

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF061323\  
 Data File : BF133732.D  
 Acq On : 13 Jun 2023 15:48  
 Operator : CG\JU  
 Sample : 03069-05  
 Misc :  
 ALS Vial : 13 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 SB35B

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-BF060923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133732.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         | 3.875       | 299           | 304         | 309          | rVB      | 15050          | 20196         | 1.64%           | 0.203%        |
| 2         | 5.040       | 498           | 502         | 509          | rVB      | 30795          | 33704         | 2.74%           | 0.340%        |
| 3         | 5.446       | 567           | 571         | 574          | rBV      | 1337651        | 1144250       | 92.94%          | 11.526%       |
| 4         | 6.457       | 739           | 743         | 746          | rBV      | 1190449        | 1058212       | 85.95%          | 10.660%       |
| 5         | 6.834       | 803           | 807         | 810          | rBV      | 611172         | 467797        | 37.99%          | 4.712%        |
| 6         | 7.393       | 898           | 902         | 905          | rBV      | 834740         | 655738        | 53.26%          | 6.605%        |
| 7         | 8.116       | 1021          | 1025        | 1028         | rBV      | 654088         | 494047        | 40.13%          | 4.977%        |
| 8         | 9.192       | 1204          | 1208        | 1211         | rBV      | 1247507        | 985488        | 80.04%          | 9.927%        |
| 9         | 9.875       | 1320          | 1324        | 1327         | rBV      | 564084         | 496381        | 40.32%          | 5.000%        |
| 10        | 10.587      | 1441          | 1445        | 1449         | rBV      | 77997          | 64763         | 5.26%           | 0.652%        |
| 11        | 10.663      | 1454          | 1458        | 1461         | rBV      | 817367         | 754107        | 61.25%          | 7.596%        |
| 12        | 11.363      | 1573          | 1577        | 1580         | rBV      | 717000         | 598335        | 48.60%          | 6.027%        |
| 13        | 11.886      | 1663          | 1666        | 1672         | rBV2     | 116068         | 104375        | 8.48%           | 1.051%        |
| 14        | 12.575      | 1780          | 1783        | 1788         | rBV      | 58671          | 62336         | 5.06%           | 0.628%        |
| 15        | 12.675      | 1797          | 1800        | 1803         | rBV4     | 23603          | 26581         | 2.16%           | 0.268%        |
| 16        | 12.804      | 1819          | 1822        | 1828         | rVB      | 56030          | 53747         | 4.37%           | 0.541%        |
| 17        | 12.951      | 1843          | 1847        | 1850         | rBV      | 1505228        | 1231209       | 100.00%         | 12.402%       |
| 18        | 13.527      | 1942          | 1945        | 1948         | rVB      | 16588          | 16172         | 1.31%           | 0.163%        |
| 19        | 13.851      | 1996          | 2000        | 2006         | rBV2     | 163098         | 209382        | 17.01%          | 2.109%        |
| 20        | 14.010      | 2022          | 2027        | 2030         | rBV      | 721270         | 675292        | 54.85%          | 6.802%        |
| 21        | 14.033      | 2030          | 2031        | 2033         | rVB      | 33644          | 17490         | 1.42%           | 0.176%        |
| 22        | 14.169      | 2052          | 2054        | 2057         | rVB      | 31481          | 30611         | 2.49%           | 0.308%        |
| 23        | 14.480      | 2104          | 2107        | 2114         | rBV2     | 95356          | 137284        | 11.15%          | 1.383%        |
| 24        | 14.927      | 2181          | 2183        | 2189         | rVB      | 62716          | 67200         | 5.46%           | 0.677%        |
| 25        | 15.122      | 2213          | 2216        | 2219         | rBV      | 91533          | 100196        | 8.14%           | 1.009%        |
| 26        | 15.474      | 2271          | 2276        | 2280         | rBV      | 339681         | 422461        | 34.31%          | 4.256%        |

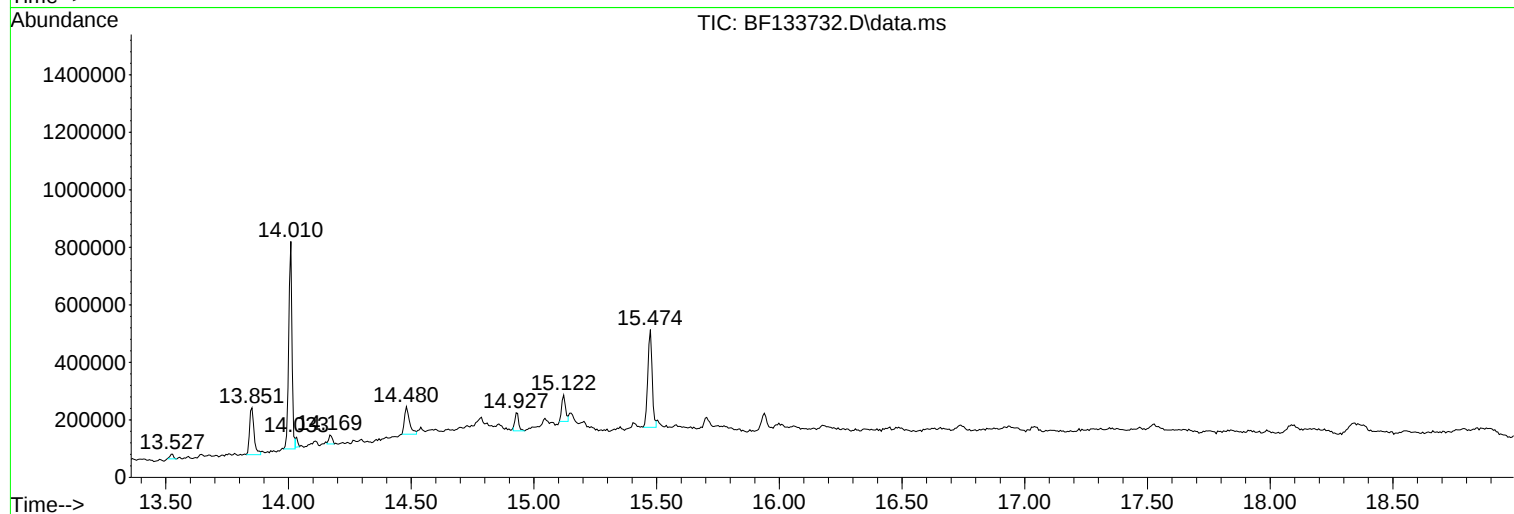
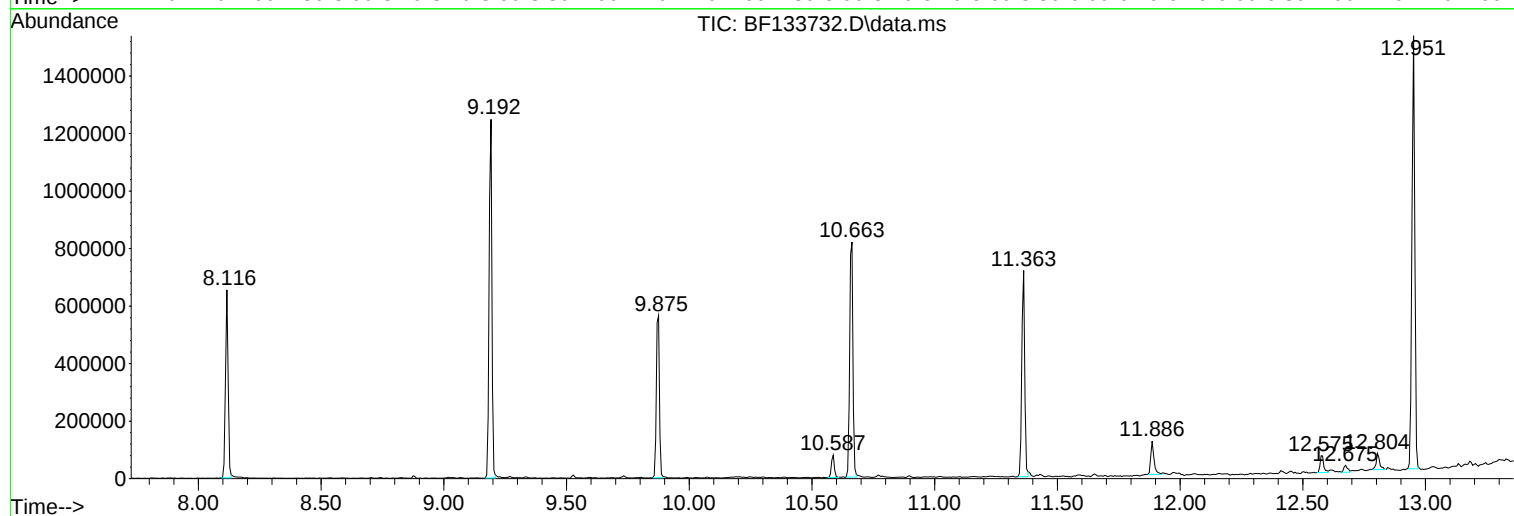
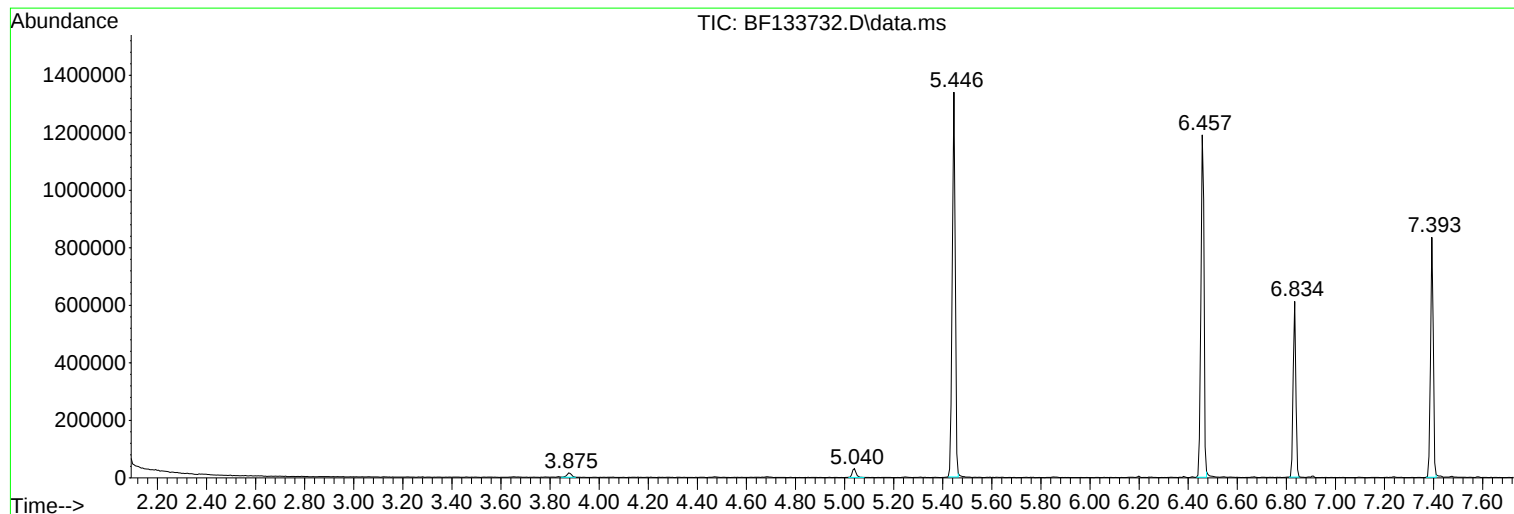
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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF060923.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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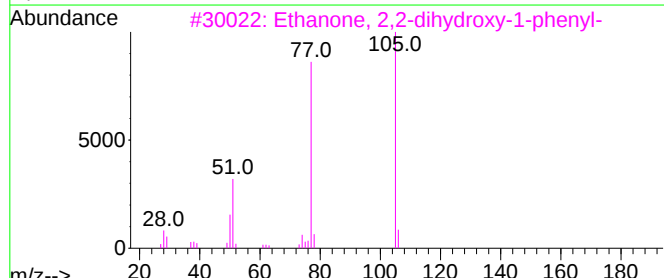
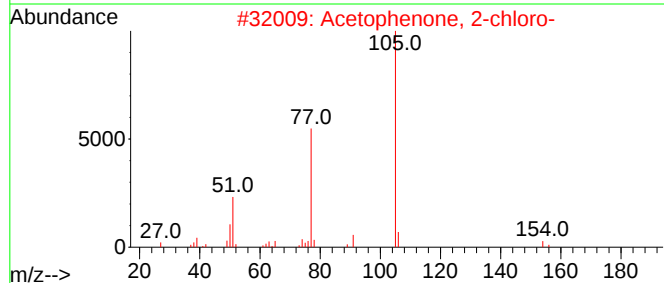
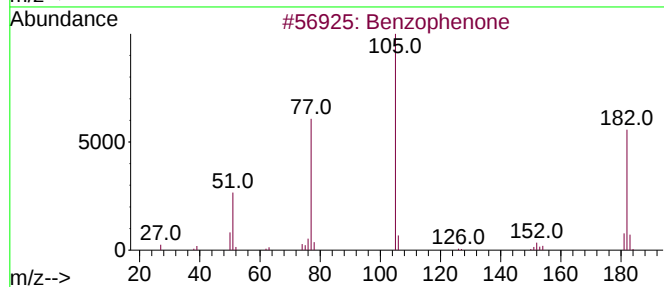
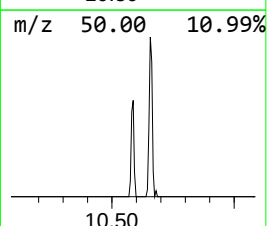
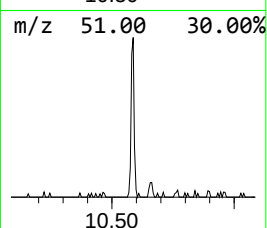
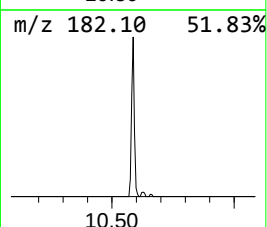
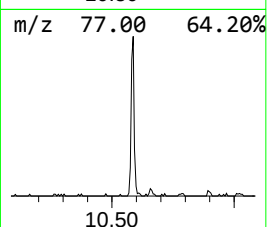
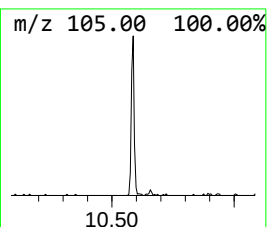
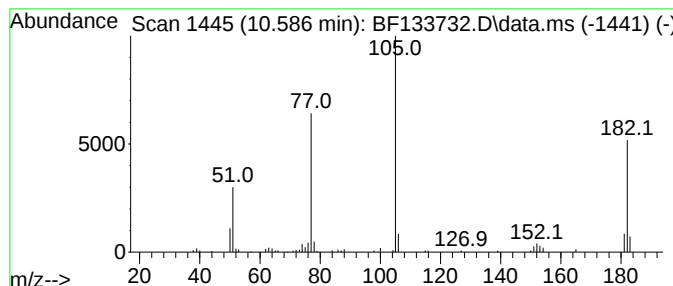
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF060923.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 Benzophenone Concentration Rank 6

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.  |
|--------|---------|-------|------------------|-------|
| 10.586 | 2.61 ng | 64763 | Acenaphthene-d10 | 9.875 |

| Hit# | of | 5 | Tentative ID                       | MW  | MolForm  | CAS#        | Qual |
|------|----|---|------------------------------------|-----|----------|-------------|------|
| 1    |    |   | Benzophenone                       | 182 | C13H10O  | 000119-61-9 | 95   |
| 2    |    |   | Acetophenone, 2-chloro-            | 154 | C8H7ClO  | 000532-27-4 | 52   |
| 3    |    |   | Ethanone, 2,2-dihydroxy-1-phenyl-  | 152 | C8H8O3   | 001075-06-5 | 52   |
| 4    |    |   | Benzoic acid, phenyl ester         | 198 | C13H10O2 | 000093-99-2 | 50   |
| 5    |    |   | Benzenepropanenitrile, .beta.-oxo- | 145 | C9H7NO   | 000614-16-4 | 50   |



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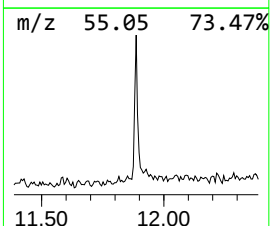
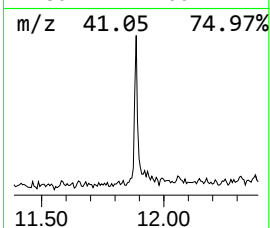
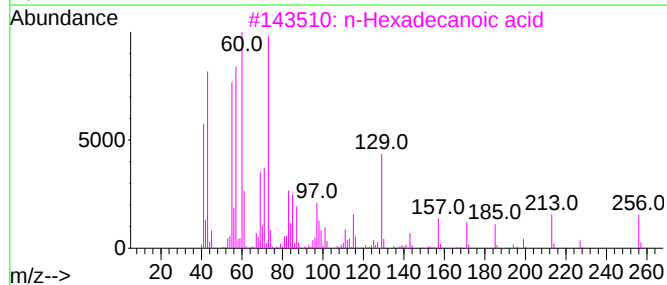
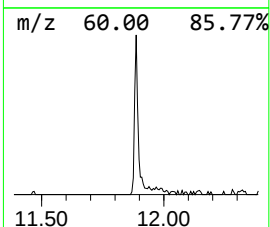
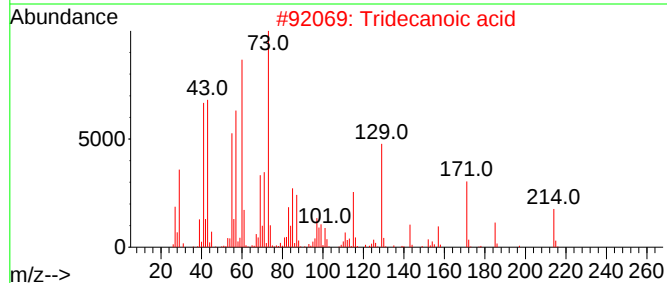
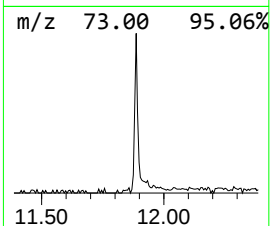
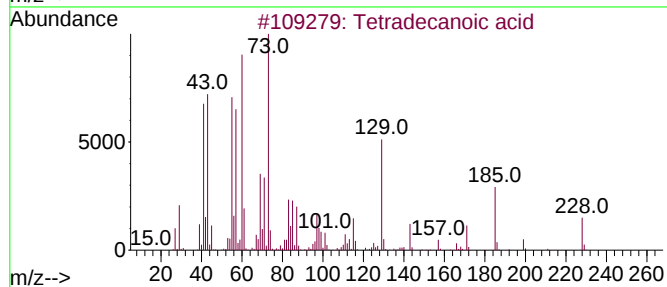
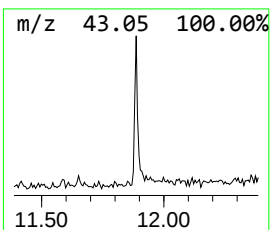
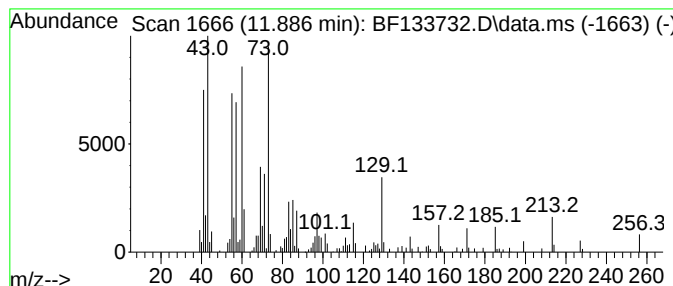
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF060923.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 2 Tetradecanoic acid Concentration Rank 4

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 11.886 | 3.49 ng | 104375 | Phenanthrene-d10 | 11.363 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 97   |
| 2    |    |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 95   |
| 3    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 95   |
| 4    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 90   |
| 5    |    |   | Undecanoic acid     | 186 | C11H22O2 | 000112-37-8 | 76   |



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ALS Vial : 13 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
SB35B

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF060923.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

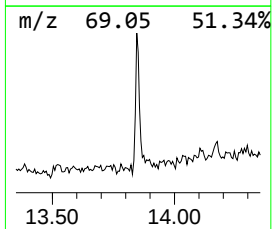
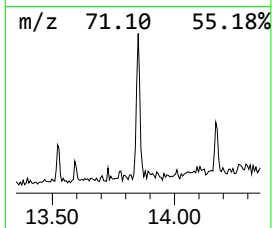
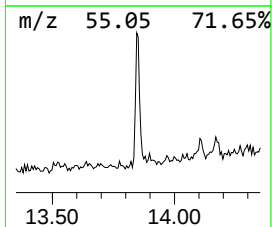
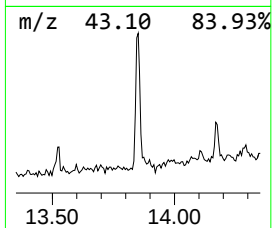
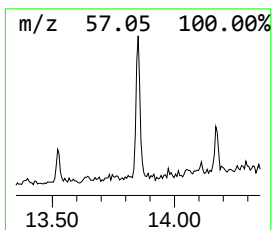
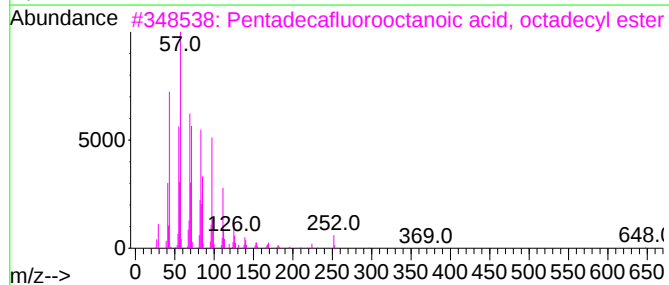
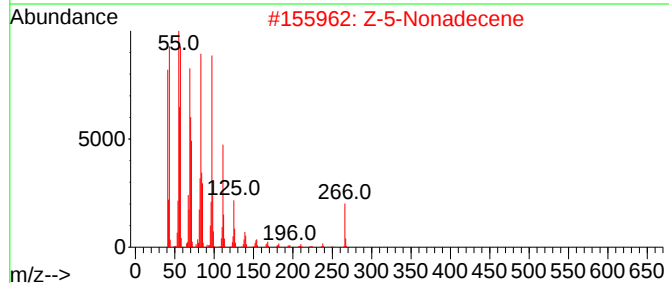
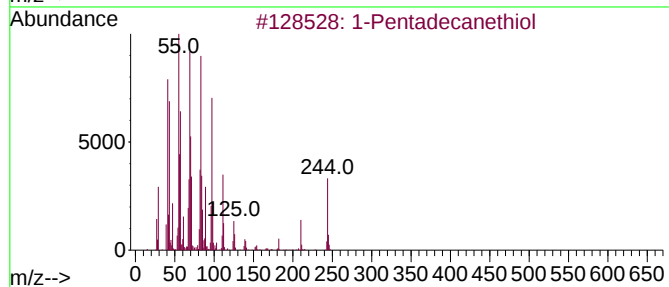
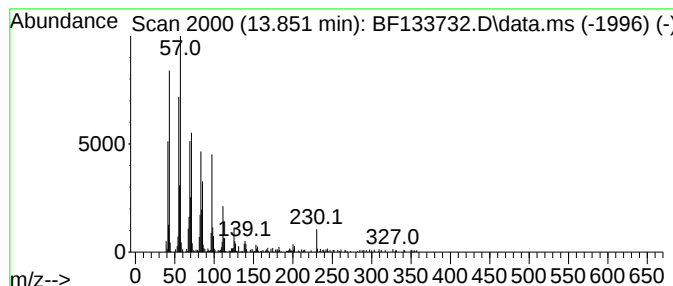
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 1-Pentadecanethiol Concentration Rank 1

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 13.851 | 6.20 ng | 209382 | Chrysene-d12     | 14.010 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm     | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|-------------|--------------|------|
| 1    |    |   | 1-Pentadecanethiol                  | 244 | C15H32S     | 025276-70-4  | 96   |
| 2    |    |   | Z-5-Nonadecene                      | 266 | C19H38      | 1000131-11-8 | 95   |
| 3    |    |   | Pentadecafluorooctanoic acid, oc... | 666 | C26H37F15O2 | 1000406-04-8 | 94   |
| 4    |    |   | Pentadecafluorooctanoic acid, he... | 652 | C25H35F15O2 | 1000406-04-7 | 91   |
| 5    |    |   | Oxalic acid, octadecyl propyl ester | 384 | C23H44O4    | 1000309-27-0 | 91   |



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ClientSampleId :  
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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF060923.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

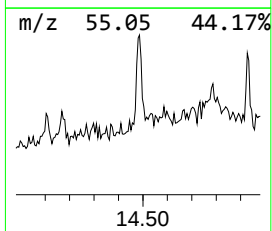
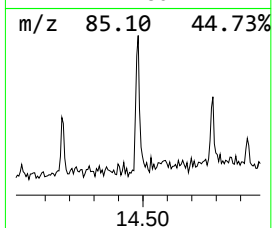
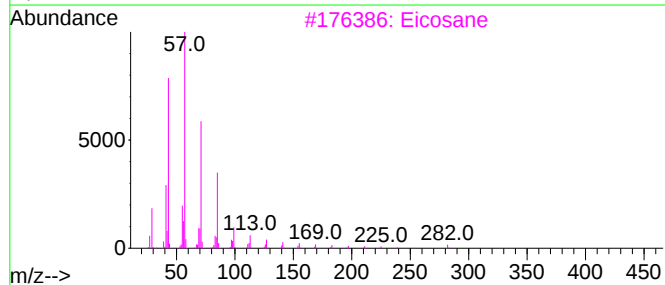
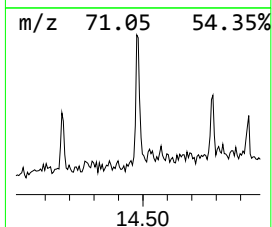
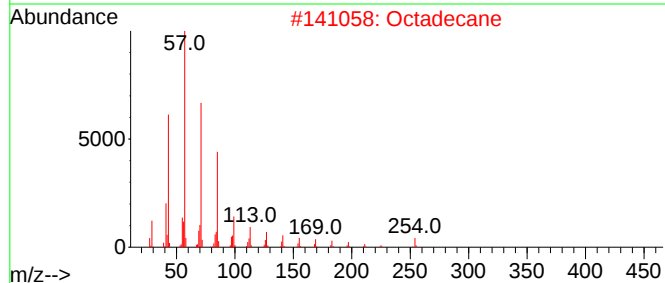
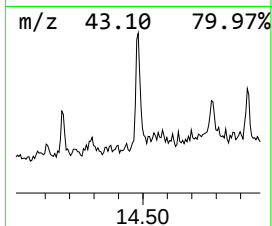
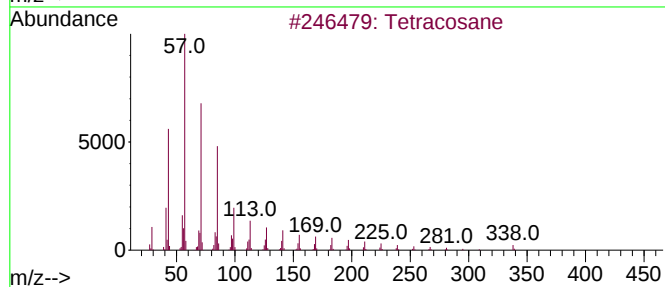
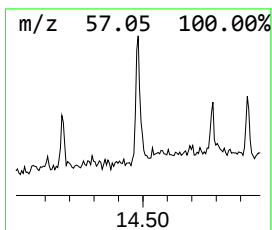
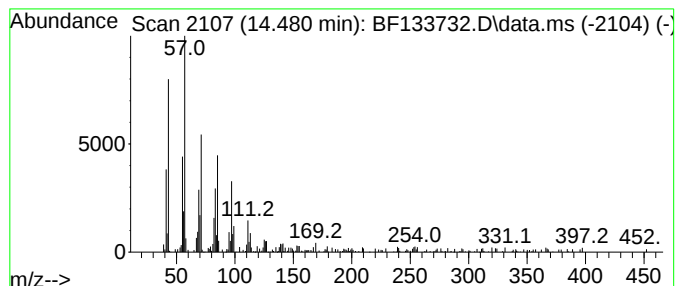
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 Tetracosane Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 14.480 | 4.07 ng | 137284 | Chrysene-d12     | 14.010 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|-----------|--------------|------|
| 1    |    |   | Tetracosane                         | 338 | C24H50    | 000646-31-1  | 92   |
| 2    |    |   | Octadecane                          | 254 | C18H38    | 000593-45-3  | 91   |
| 3    |    |   | Eicosane                            | 282 | C20H42    | 000112-95-8  | 91   |
| 4    |    |   | Tricosane                           | 324 | C23H48    | 000638-67-5  | 87   |
| 5    |    |   | Sulfurous acid, octadecyl 2-prop... | 376 | C21H44O3S | 1000309-12-7 | 83   |



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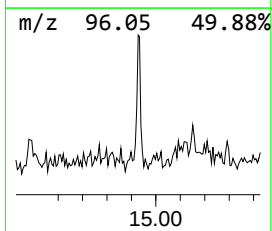
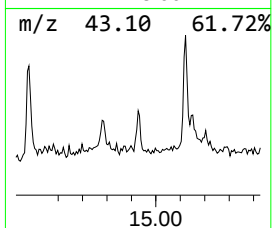
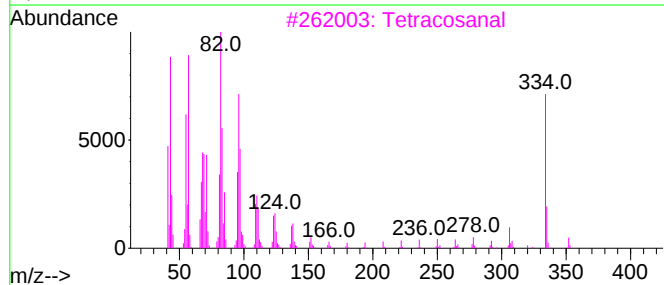
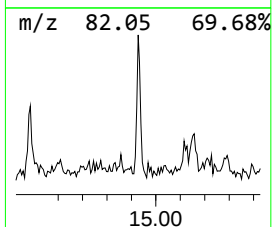
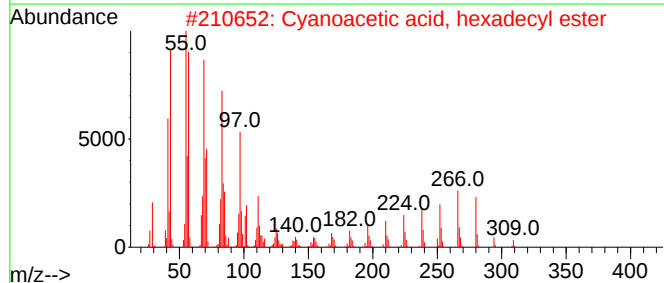
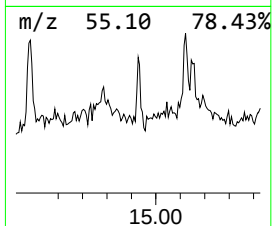
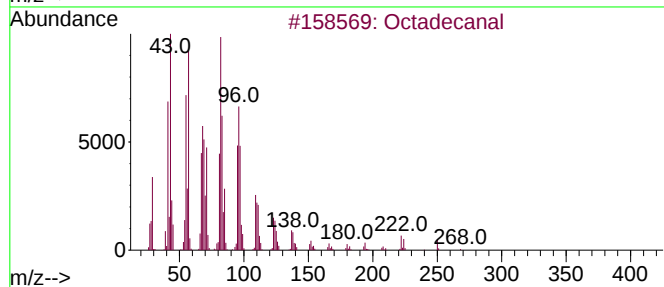
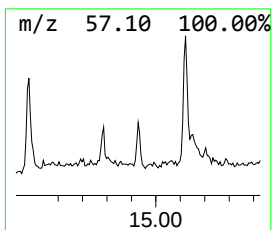
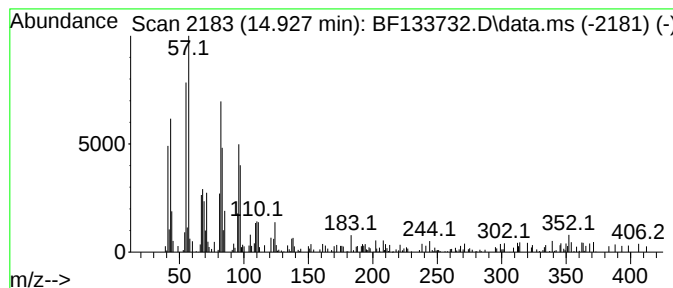
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 6 Octadecanal Concentration Rank 5

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 14.927 | 3.18 ng | 67200 | Perylene-d12     | 15.474 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|-----------|--------------|------|
| 1    |    |   | Octadecanal                         | 268 | C18H36O   | 000638-66-4  | 58   |
| 2    |    |   | Cyanoacetic acid, hexadecyl ester   | 309 | C19H35NO2 | 1000406-23-3 | 50   |
| 3    |    |   | Tetracosanal                        | 352 | C24H48O   | 057866-08-7  | 50   |
| 4    |    |   | Z-11(13-Methyl)tetradecen-1-ol a... | 268 | C17H32O2  | 1000131-33-3 | 49   |
| 5    |    |   | 7-Azabicyclo[4.1.0]heptane, 1-me... | 111 | C7H13N    | 025022-25-7  | 45   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF061323\  
Data File : BF133732.D  
Acq On : 13 Jun 2023 15:48  
Operator : CG\JU  
Sample : 03069-05  
Misc :  
ALS Vial : 13 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
SB35B

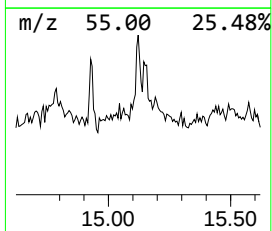
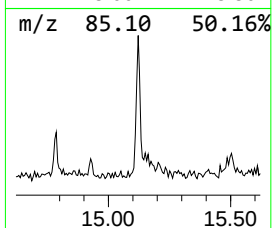
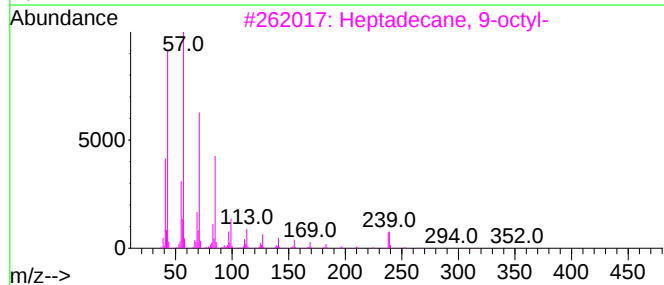
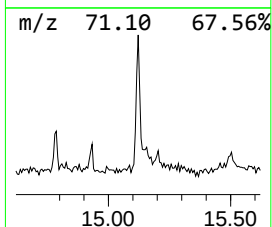
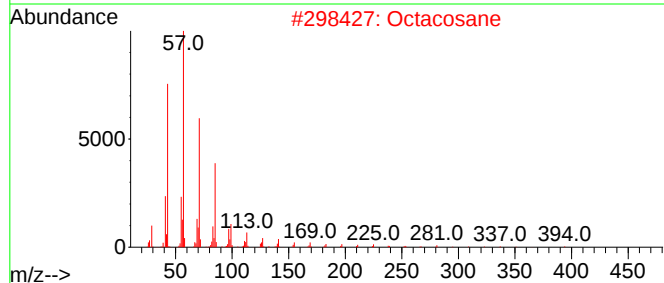
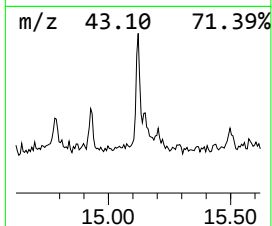
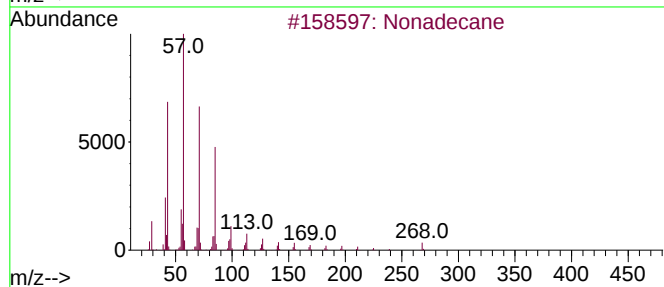
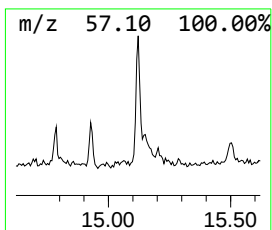
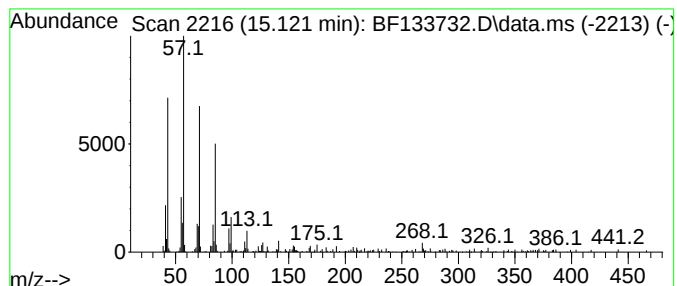
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 7 Nonadecane Concentration Rank 2

| R.T.      | EstConc                  | Area   | Relative to ISTD | R.T.        |      |
|-----------|--------------------------|--------|------------------|-------------|------|
| 15.121    | 4.74 ng                  | 100196 | Perylene-d12     | 15.474      |      |
| Hit# of 5 | Tentative ID             | MW     | MolForm          | CAS#        | Qual |
| 1         | Nonadecane               | 268    | C19H40           | 000629-92-5 | 91   |
| 2         | Octacosane               | 394    | C28H58           | 000630-02-4 | 87   |
| 3         | Heptadecane, 9-octyl-    | 352    | C25H52           | 007225-64-1 | 87   |
| 4         | Hexadecane, 1-iodo-      | 352    | C16H33I          | 000544-77-4 | 72   |
| 5         | Undecane, 2,10-dimethyl- | 184    | C13H28           | 017301-27-8 | 72   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF061323\  
Data File : BF133732.D  
Acq On : 13 Jun 2023 15:48  
Operator : CG\JU  
Sample : 03069-05  
Misc :  
ALS Vial : 13 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
SB35B

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF060923.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 |
| Benzophenone       | 10.586 | 2.6     | ng    | 64763    | 3                     | 9.875  | 496381 | 20.0 |
| Tetradecanoic acid | 11.886 | 3.5     | ng    | 104375   | 4                     | 11.363 | 598335 | 20.0 |
| 1-Pentadecanethiol | 13.851 | 6.2     | ng    | 209382   | 5                     | 14.010 | 675292 | 20.0 |
| Tetracosane        | 14.480 | 4.1     | ng    | 137284   | 5                     | 14.010 | 675292 | 20.0 |
| Octadecanal        | 14.927 | 3.2     | ng    | 67200    | 6                     | 15.474 | 422461 | 20.0 |
| Nonadecane         | 15.121 | 4.7     | ng    | 100196   | 6                     | 15.474 | 422461 | 20.0 |