

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF101323\  
 Data File : BF135758.D  
 Acq On : 13 Oct 2023 18:08  
 Operator : CG\JU  
 Sample : 04844-05  
 Misc :  
 ALS Vial : 13 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 OR-603-COMP-06

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-BF101323.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135758.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         | 4.969       | 487           | 490         | 506          | rBV      | 103467         | 156765        | 6.33%           | 0.861%        |
| 2         | 5.369       | 555           | 558         | 587          | rBV      | 2111911        | 2476351       | 100.00%         | 13.598%       |
| 3         | 6.387       | 728           | 731         | 759          | rBV      | 2071978        | 2321030       | 93.73%          | 12.745%       |
| 4         | 6.734       | 787           | 790         | 800          | rVB      | 696225         | 641388        | 25.90%          | 3.522%        |
| 5         | 7.304       | 884           | 887         | 901          | rBV      | 1669318        | 1471989       | 59.44%          | 8.083%        |
| 6         | 8.016       | 1005          | 1008        | 1016         | rVB      | 932786         | 773365        | 31.23%          | 4.247%        |
| 7         | 8.604       | 1105          | 1108        | 1112         | rBV      | 45089          | 36612         | 1.48%           | 0.201%        |
| 8         | 9.092       | 1188          | 1191        | 1195         | rBV      | 2746631        | 2436731       | 98.40%          | 13.381%       |
| 9         | 9.175       | 1202          | 1205        | 1207         | rVB      | 44554          | 38480         | 1.55%           | 0.211%        |
| 10        | 9.216       | 1208          | 1212        | 1216         | rBV      | 41914          | 40884         | 1.65%           | 0.225%        |
| 11        | 9.704       | 1292          | 1295        | 1300         | rBV      | 31215          | 27154         | 1.10%           | 0.149%        |
| 12        | 9.775       | 1303          | 1307        | 1312         | rBV      | 988742         | 839897        | 33.92%          | 4.612%        |
| 13        | 10.204      | 1373          | 1380        | 1383         | rBV2     | 28755          | 33882         | 1.37%           | 0.186%        |
| 14        | 10.569      | 1438          | 1442        | 1458         | rBV      | 1548881        | 1451829       | 58.63%          | 7.972%        |
| 15        | 11.269      | 1558          | 1561        | 1564         | rBV      | 982733         | 821895        | 33.19%          | 4.513%        |
| 16        | 11.292      | 1564          | 1565        | 1570         | rVB      | 50808          | 41544         | 1.68%           | 0.228%        |
| 17        | 11.804      | 1649          | 1652        | 1661         | rBV      | 217275         | 246573        | 9.96%           | 1.354%        |
| 18        | 12.498      | 1767          | 1770        | 1779         | rBV      | 37591          | 53571         | 2.16%           | 0.294%        |
| 19        | 12.598      | 1784          | 1787        | 1795         | rBV3     | 33216          | 56178         | 2.27%           | 0.308%        |
| 20        | 12.727      | 1807          | 1809        | 1813         | rVB      | 29718          | 28229         | 1.14%           | 0.155%        |
| 21        | 12.863      | 1828          | 1832        | 1836         | rBV      | 1998275        | 1922692       | 77.64%          | 10.558%       |
| 22        | 13.351      | 1910          | 1915        | 1926         | rBV      | 509764         | 501012        | 20.23%          | 2.751%        |
| 23        | 13.439      | 1926          | 1930        | 1933         | rBV2     | 26057          | 30284         | 1.22%           | 0.166%        |
| 24        | 13.768      | 1983          | 1986        | 1991         | rBV      | 29878          | 28598         | 1.15%           | 0.157%        |
| 25        | 13.851      | 1991          | 2000        | 2006         | rBV7     | 25842          | 86734         | 3.50%           | 0.476%        |
| 26        | 13.933      | 2011          | 2014        | 2025         | rVB      | 541003         | 533308        | 21.54%          | 2.929%        |
| 27        | 14.092      | 2037          | 2041        | 2044         | rBV      | 30197          | 31165         | 1.26%           | 0.171%        |
| 28        | 14.398      | 2089          | 2093        | 2097         | rBV      | 43080          | 40046         | 1.62%           | 0.220%        |
| 29        | 14.704      | 2140          | 2145        | 2150         | rBV      | 56877          | 71995         | 2.91%           | 0.395%        |
| 30        | 14.774      | 2153          | 2157        | 2162         | rVB      | 42276          | 48283         | 1.95%           | 0.265%        |
| 31        | 15.033      | 2197          | 2201        | 2206         | rVB      | 68187          | 88873         | 3.59%           | 0.488%        |
| 32        | 15.410      | 2260          | 2265        | 2276         | rBV      | 493963         | 662229        | 26.74%          | 3.636%        |
| 33        | 15.845      | 2333          | 2339        | 2346         | rBV2     | 45724          | 80412         | 3.25%           | 0.442%        |
| 34        | 16.351      | 2420          | 2425        | 2431         | rBV4     | 26682          | 50725         | 2.05%           | 0.279%        |
| 35        | 16.951      | 2522          | 2527        | 2534         | rVB5     | 18957          | 40180         | 1.62%           | 0.221%        |

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Sample : 04844-05  
Misc :  
ALS Vial : 13 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
OR-603-COMP-06

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-BF101323.M  
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

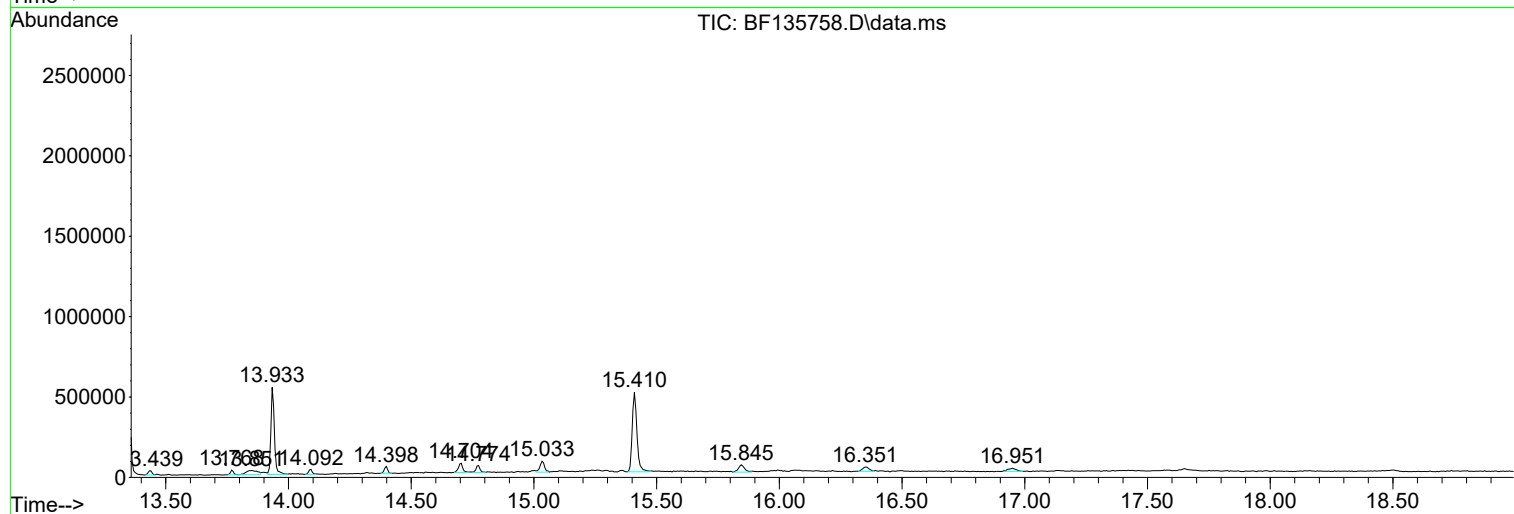
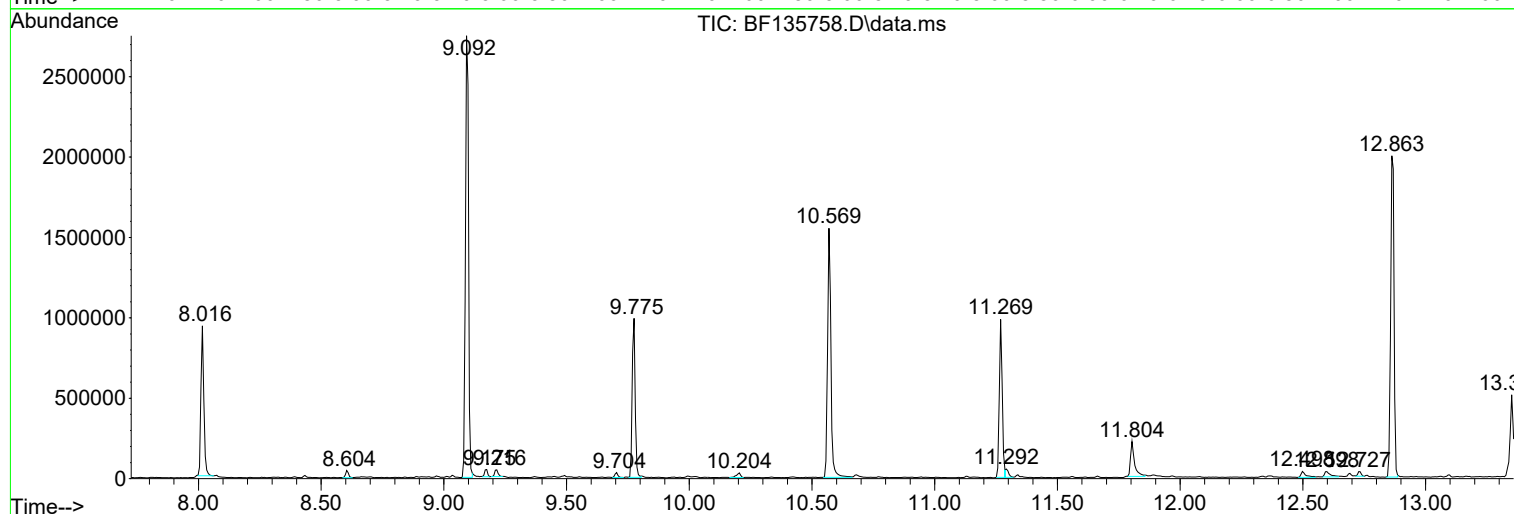
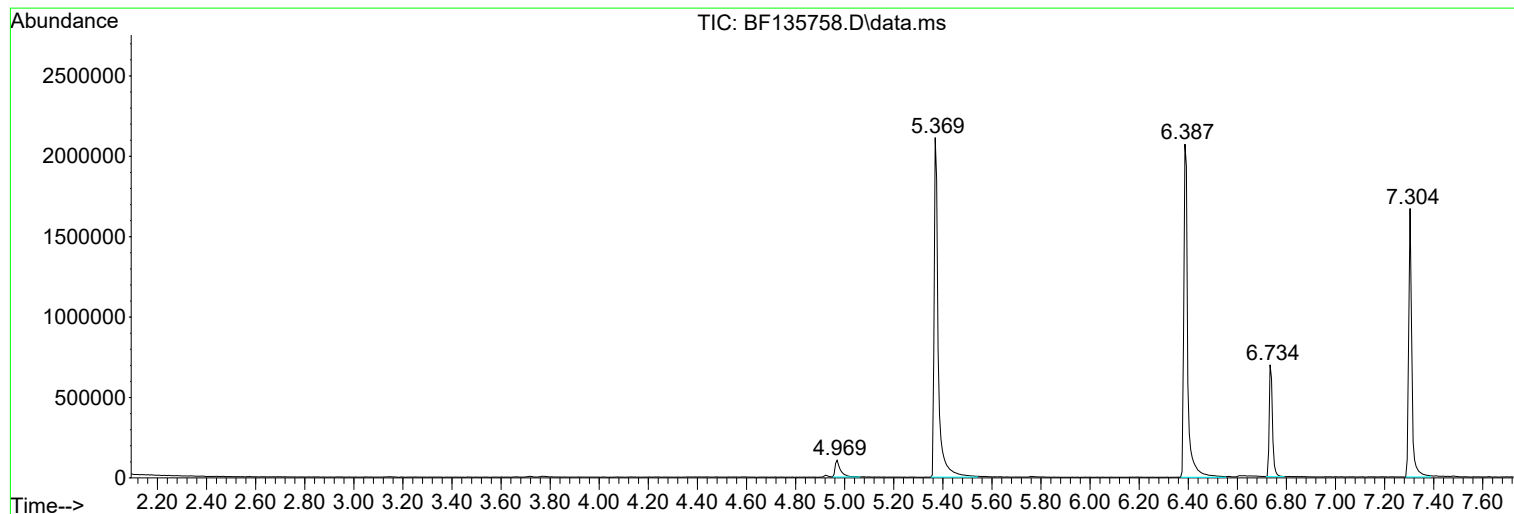
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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF101323.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Operator : CG\JU  
Sample : 04844-05  
Misc :  
ALS Vial : 13 Sample Multiplier: 1

Instrument :  
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ClientSampleId :  
OR-603-COMP-06

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF101323.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

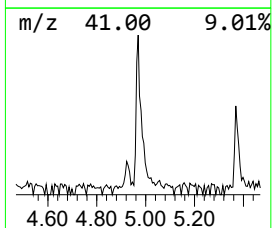
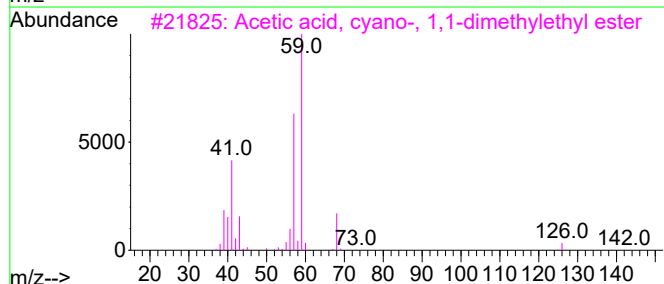
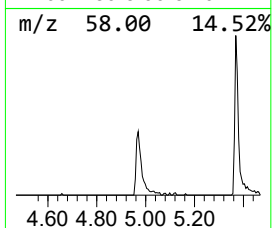
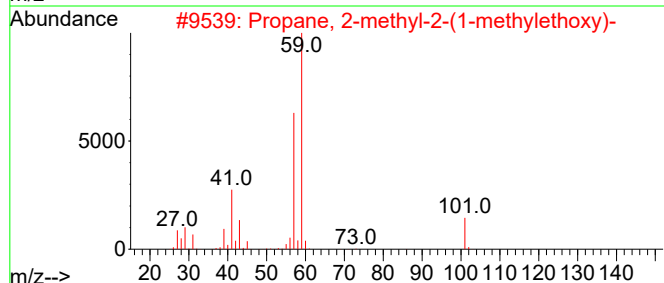
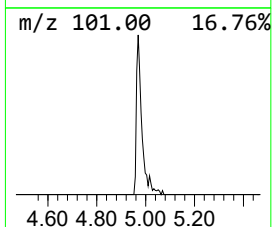
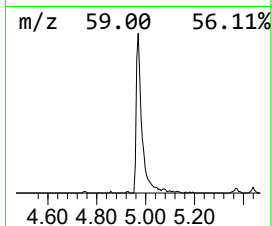
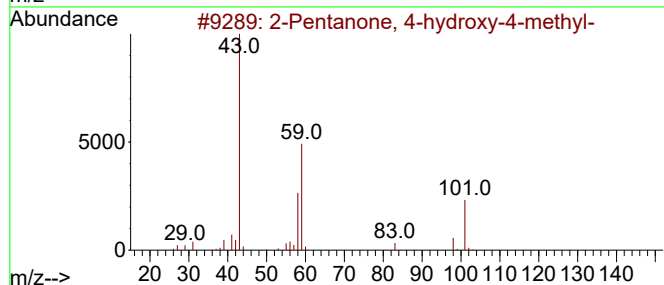
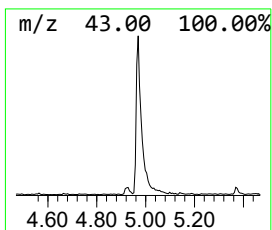
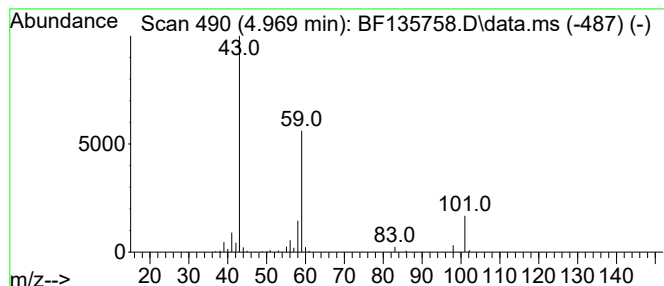
TIC Library : C:\Database\NIST0.L  
TIC Integration Parameters: LSCINT.P

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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.  |
|-------|---------|--------|------------------------|-------|
| 4.969 | 4.89 ng | 156765 | 1,4-Dichlorobenzene-d4 | 6.734 |

| Hit# | of                                  | 5   | Tentative ID | MW          | MolForm | CAS# | Qual |
|------|-------------------------------------|-----|--------------|-------------|---------|------|------|
| 1    | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2      | 000123-42-2 | 64      |      |      |
| 2    | Propane, 2-methyl-2-(1-methyleth... | 116 | C7H16O       | 017348-59-3 | 53      |      |      |
| 3    | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2     | 001116-98-9 | 32      |      |      |
| 4    | 2-Hexanol, 2-methyl-                | 116 | C7H16O       | 000625-23-0 | 28      |      |      |
| 5    | 1-Propen-2-ol, acetate              | 100 | C5H8O2       | 000108-22-5 | 10      |      |      |



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OR-603-COMP-06

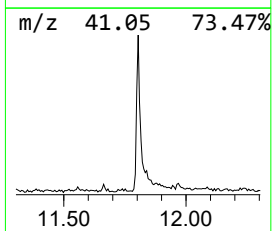
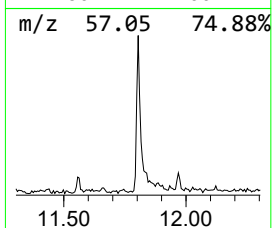
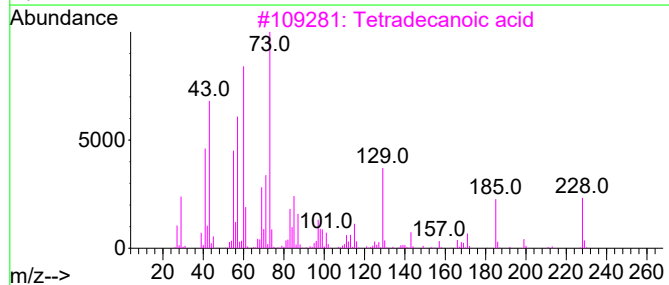
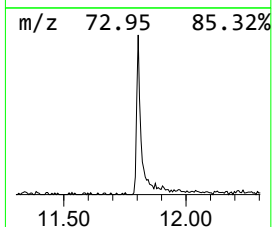
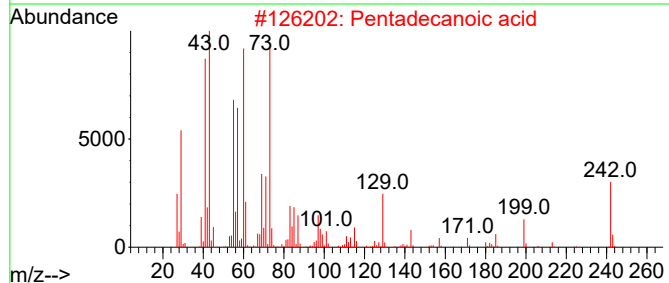
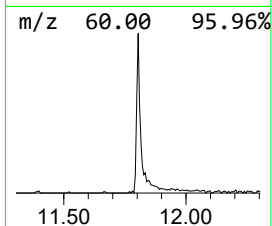
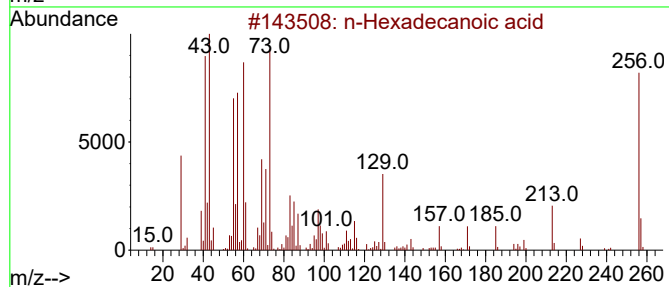
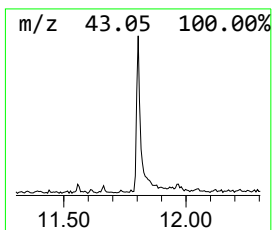
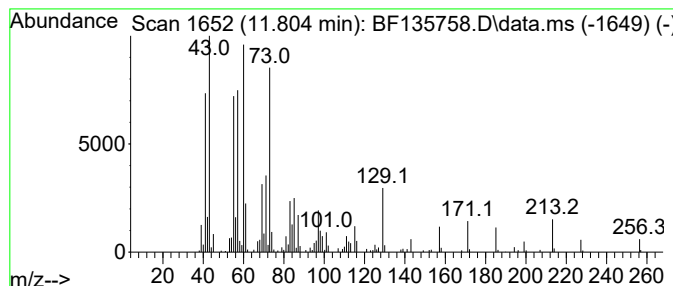
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF101323.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 11.804 | 6.00 ng | 246573 | Phenanthrene-d10 | 11.269 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 98   |
| 2    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 87   |
| 3    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 72   |
| 4    |    |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 72   |
| 5    |    |   | Dodecanoic acid     | 200 | C12H24O2 | 000143-07-7 | 59   |



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ALS Vial : 13 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
OR-603-COMP-06

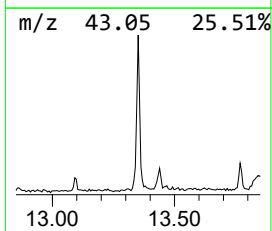
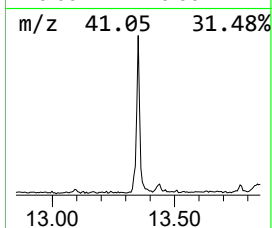
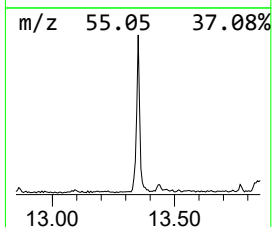
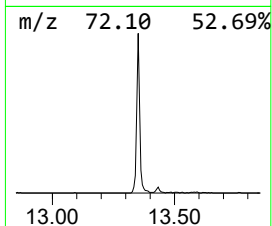
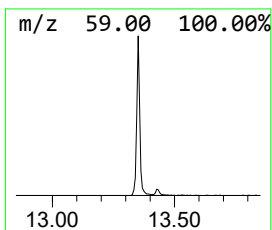
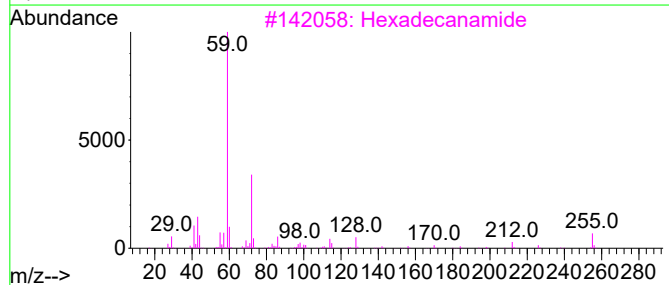
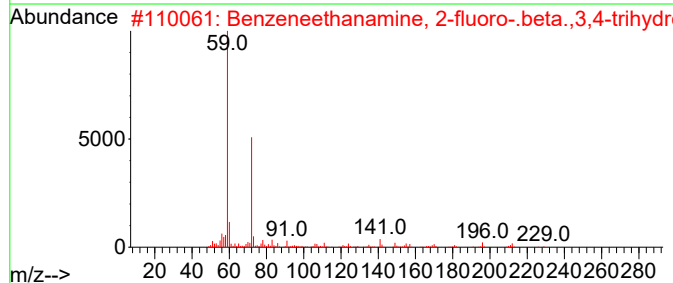
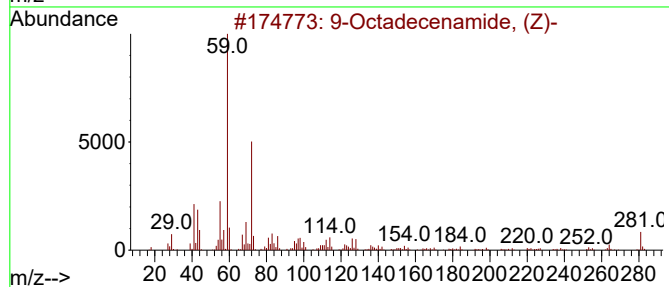
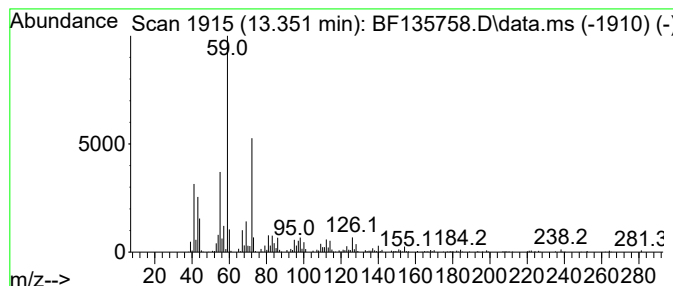
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF101323.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 3 9-Octadecenamide, (Z)- Concentration Rank 1

| R.T.   | EstConc  | Area   | Relative to ISTD | R.T.   |
|--------|----------|--------|------------------|--------|
| 13.351 | 18.79 ng | 501012 | Chrysene-d12     | 13.933 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|------------|-------------|------|
| 1    |    |   | 9-Octadecenamide, (Z)-              | 281 | C18H35NO   | 000301-02-0 | 94   |
| 2    |    |   | Benzeneethanamine, 2-fluoro-.bet... | 229 | C11H16FNO3 | 061338-98-5 | 64   |
| 3    |    |   | Hexadecanamide                      | 255 | C16H33NO   | 000629-54-9 | 64   |
| 4    |    |   | Pentanamide                         | 101 | C5H11NO    | 000626-97-1 | 59   |
| 5    |    |   | Nonanamide                          | 157 | C9H19NO    | 001120-07-6 | 59   |



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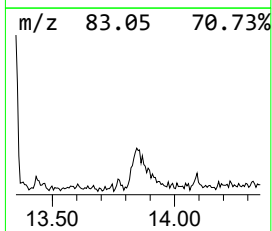
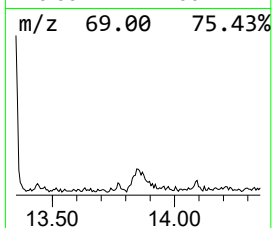
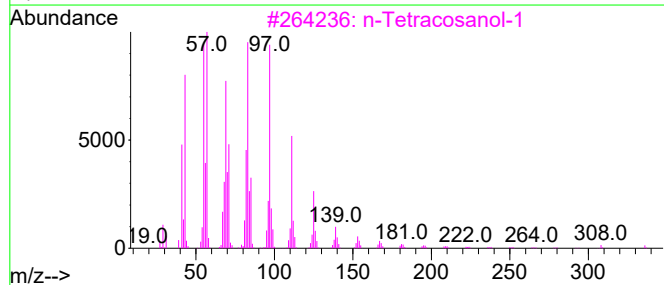
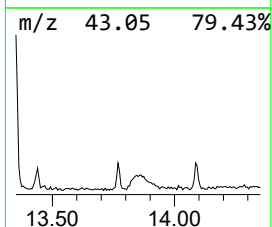
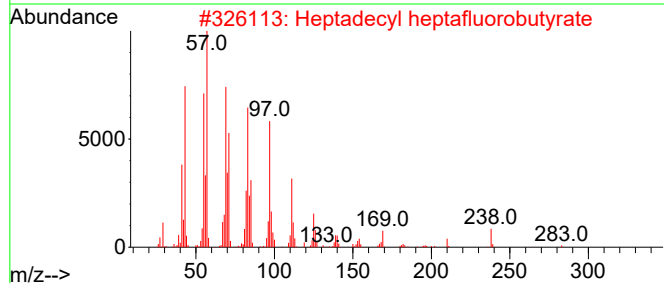
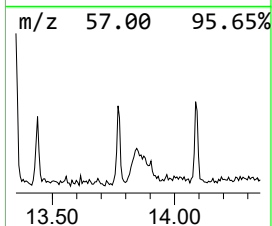
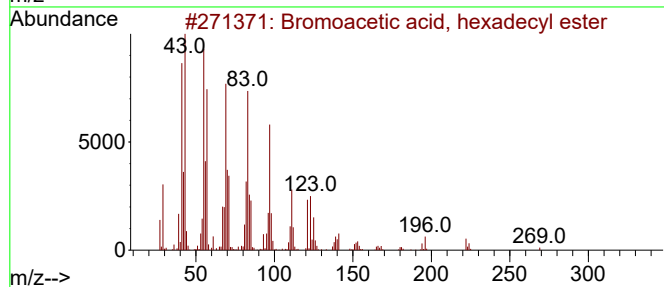
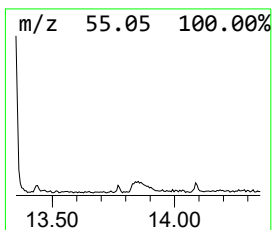
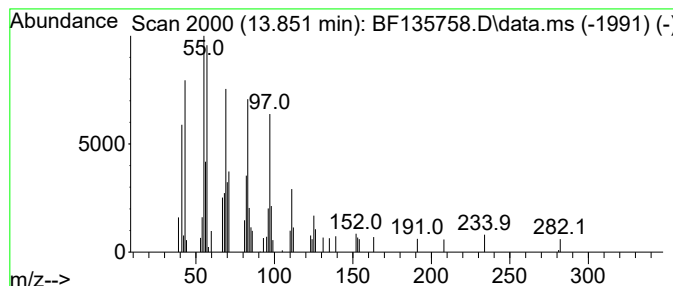
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF101323.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L  
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Peak Number 4 Bromoacetic acid, hexadecyl... Concentration Rank 4

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 13.851 | 3.25 ng | 86734 | Chrysene-d12     | 13.933 |

| Hit# | of | 5 | Tentative ID                      | MW  | MolForm    | CAS#        | Qual |
|------|----|---|-----------------------------------|-----|------------|-------------|------|
| 1    |    |   | Bromoacetic acid, hexadecyl ester | 362 | C18H35BrO2 | 005454-48-8 | 90   |
| 2    |    |   | Heptadecyl heptafluorobutyrate    | 452 | C21H35F7O2 | 959085-66-6 | 90   |
| 3    |    |   | n-Tetracosanol-1                  | 354 | C24H50O    | 000506-51-4 | 87   |
| 4    |    |   | 1-Hexadecanol                     | 242 | C16H34O    | 036653-82-4 | 87   |
| 5    |    |   | 17-Pentatriacontene               | 491 | C35H70     | 006971-40-0 | 87   |



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ClientSampleId :  
OR-603-COMP-06

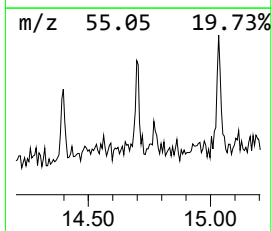
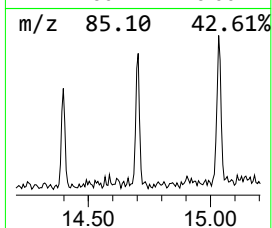
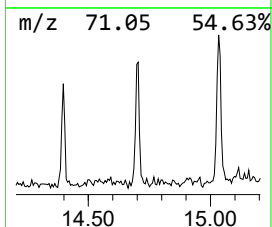
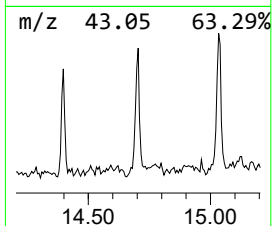
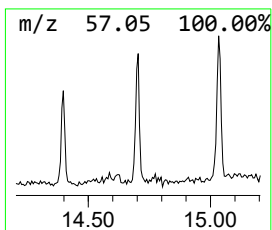
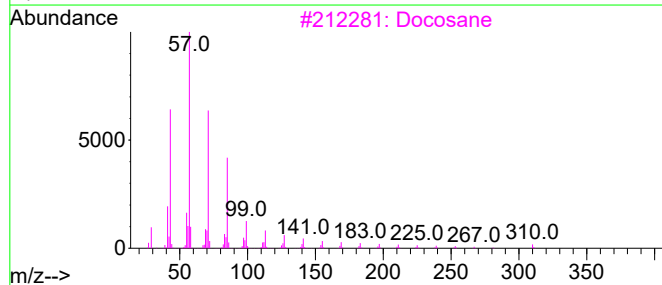
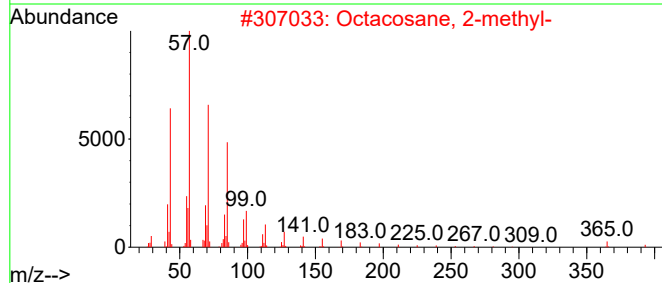
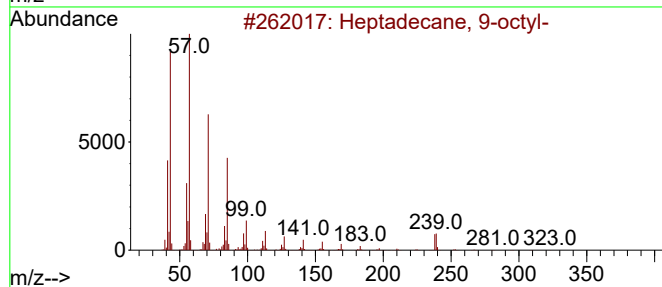
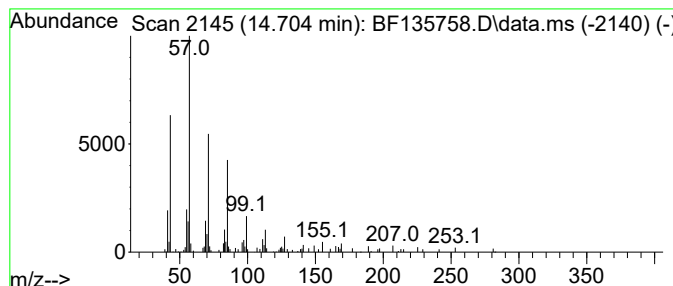
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 Heptadecane, 9-octyl- Concentration Rank 7

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 14.704 | 2.17 ng | 71995 | Perylene-d12     | 15.410 |

| Hit# | of | 5 | Tentative ID          | MW  | MolForm | CAS#        | Qual |
|------|----|---|-----------------------|-----|---------|-------------|------|
| 1    |    |   | Heptadecane, 9-octyl- | 352 | C25H52  | 007225-64-1 | 91   |
| 2    |    |   | Octacosane, 2-methyl- | 408 | C29H60  | 001560-98-1 | 91   |
| 3    |    |   | Docosane              | 310 | C22H46  | 000629-97-0 | 91   |
| 4    |    |   | Pentacosane           | 352 | C25H52  | 000629-99-2 | 90   |
| 5    |    |   | Nonadecane, 2-methyl- | 282 | C20H42  | 001560-86-7 | 90   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF101323\  
Data File : BF135758.D  
Acq On : 13 Oct 2023 18:08  
Operator : CG\JU  
Sample : 04844-05  
Misc :  
ALS Vial : 13 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
OR-603-COMP-06

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF101323.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

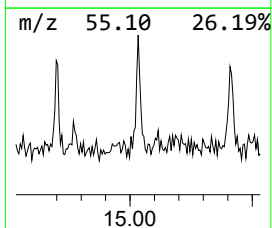
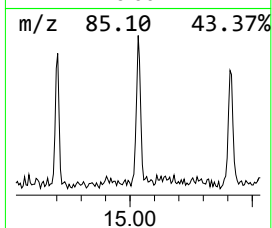
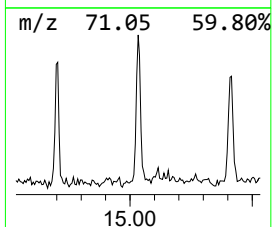
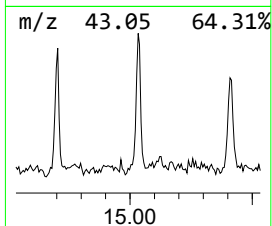
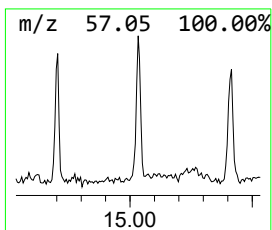
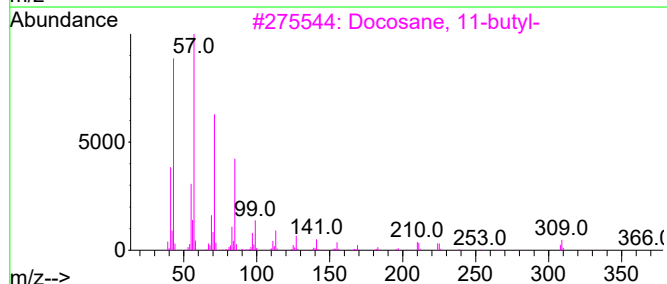
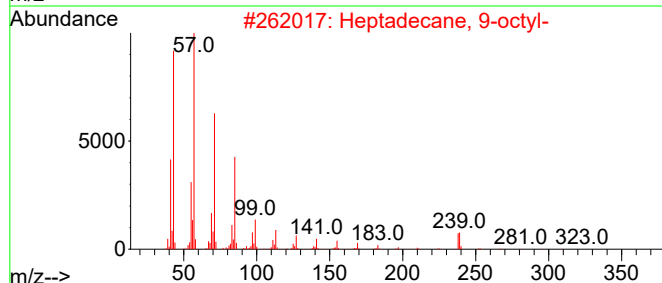
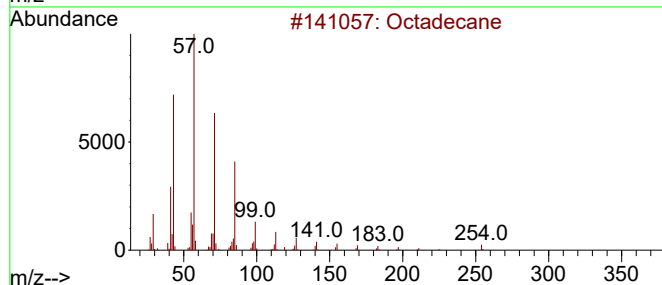
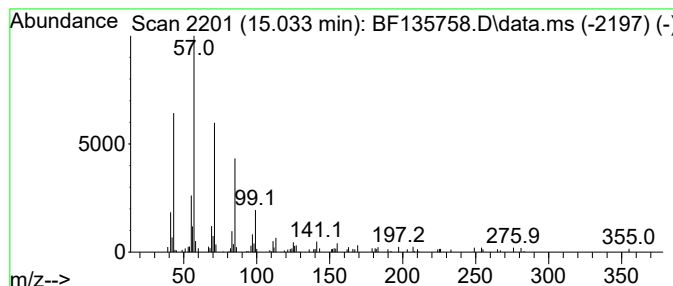
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 6 Octadecane Concentration Rank 5

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 15.033 | 2.68 ng | 88873 | Perylene-d12     | 15.410 |

| Hit# | of | 5 | Tentative ID          | MW  | MolForm | CAS#         | Qual |
|------|----|---|-----------------------|-----|---------|--------------|------|
| 1    |    |   | Octadecane            | 254 | C18H38  | 000593-45-3  | 90   |
| 2    |    |   | Heptadecane, 9-octyl- | 352 | C25H52  | 007225-64-1  | 72   |
| 3    |    |   | Docosane, 11-butyl-   | 366 | C26H54  | 013475-76-8  | 72   |
| 4    |    |   | Hexadecane, 1-iodo-   | 352 | C16H33I | 000544-77-4  | 72   |
| 5    |    |   | Docosane, 1-iodo-     | 436 | C22H45I | 1000406-31-9 | 64   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF101323\  
Data File : BF135758.D  
Acq On : 13 Oct 2023 18:08  
Operator : CG\JU  
Sample : 04844-05  
Misc :  
ALS Vial : 13 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
OR-603-COMP-06

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF101323.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

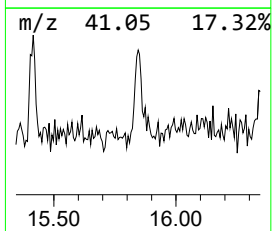
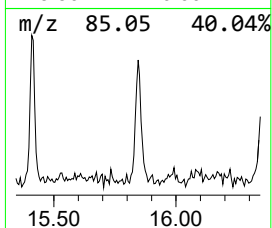
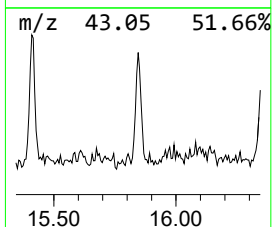
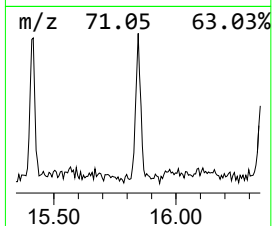
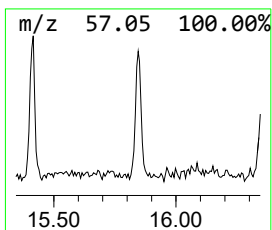
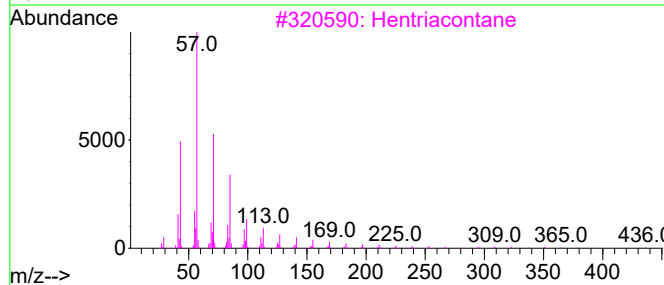
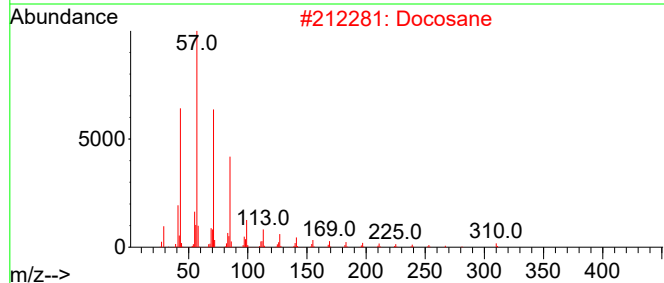
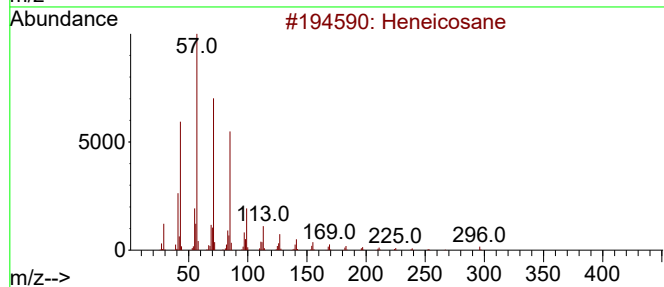
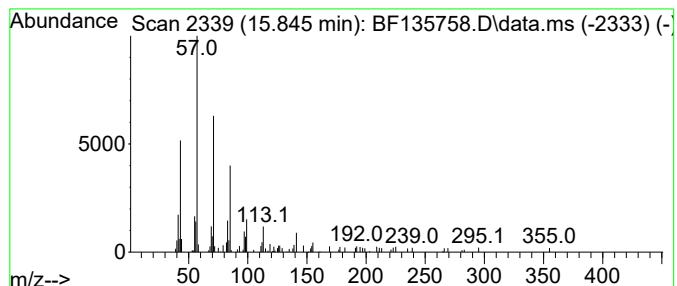
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Peak Number 7 Heneicosane Concentration Rank 6

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 15.845 | 2.43 ng | 80412 | Perylene-d12     | 15.410 |

| Hit# | of | 5 | Tentative ID       | MW  | MolForm | CAS#        | Qual |
|------|----|---|--------------------|-----|---------|-------------|------|
| 1    |    |   | Heneicosane        | 296 | C21H44  | 000629-94-7 | 87   |
| 2    |    |   | Docosane           | 310 | C22H46  | 000629-97-0 | 87   |
| 3    |    |   | Hentriacontane     | 437 | C31H64  | 000630-04-6 | 86   |
| 4    |    |   | Docosane, 7-hexyl- | 394 | C28H58  | 055373-86-9 | 86   |
| 5    |    |   | Octadecane         | 254 | C18H38  | 000593-45-3 | 86   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF101323\  
Data File : BF135758.D  
Acq On : 13 Oct 2023 18:08  
Operator : CG\JU  
Sample : 04844-05  
Misc :  
ALS Vial : 13 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
OR-603-COMP-06

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF101323.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| 2-Pentanone, 4-... | 4.969  | 4.9     | ng    | 156765   | 1                     | 6.734  | 641388 | 20.0 |
| n-Hexadecanoic ... | 11.804 | 6.0     | ng    | 246573   | 4                     | 11.269 | 821895 | 20.0 |
| 9-Octadecenamid... | 13.351 | 18.8    | ng    | 501012   | 5                     | 13.933 | 533308 | 20.0 |
| Bromoacetic aci... | 13.851 | 3.3     | ng    | 86734    | 5                     | 13.933 | 533308 | 20.0 |
| Heptadecane, 9-... | 14.704 | 2.2     | ng    | 71995    | 6                     | 15.410 | 662229 | 20.0 |
| Octadecane         | 15.033 | 2.7     | ng    | 88873    | 6                     | 15.410 | 662229 | 20.0 |
| Heneicosane        | 15.845 | 2.4     | ng    | 80412    | 6                     | 15.410 | 662229 | 20.0 |