

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF102220\  
 Data File : BF122081.D  
 Acq On : 22 Oct 2020 13:56  
 Operator : JU/CG  
 Sample : L4436-08  
 Misc :  
 ALS Vial : 9 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 36A

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-BF101220.M  
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122081.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         | 4.946       | 483           | 486         | 497          | rBV      | 29586          | 45400         | 1.39%           | 0.209%        |
| 2         | 5.351       | 551           | 555         | 581          | rBV      | 2308519        | 2509715       | 76.92%          | 11.544%       |
| 3         | 6.381       | 726           | 730         | 759          | rBV      | 2458915        | 2559814       | 78.45%          | 11.775%       |
| 4         | 6.581       | 762           | 764         | 773          | rBV      | 37205          | 67681         | 2.07%           | 0.311%        |
| 5         | 6.728       | 786           | 789         | 797          | rVB      | 722060         | 611743        | 18.75%          | 2.814%        |
| 6         | 7.298       | 882           | 886         | 889          | rBV      | 1870416        | 1678211       | 51.43%          | 7.719%        |
| 7         | 8.010       | 1003          | 1007        | 1021         | rBV      | 891616         | 822875        | 25.22%          | 3.785%        |
| 8         | 9.086       | 1185          | 1190        | 1201         | rBV      | 3172345        | 3014640       | 92.39%          | 13.867%       |
| 9         | 9.481       | 1254          | 1257        | 1269         | rBV      | 412305         | 377003        | 11.55%          | 1.734%        |
| 10        | 9.757       | 1301          | 1304        | 1320         | rVB      | 1023186        | 965994        | 29.61%          | 4.443%        |
| 11        | 10.551      | 1435          | 1439        | 1455         | rBV      | 1880168        | 1973368       | 60.48%          | 9.077%        |
| 12        | 11.245      | 1553          | 1557        | 1564         | rBV      | 1109430        | 1018066       | 31.20%          | 4.683%        |
| 13        | 11.775      | 1644          | 1647        | 1654         | rBV3     | 74439          | 74734         | 2.29%           | 0.344%        |
| 14        | 12.463      | 1760          | 1764        | 1770         | rBV      | 80359          | 76391         | 2.34%           | 0.351%        |
| 15        | 12.692      | 1798          | 1803        | 1806         | rVB      | 67125          | 68821         | 2.11%           | 0.317%        |
| 16        | 12.827      | 1822          | 1826        | 1830         | rBV      | 3273683        | 3262831       | 100.00%         | 15.008%       |
| 17        | 13.721      | 1975          | 1978        | 1988         | rBV      | 246944         | 497471        | 15.25%          | 2.288%        |
| 18        | 13.886      | 2002          | 2006        | 2009         | rBV      | 845097         | 771421        | 23.64%          | 3.548%        |
| 19        | 13.910      | 2009          | 2010        | 2015         | rVB2     | 53596          | 47173         | 1.45%           | 0.217%        |
| 20        | 14.339      | 2080          | 2083        | 2085         | rBV2     | 37954          | 38788         | 1.19%           | 0.178%        |
| 21        | 14.374      | 2085          | 2089        | 2096         | rVV8     | 27833          | 64247         | 1.97%           | 0.296%        |
| 22        | 14.633      | 2130          | 2133        | 2138         | rBV      | 33250          | 33269         | 1.02%           | 0.153%        |
| 23        | 14.774      | 2154          | 2157        | 2161         | rVB      | 58491          | 56731         | 1.74%           | 0.261%        |
| 24        | 14.915      | 2178          | 2181        | 2184         | rBV      | 31478          | 40244         | 1.23%           | 0.185%        |
| 25        | 14.951      | 2184          | 2187        | 2191         | rVV2     | 58592          | 71120         | 2.18%           | 0.327%        |
| 26        | 15.015      | 2192          | 2198        | 2207         | rVV6     | 40057          | 110372        | 3.38%           | 0.508%        |
| 27        | 15.321      | 2245          | 2250        | 2258         | rBV      | 490068         | 682363        | 20.91%          | 3.139%        |
| 28        | 15.715      | 2313          | 2317        | 2323         | rVB      | 55484          | 77566         | 2.38%           | 0.357%        |
| 29        | 15.804      | 2326          | 2332        | 2333         | rBV3     | 36421          | 61498         | 1.88%           | 0.283%        |
| 30        | 16.733      | 2485          | 2490        | 2498         | rVB6     | 26155          | 60660         | 1.86%           | 0.279%        |

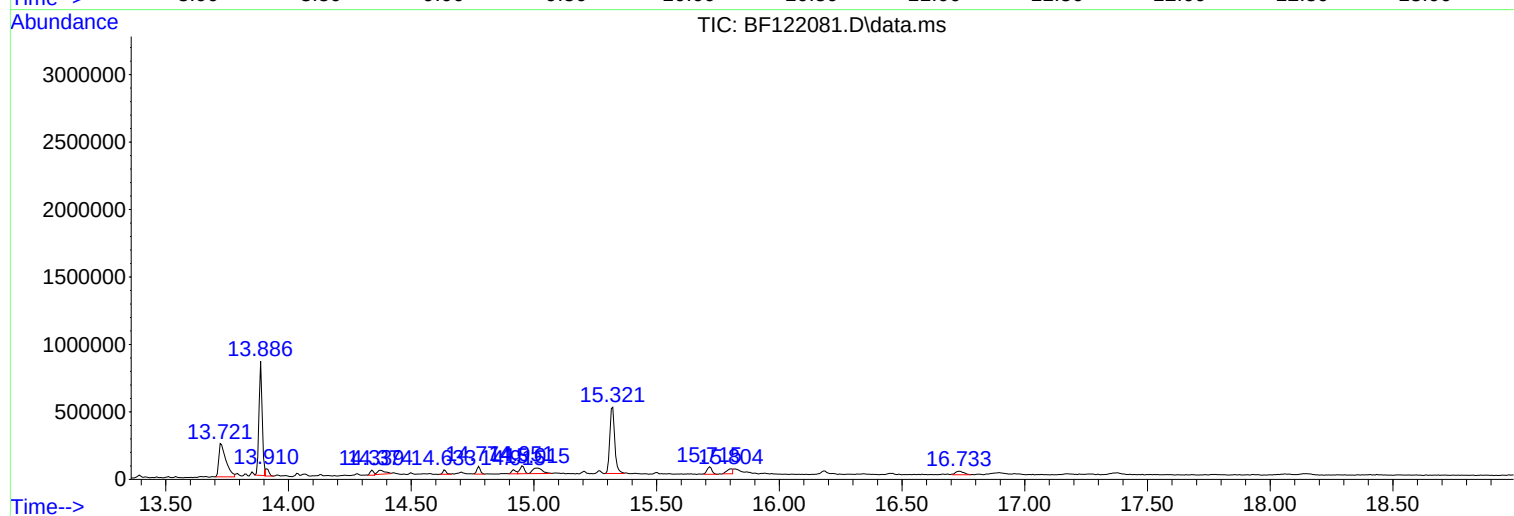
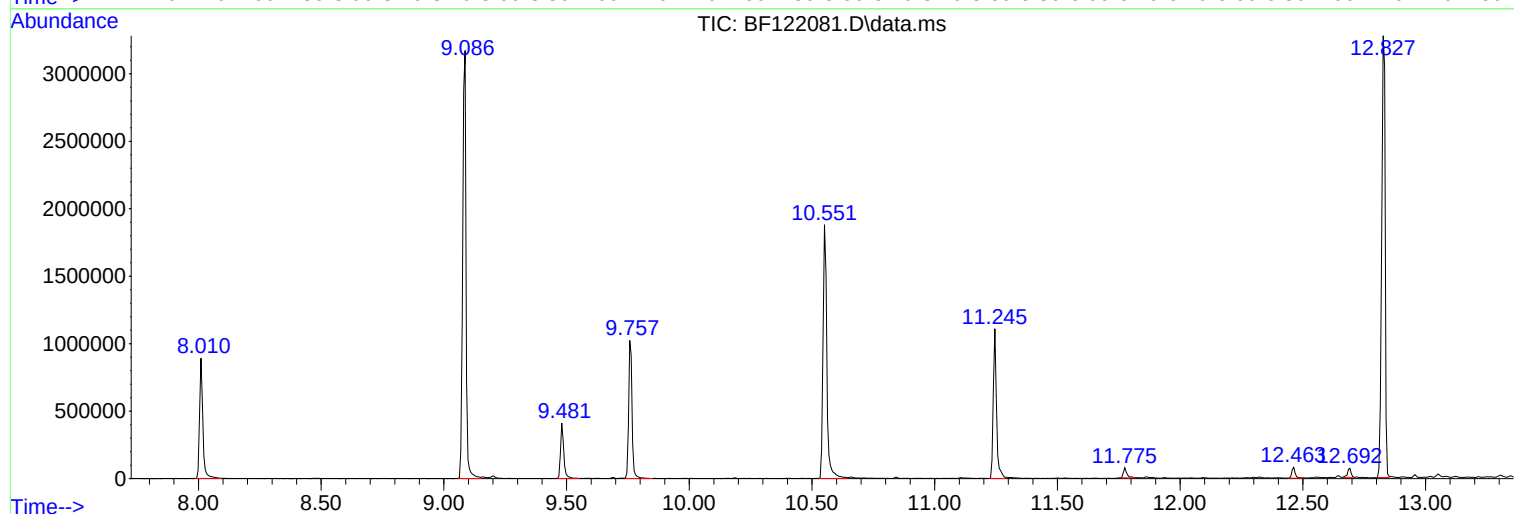
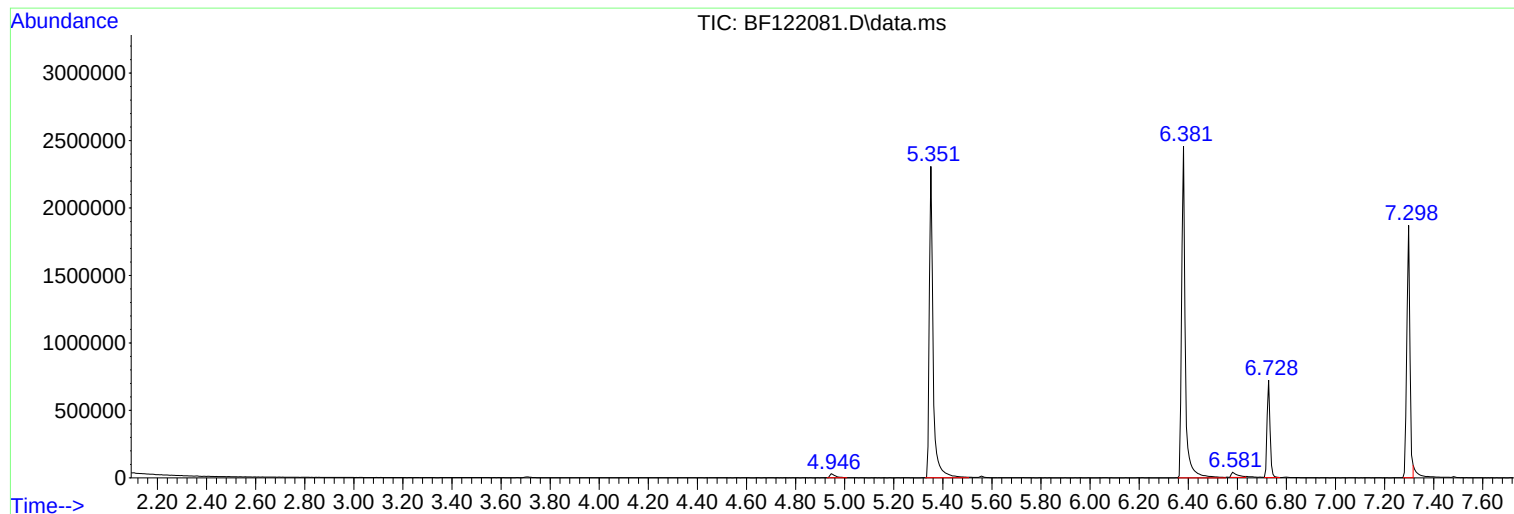
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Misc :  
ALS Vial : 9 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
36A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF101220.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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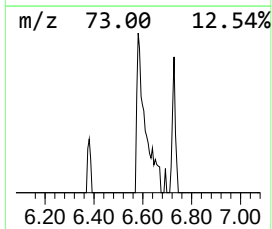
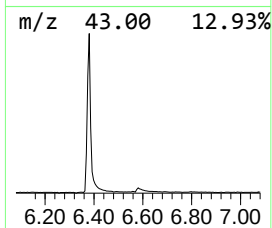
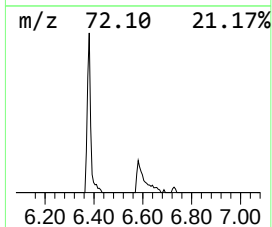
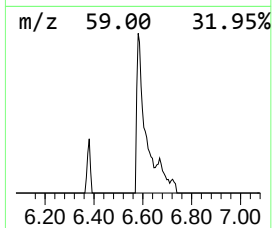
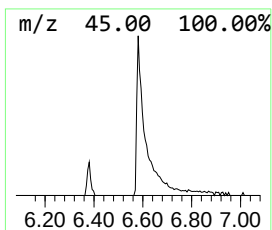
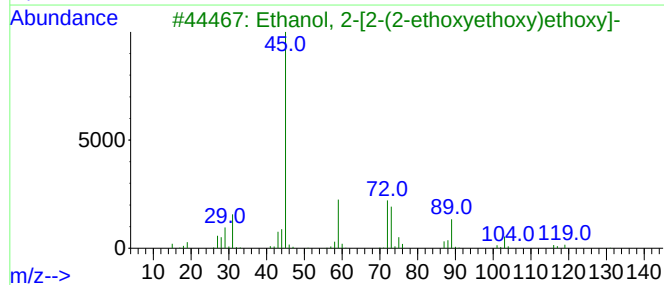
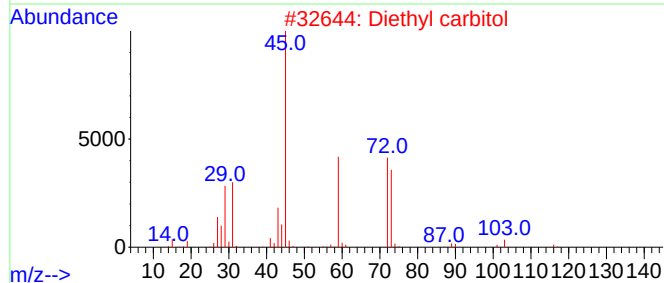
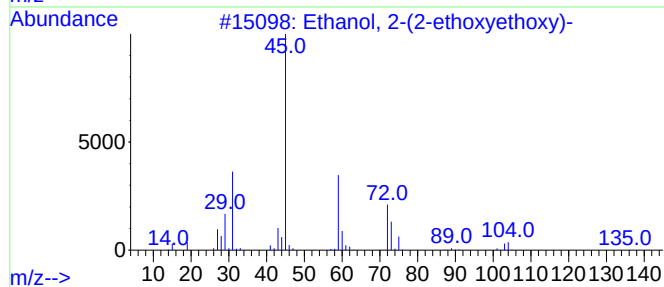
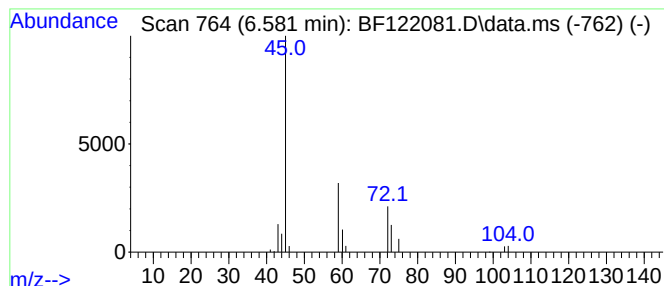
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 4

| R.T.  | EstConc | Area  | Relative to ISTD       | R.T.  |
|-------|---------|-------|------------------------|-------|
| 6.581 | 2.21 ng | 67681 | 1,4-Dichlorobenzene-d4 | 6.728 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|---------|-------------|------|
| 1    |    |   | Ethanol, 2-(2-ethoxyethoxy)-        | 134 | C6H14O3 | 000111-90-0 | 83   |
| 2    |    |   | Diethyl carbitol                    | 162 | C8H18O3 | 000112-36-7 | 72   |
| 3    |    |   | Ethanol, 2-[2-(2-ethoxyethoxy)et... | 178 | C8H18O4 | 000112-50-5 | 39   |
| 4    |    |   | 2-Propanol, 1-(1-methylethoxy)-     | 118 | C6H14O2 | 003944-36-3 | 38   |
| 5    |    |   | Ethanol, 2-(2-methoxyethoxy)-       | 120 | C5H12O3 | 000111-77-3 | 36   |



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TIC Library : C:\DATABASE\NIST11.L  
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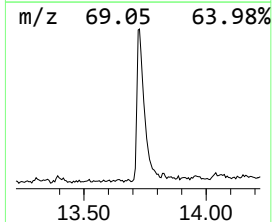
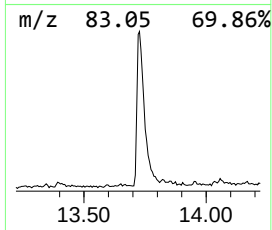
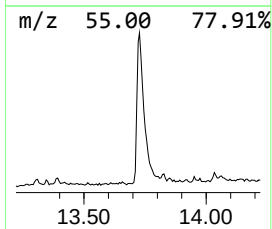
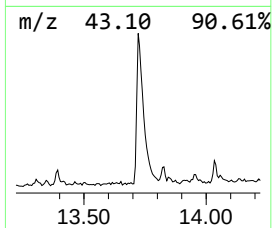
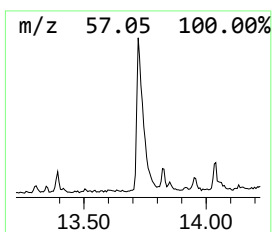
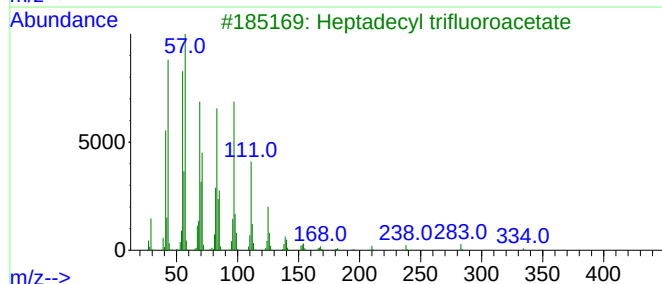
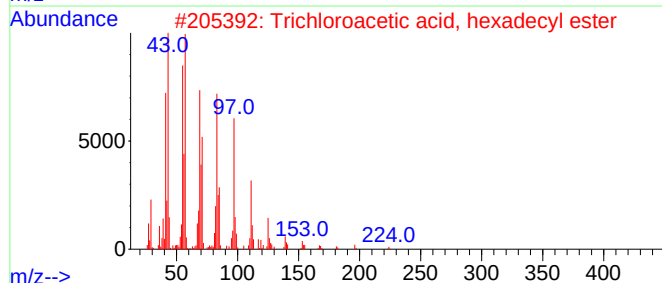
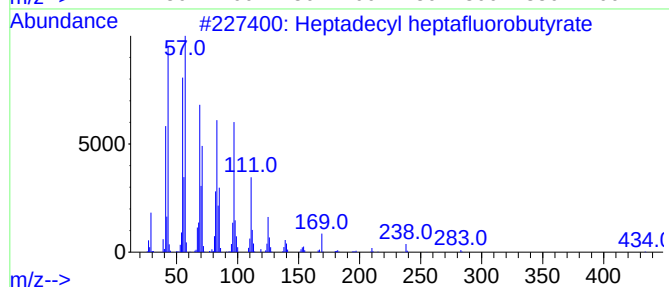
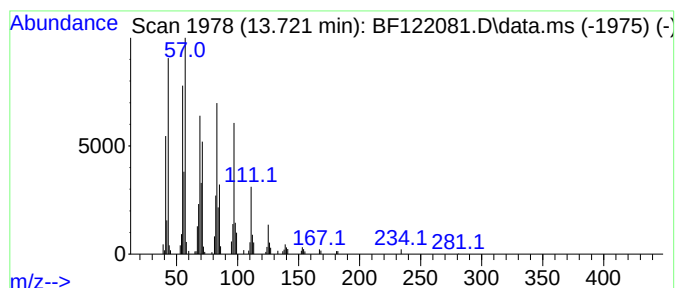
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Peak Number 2 Heptadecyl heptafluorobutyrate Concentration Rank 1

| R.T.   | EstConc  | Area   | Relative to ISTD | R.T.   |
|--------|----------|--------|------------------|--------|
| 13.721 | 12.90 ng | 497471 | Chrysene-d12     | 13.886 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm     | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|-------------|--------------|------|
| 1    |    |   | Heptadecyl heptafluorobutyrate      | 452 | C21H35F7O2  | 959085-66-6  | 95   |
| 2    |    |   | Trichloroacetic acid, hexadecyl ... | 386 | C18H33Cl3O2 | 074339-54-1  | 95   |
| 3    |    |   | Heptadecyl trifluoroacetate         | 352 | C19H35F3O2  | 1000351-87-0 | 94   |
| 4    |    |   | 1-Heptacosanol                      | 396 | C27H56O     | 002004-39-9  | 91   |
| 5    |    |   | Pentafluoropropionic acid, hepta... | 402 | C20H35F5O2  | 959218-78-1  | 91   |



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Sample : L4436-08  
Misc :  
ALS Vial : 9 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampled :  
36A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF101220.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

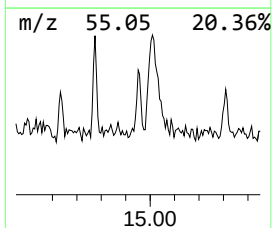
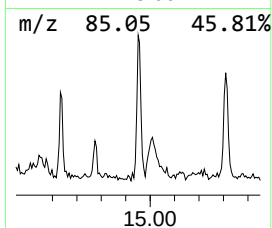
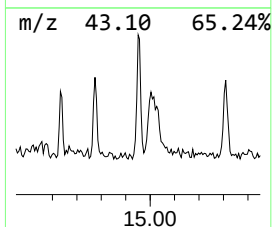
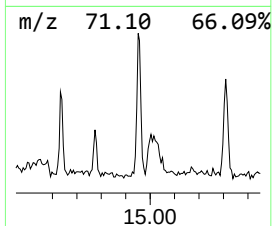
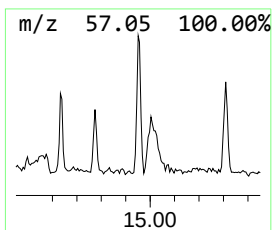
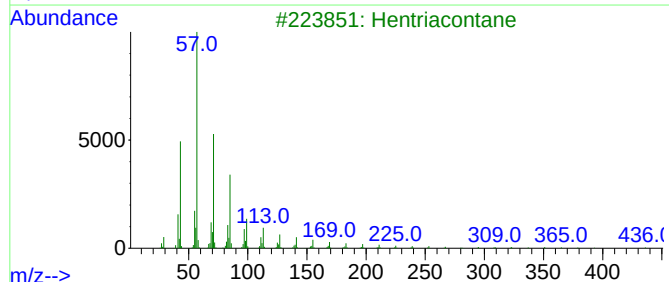
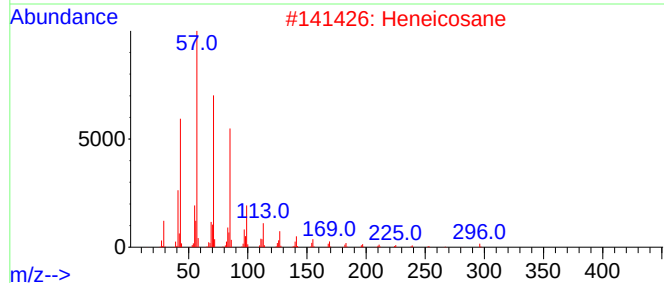
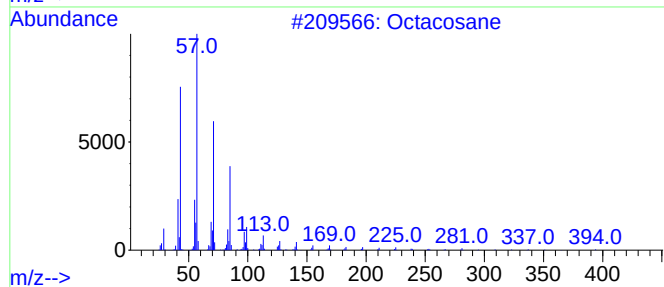
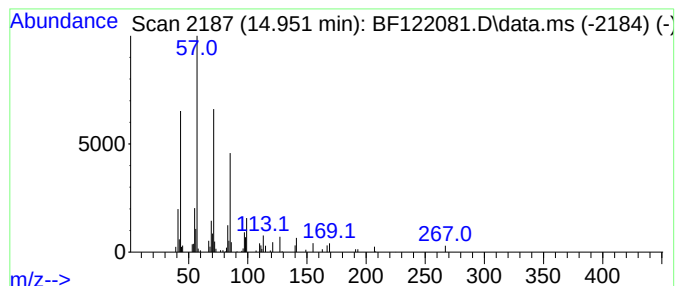
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 Octacosane Concentration Rank 5

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 14.951 | 2.08 ng | 71120 | Perylene-d12     | 15.321 |

| Hit# | of | 5 | Tentative ID          | MW  | MolForm | CAS#        | Qual |
|------|----|---|-----------------------|-----|---------|-------------|------|
| 1    |    |   | Octacosane            | 394 | C28H58  | 000630-02-4 | 91   |
| 2    |    |   | Heneicosane           | 296 | C21H44  | 000629-94-7 | 90   |
| 3    |    |   | Hentriacontane        | 437 | C31H64  | 000630-04-6 | 90   |
| 4    |    |   | Docosane              | 310 | C22H46  | 000629-97-0 | 90   |
| 5    |    |   | Nonadecane, 2-methyl- | 282 | C20H42  | 001560-86-7 | 90   |



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ALS Vial : 9 Sample Multiplier: 1

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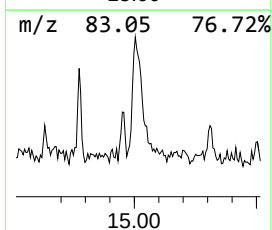
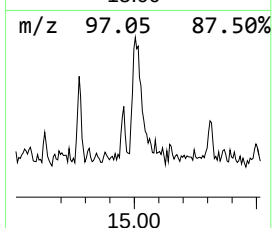
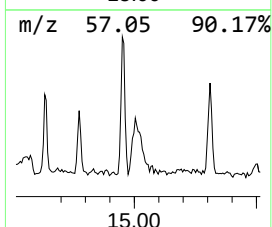
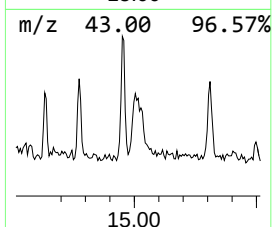
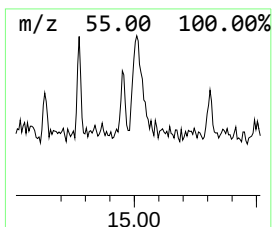
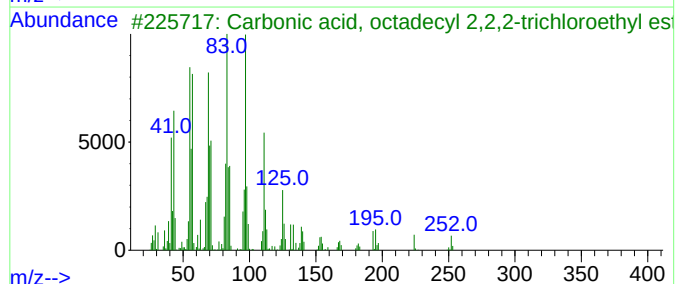
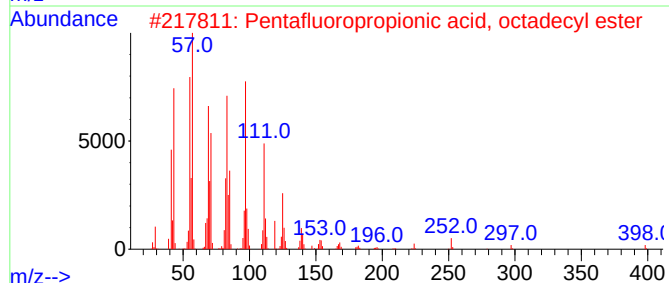
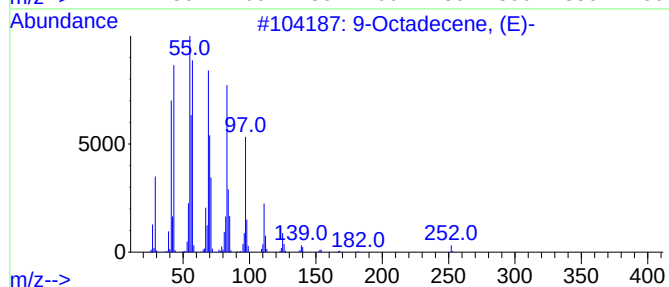
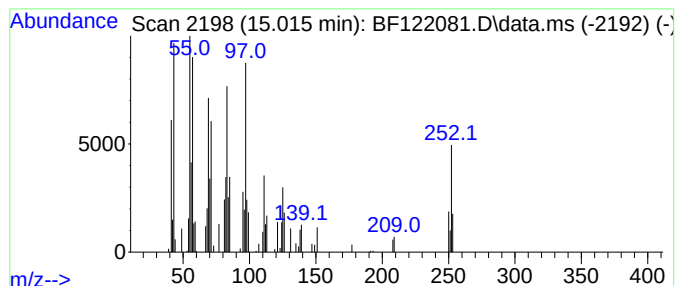
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TIC Library : C:\DATABASE\NIST11.L  
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Peak Number 4 9-Octadecene, (E)- Concentration Rank 2

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 15.015 | 3.23 ng | 110372 | Perylene-d12     | 15.321 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm     | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|-------------|--------------|------|
| 1    |    |   | 9-Octadecene, (E)-                  | 252 | C18H36      | 007206-25-9  | 90   |
| 2    |    |   | Pentafluoropropionic acid, octad... | 416 | C21H37F5O2  | 959261-25-7  | 86   |
| 3    |    |   | Carbonic acid, octadecyl 2,2,2-t... | 444 | C21H39Cl3O3 | 1000314-56-3 | 76   |
| 4    |    |   | Heptafluorobutyric acid, pentade... | 424 | C19H31F7O2  | 959261-23-5  | 70   |
| 5    |    |   | Pentafluoropropionic acid, penta... | 374 | C18H31F5O2  | 959092-08-1  | 70   |



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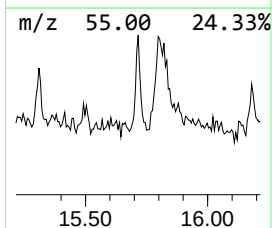
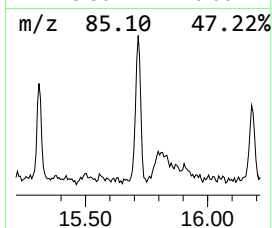
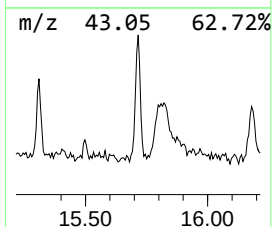
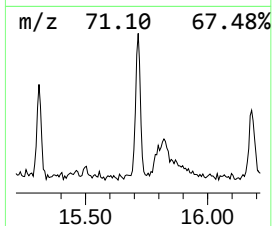
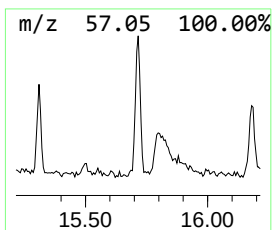
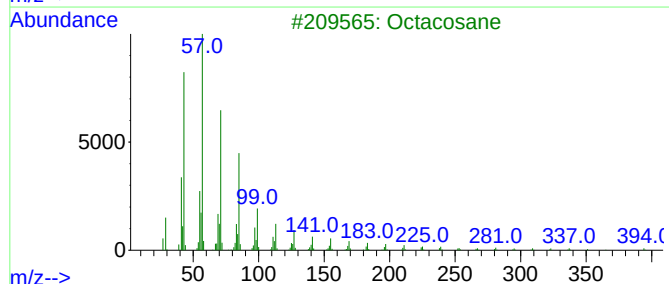
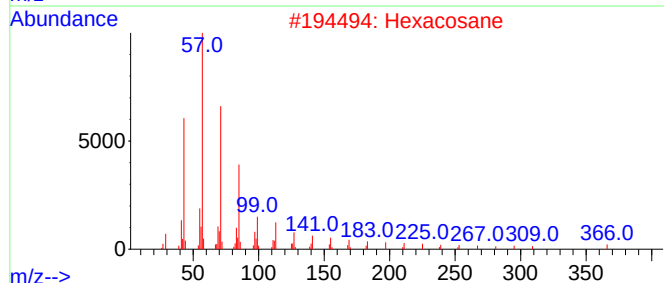
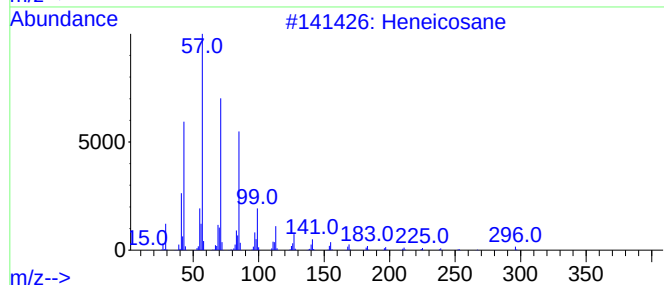
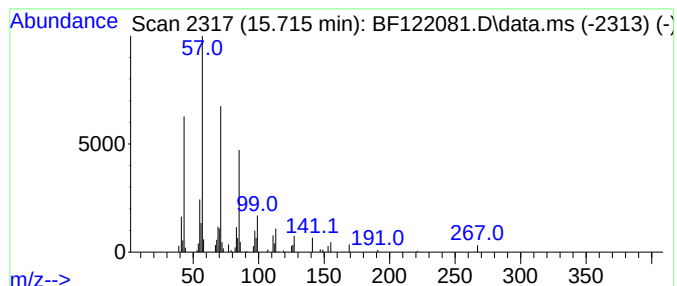
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 Heneicosane Concentration Rank 3

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 15.715 | 2.27 ng | 77566 | Perylene-d12     | 15.321 |

| Hit# | of | 5 | Tentative ID          | MW  | MolForm | CAS#        | Qual |
|------|----|---|-----------------------|-----|---------|-------------|------|
| 1    |    |   | Heneicosane           | 296 | C21H44  | 000629-94-7 | 91   |
| 2    |    |   | Hexacosane            | 366 | C26H54  | 000630-01-3 | 91   |
| 3    |    |   | Octacosane            | 394 | C28H58  | 000630-02-4 | 91   |
| 4    |    |   | Heptadecane, 9-octyl- | 352 | C25H52  | 007225-64-1 | 91   |
| 5    |    |   | Pentacosane           | 352 | C25H52  | 000629-99-2 | 91   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF102220\  
Data File : BF122081.D  
Acq On : 22 Oct 2020 13:56  
Operator : JU/CG  
Sample : L4436-08  
Misc :  
ALS Vial : 9 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
36A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF101220.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| Ethanol, 2-(2-e... | 6.581  | 2.2     | ng    | 67681    | 1                     | 6.728  | 611743 | 20.0 |
| Heptadecyl hept... | 13.721 | 12.9    | ng    | 497471   | 5                     | 13.886 | 771421 | 20.0 |
| Octacosane         | 14.951 | 2.1     | ng    | 71120    | 6                     | 15.321 | 682363 | 20.0 |
| 9-Octadecene, (E)- | 15.015 | 3.2     | ng    | 110372   | 6                     | 15.321 | 682363 | 20.0 |
| Heneicosane        | 15.715 | 2.3     | ng    | 77566    | 6                     | 15.321 | 682363 | 20.0 |