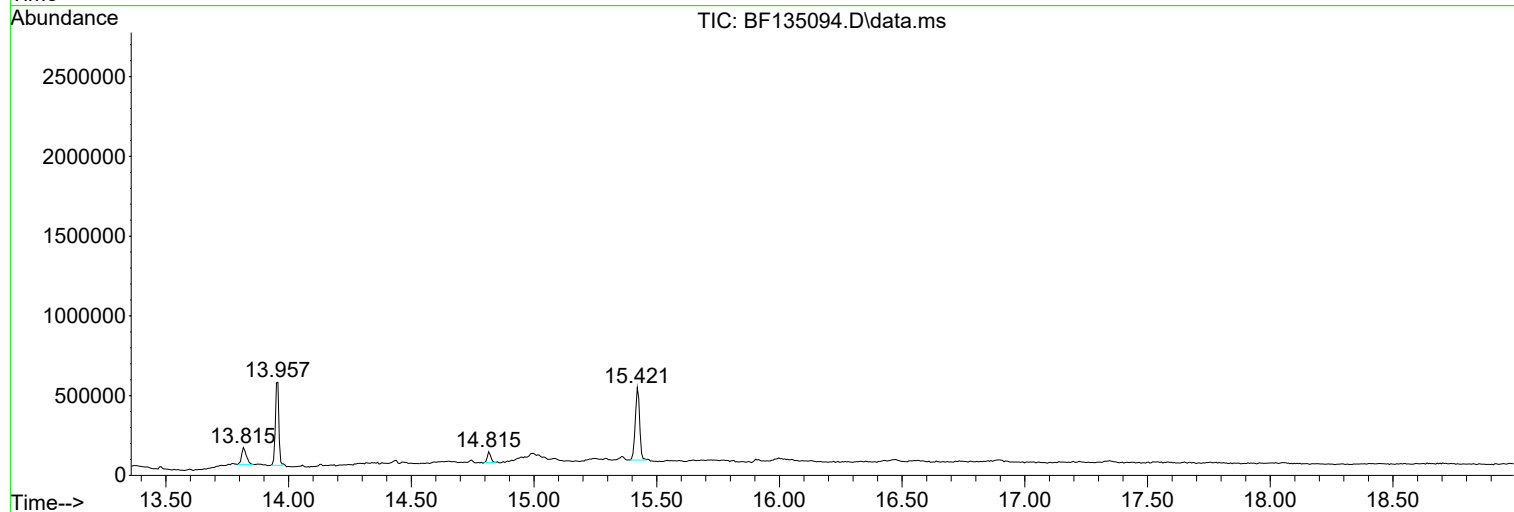
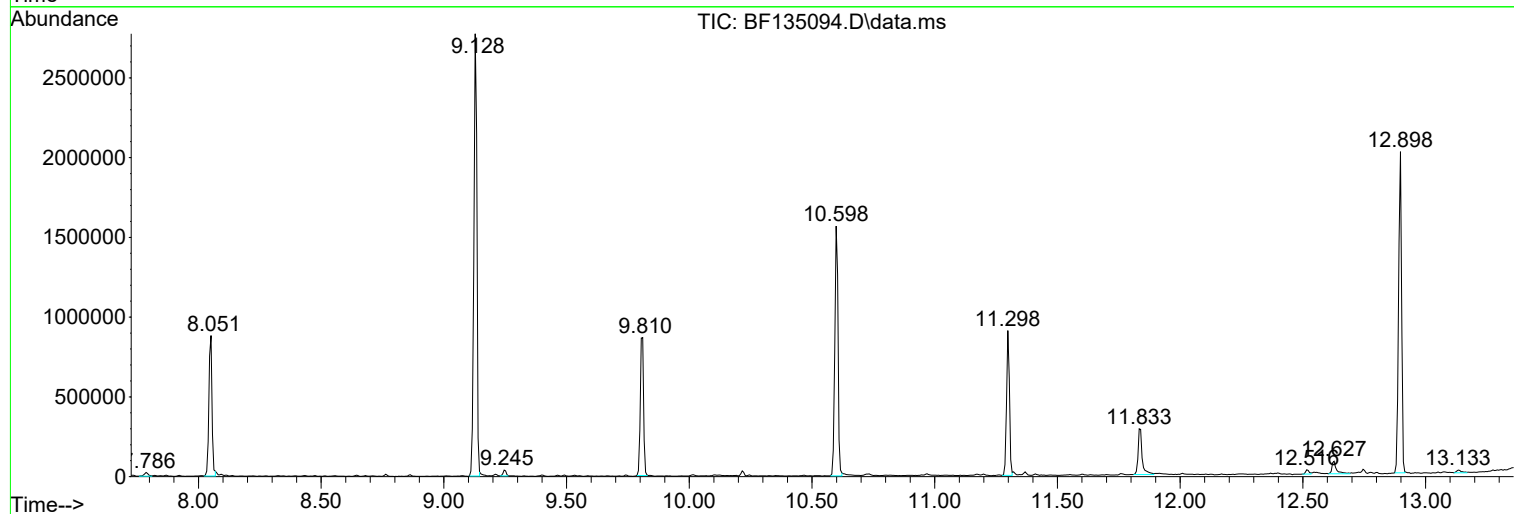
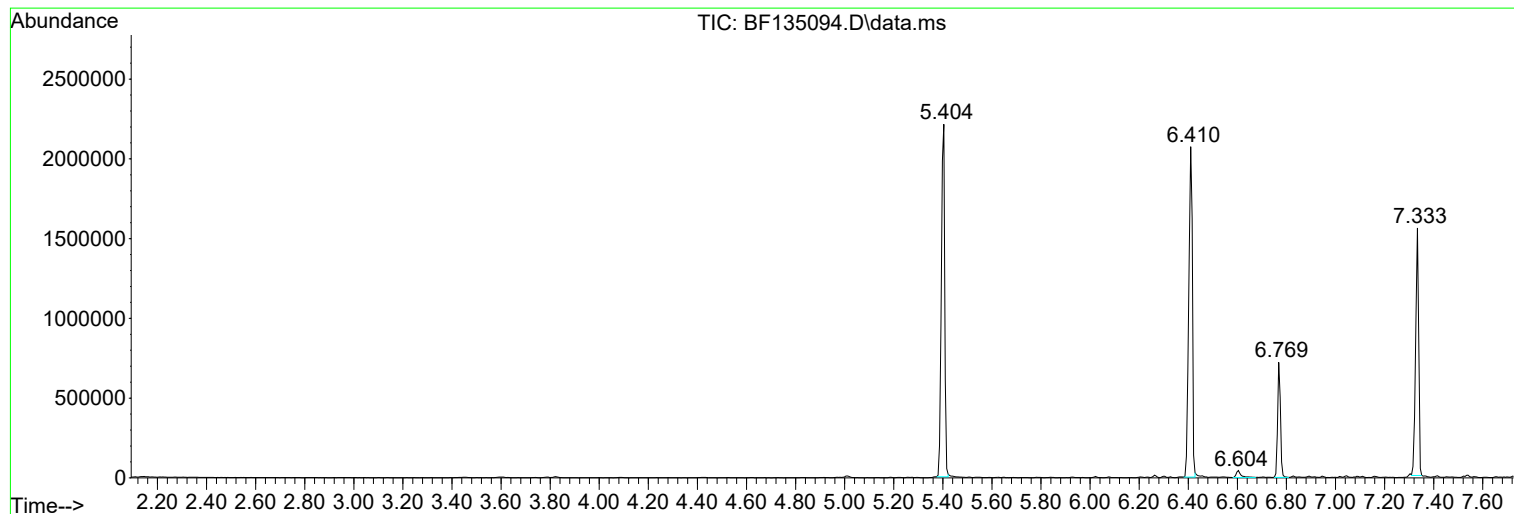
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TP-01(6-7)

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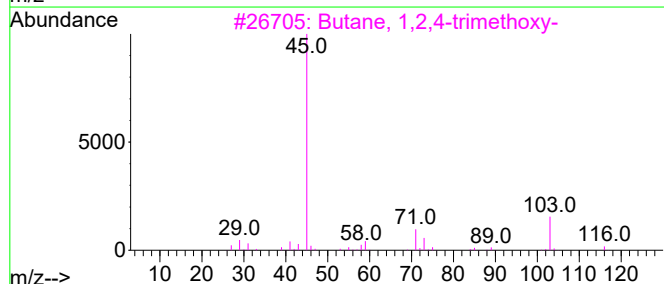
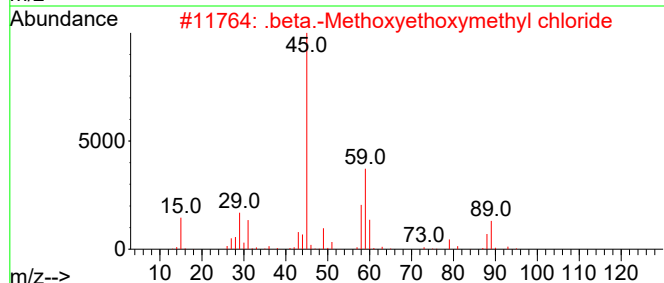
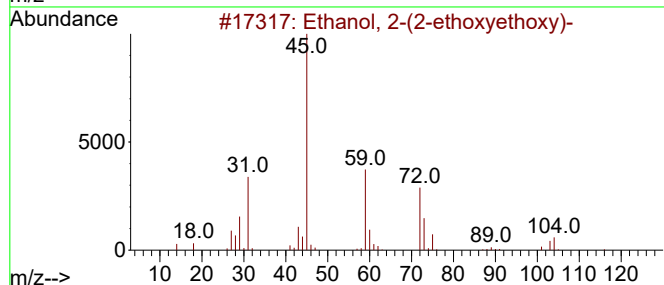
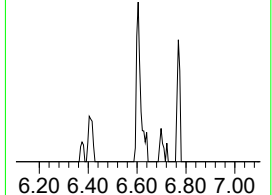
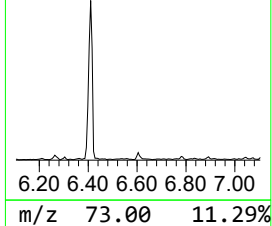
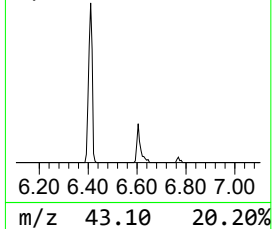
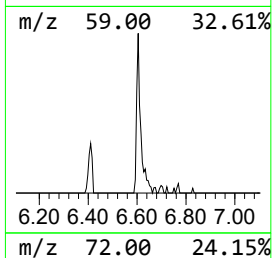
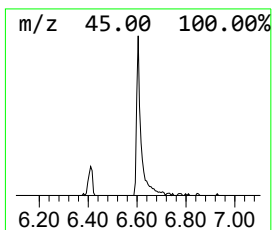
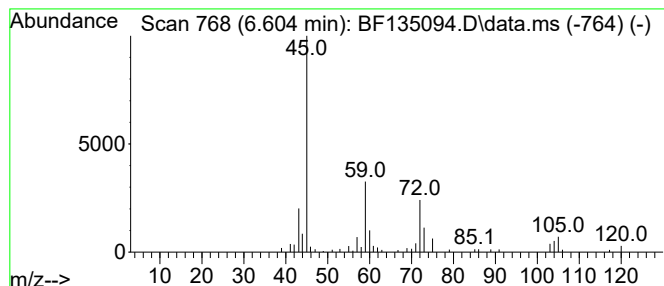
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF083023.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 5

| R.T.  | EstConc | Area  | Relative to ISTD       | R.T.  |
|-------|---------|-------|------------------------|-------|
| 6.604 | 2.15 ng | 62059 | 1,4-Dichlorobenzene-d4 | 6.769 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | Ethanol, 2-(2-ethoxyethoxy)-        | 134 | C6H14O3  | 000111-90-0 | 90   |
| 2    |    |   | .beta.-Methoxyethoxymethyl chloride | 124 | C4H9ClO2 | 003970-21-6 | 42   |
| 3    |    |   | Butane, 1,2,4-trimethoxy-           | 148 | C7H16O3  | 020637-48-3 | 40   |
| 4    |    |   | 2-Pentanol                          | 88  | C5H12O   | 006032-29-7 | 38   |
| 5    |    |   | 1-Butene, 4-methoxy                 | 86  | C5H10O   | 004696-30-4 | 38   |



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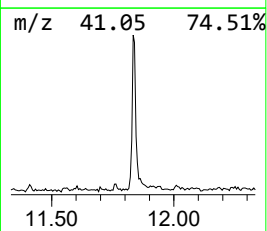
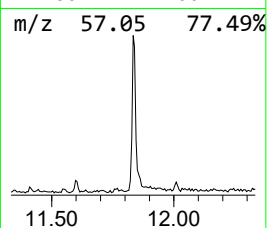
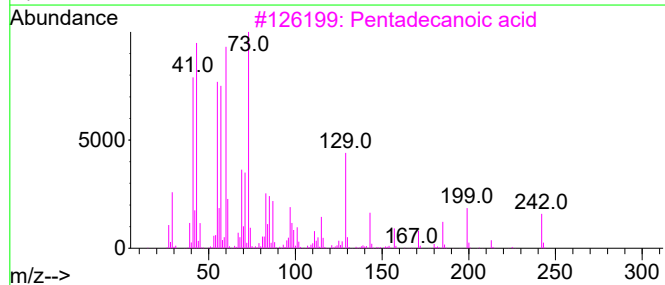
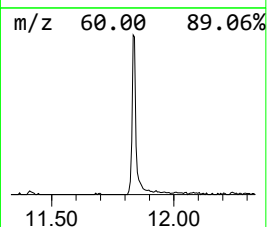
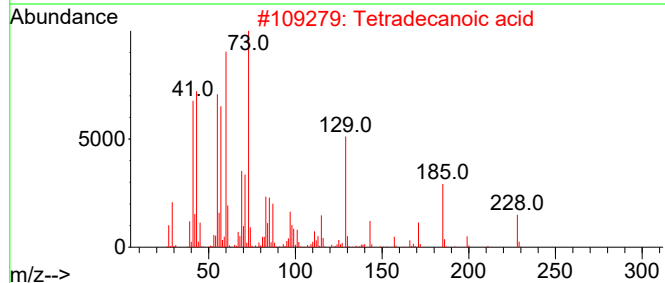
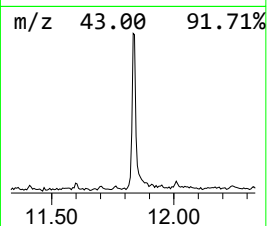
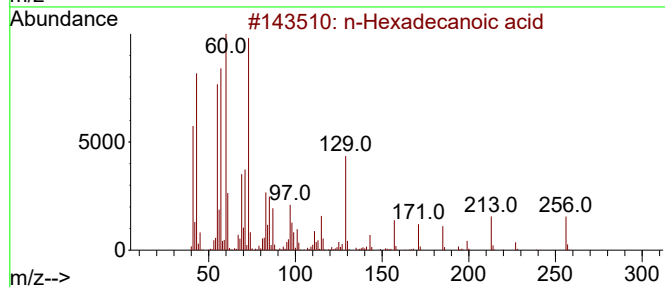
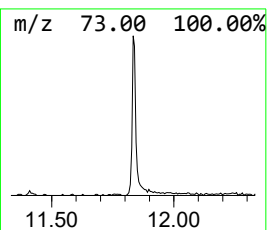
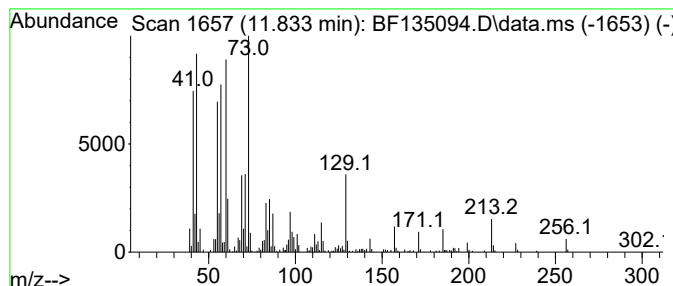
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF083023.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.   |
|--------|---------|--------|------------------|--------|
| 11.833 | 8.86 ng | 332017 | Phenanthrene-d10 | 11.298 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 99   |
| 2    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 96   |
| 3    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 90   |
| 4    |    |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 81   |
| 5    |    |   | Dodecanoic acid     | 200 | C12H24O2 | 000143-07-7 | 59   |



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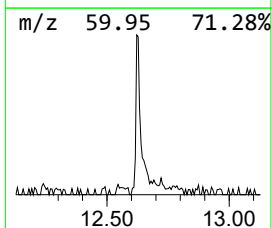
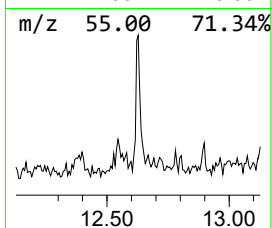
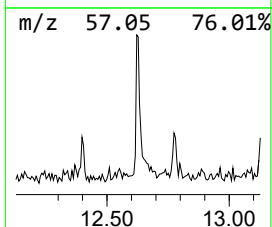
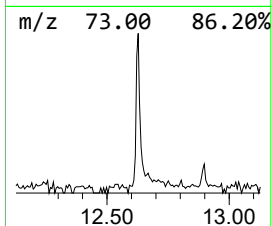
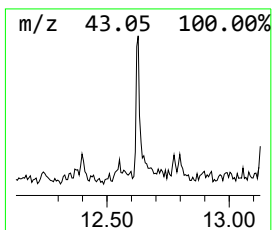
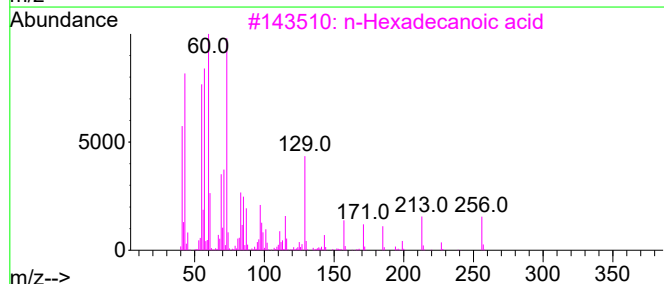
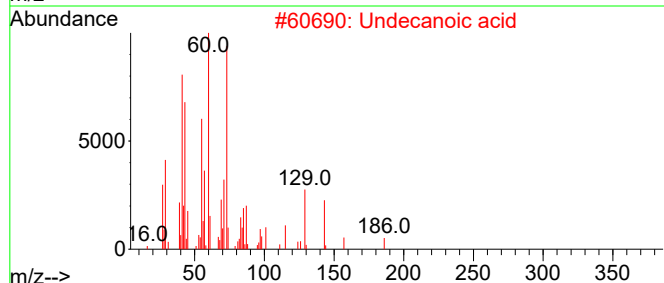
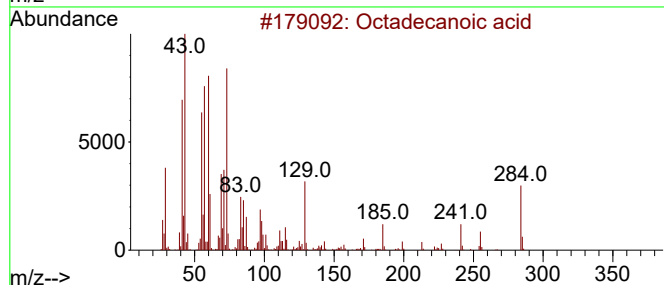
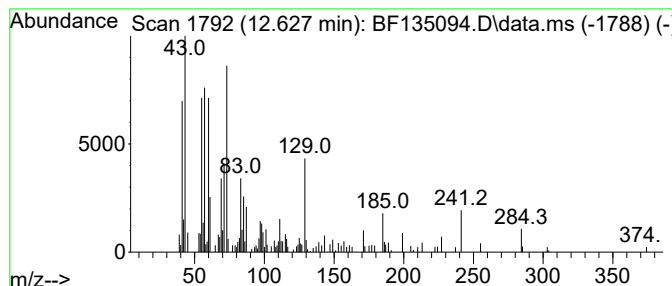
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF083023.M  
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TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 Octadecanoic acid Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 12.627 | 2.75 ng | 103010 | Phenanthrene-d10 | 11.298 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | Octadecanoic acid   | 284 | C18H36O2 | 000057-11-4 | 93   |
| 2    |    |   | Undecanoic acid     | 186 | C11H22O2 | 000112-37-8 | 78   |
| 3    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 52   |
| 4    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 52   |
| 5    |    |   | n-Decanoic acid     | 172 | C10H20O2 | 000334-48-5 | 43   |



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Instrument :  
BNA\_F  
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TP-01(6-7)

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

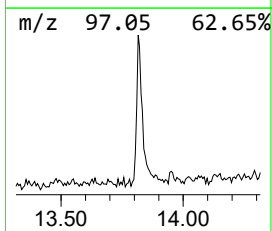
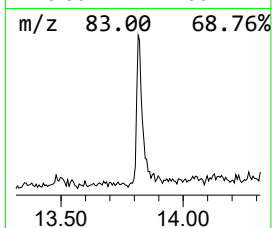
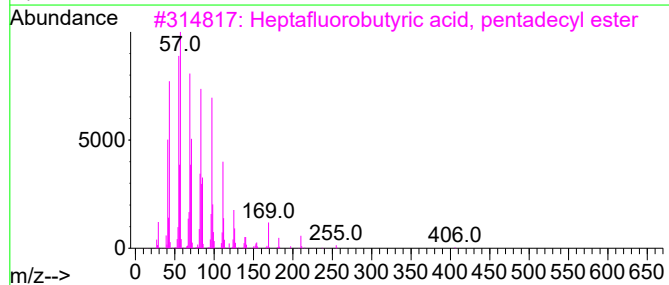
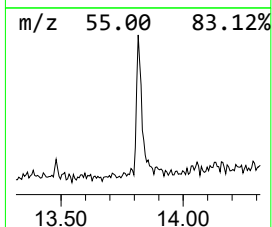
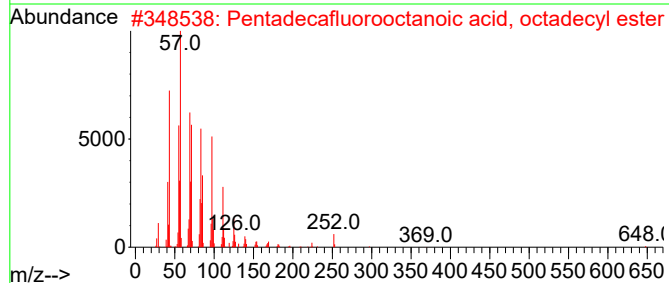
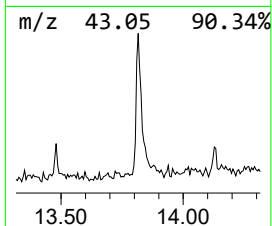
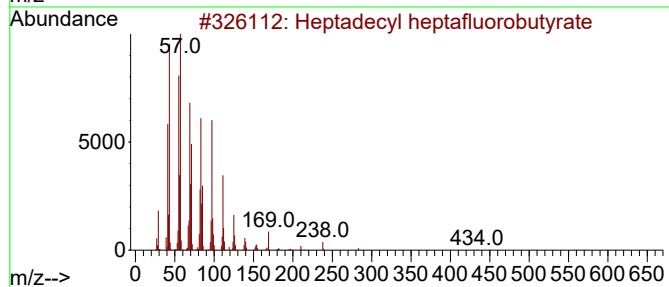
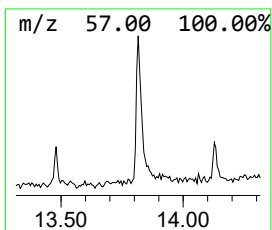
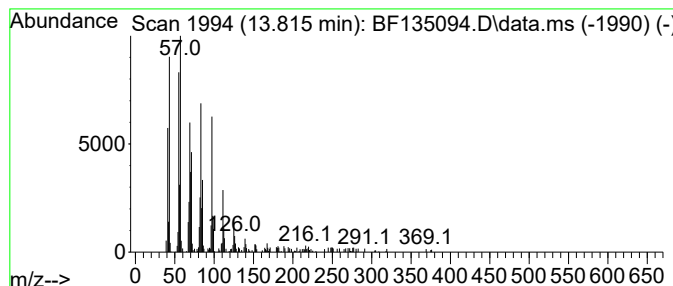
TIC Library : C:\Database\NIST20.L  
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Peak Number 4 Heptadecyl heptafluorobutyrate Concentration Rank 2

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 13.815 | 5.78 ng | 149103 | Chrysene-d12     | 13.957 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm     | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|-------------|--------------|------|
| 1    |    |   | Heptadecyl heptafluorobutyrate      | 452 | C21H35F7O2  | 959085-66-6  | 95   |
| 2    |    |   | Pentadecafluorooctanoic acid, oc... | 666 | C26H37F15O2 | 1000406-04-8 | 94   |
| 3    |    |   | Heptafluorobutyric acid, pentade... | 424 | C19H31F7O2  | 959261-23-5  | 94   |
| 4    |    |   | Pentafluoropropionic acid, penta... | 374 | C18H31F5O2  | 959092-08-1  | 94   |
| 5    |    |   | Pentafluoropropionic acid, hepta... | 402 | C20H35F5O2  | 959218-78-1  | 91   |



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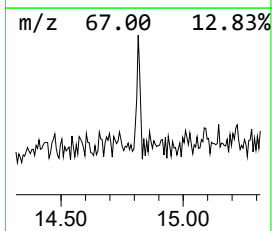
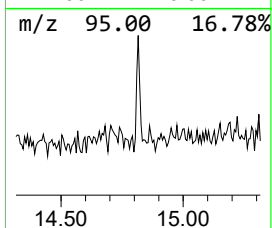
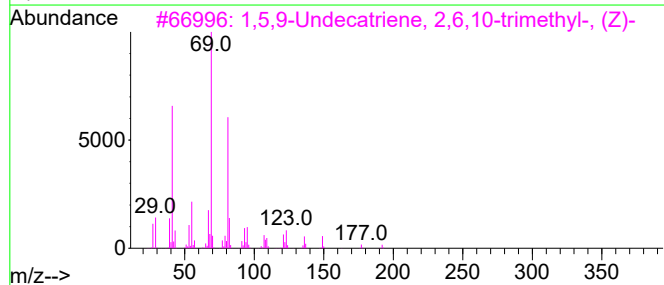
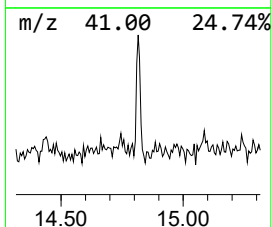
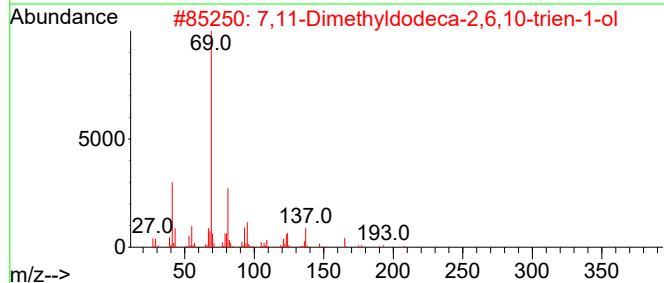
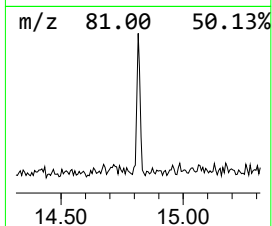
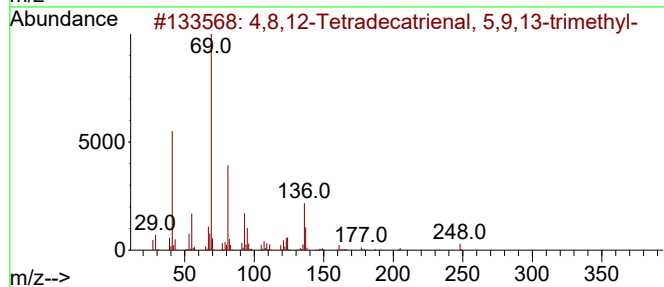
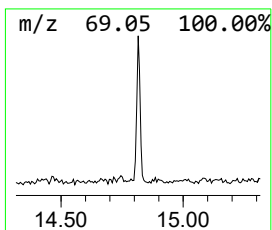
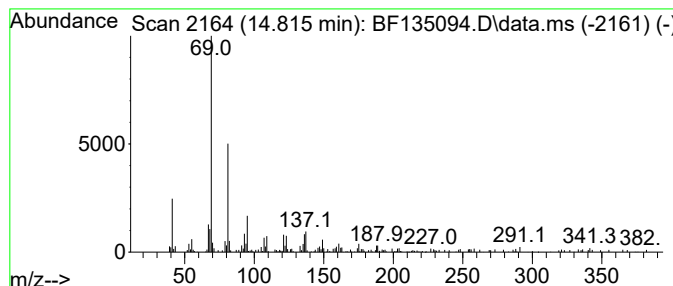
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Peak Number 5 4,8,12-Tetradecatrienal, 5,... Concentration Rank 4

| R.T.      | EstConc                             | Area  | Relative to ISTD | R.T.        |      |
|-----------|-------------------------------------|-------|------------------|-------------|------|
| 14.815    | 2.38 ng                             | 66418 | Perylene-d12     | 15.421      |      |
| Hit# of 5 | Tentative ID                        | MW    | MolForm          | CAS#        | Qual |
| 1         | 4,8,12-Tetradecatrienal, 5,9,13-... | 248   | C17H28O          | 066408-55-7 | 72   |
| 2         | 7,11-Dimethyldodeca-2,6,10-trien... | 208   | C14H24O          | 125529-10-4 | 72   |
| 3         | 1,5,9-Undecatriene, 2,6,10-trime... | 192   | C14H24           | 062951-96-6 | 70   |
| 4         | Supraene                            | 410   | C30H50           | 007683-64-9 | 64   |
| 5         | Geranyl citronellate                | 306   | C20H34O2         | 107811-06-3 | 64   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF090523\  
Data File : BF135094.D  
Acq On : 05 Sep 2023 14:26  
Operator : CG\JU  
Sample : 04109-01  
Misc :  
ALS Vial : 8 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
TP-01(6-7)

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

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| Ethanol, 2-(2-e... | 6.604  | 2.1     | ng    | 62059    | 1                     | 6.769  | 576511 | 20.0 |
| n-Hexadecanoic ... | 11.833 | 8.9     | ng    | 332017   | 4                     | 11.298 | 749249 | 20.0 |
| Octadecanoic acid  | 12.627 | 2.8     | ng    | 103010   | 4                     | 11.298 | 749249 | 20.0 |
| Heptadecyl hept... | 13.815 | 5.8     | ng    | 149103   | 5                     | 13.957 | 515680 | 20.0 |
| 4,8,12-Tetradec... | 14.815 | 2.4     | ng    | 66418    | 6                     | 15.421 | 559304 | 20.0 |