

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF081623\  
 Data File : BF134798.D  
 Acq On : 16 Aug 2023 09:25  
 Operator : CG\JU  
 Sample : 04017-03  
 Misc :  
 ALS Vial : 4 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 JC-03-081423-B

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-BF080123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134798.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         | 5.422       | 563           | 567         | 581          | rBV      | 2106757        | 1824821       | 87.16%          | 9.510%        |
| 2         | 6.428       | 734           | 738         | 741          | rBV      | 2048695        | 1786894       | 85.35%          | 9.312%        |
| 3         | 6.798       | 797           | 801         | 804          | rBV      | 1435293        | 1104907       | 52.77%          | 5.758%        |
| 4         | 7.357       | 892           | 896         | 899          | rBV      | 1472067        | 1143375       | 54.61%          | 5.959%        |
| 5         | 8.075       | 1014          | 1018        | 1022         | rBV      | 1751131        | 1426265       | 68.12%          | 7.433%        |
| 6         | 9.151       | 1197          | 1201        | 1210         | rBV      | 2380863        | 2093633       | 100.00%         | 10.911%       |
| 7         | 9.269       | 1218          | 1221        | 1225         | rBV      | 32809          | 31831         | 1.52%           | 0.166%        |
| 8         | 9.833       | 1313          | 1317        | 1327         | rVB      | 1868652        | 1519109       | 72.56%          | 7.917%        |
| 9         | 10.033      | 1347          | 1351        | 1356         | rBV2     | 53170          | 72223         | 3.45%           | 0.376%        |
| 10        | 10.622      | 1447          | 1451        | 1462         | rBV      | 1233428        | 1136733       | 54.29%          | 5.924%        |
| 11        | 10.745      | 1469          | 1472        | 1480         | rVB3     | 28572          | 48866         | 2.33%           | 0.255%        |
| 12        | 11.222      | 1551          | 1553        | 1560         | rVB2     | 24128          | 26894         | 1.28%           | 0.140%        |
| 13        | 11.322      | 1566          | 1570        | 1573         | rBV      | 1553560        | 1278419       | 61.06%          | 6.662%        |
| 14        | 11.651      | 1623          | 1626        | 1628         | rBV4     | 19693          | 29336         | 1.40%           | 0.153%        |
| 15        | 11.680      | 1628          | 1631        | 1635         | rVV4     | 34776          | 73313         | 3.50%           | 0.382%        |
| 16        | 11.721      | 1635          | 1638        | 1644         | rVB      | 92057          | 104794        | 5.01%           | 0.546%        |
| 17        | 11.857      | 1656          | 1661        | 1670         | rBV      | 477279         | 504348        | 24.09%          | 2.628%        |
| 18        | 12.033      | 1686          | 1691        | 1694         | rVB2     | 26148          | 38816         | 1.85%           | 0.202%        |
| 19        | 12.380      | 1747          | 1750        | 1752         | rBV2     | 21236          | 24979         | 1.19%           | 0.130%        |
| 20        | 12.410      | 1752          | 1755        | 1756         | rVV3     | 48155          | 46159         | 2.20%           | 0.241%        |
| 21        | 12.433      | 1756          | 1759        | 1762         | rVB2     | 203212         | 168123        | 8.03%           | 0.876%        |
| 22        | 12.539      | 1771          | 1777        | 1780         | rBV2     | 72747          | 141284        | 6.75%           | 0.736%        |
| 23        | 12.568      | 1780          | 1782        | 1790         | rVV4     | 67221          | 100548        | 4.80%           | 0.524%        |
| 24        | 12.645      | 1791          | 1795        | 1801         | rBV      | 157470         | 182043        | 8.70%           | 0.949%        |
| 25        | 12.763      | 1813          | 1815        | 1818         | rVB      | 70825          | 63301         | 3.02%           | 0.330%        |
| 26        | 12.916      | 1837          | 1841        | 1844         | rBV      | 1860853        | 1649648       | 78.79%          | 8.597%        |
| 27        | 12.968      | 1844          | 1850        | 1858         | rVB5     | 70144          | 163675        | 7.82%           | 0.853%        |
| 28        | 13.386      | 1919          | 1921        | 1929         | rBV6     | 38828          | 66558         | 3.18%           | 0.347%        |
| 29        | 13.757      | 1980          | 1984        | 1989         | rVB3     | 79591          | 135189        | 6.46%           | 0.705%        |
| 30        | 13.833      | 1994          | 1997        | 2006         | rVB2     | 113193         | 178031        | 8.50%           | 0.928%        |
| 31        | 13.968      | 2016          | 2020        | 2024         | rBV      | 1134351        | 1127360       | 53.85%          | 5.875%        |
| 32        | 14.457      | 2100          | 2103        | 2105         | rBV      | 68948          | 63321         | 3.02%           | 0.330%        |
| 33        | 15.445      | 2266          | 2271        | 2277         | rBV      | 623965         | 833729        | 39.82%          | 4.345%        |

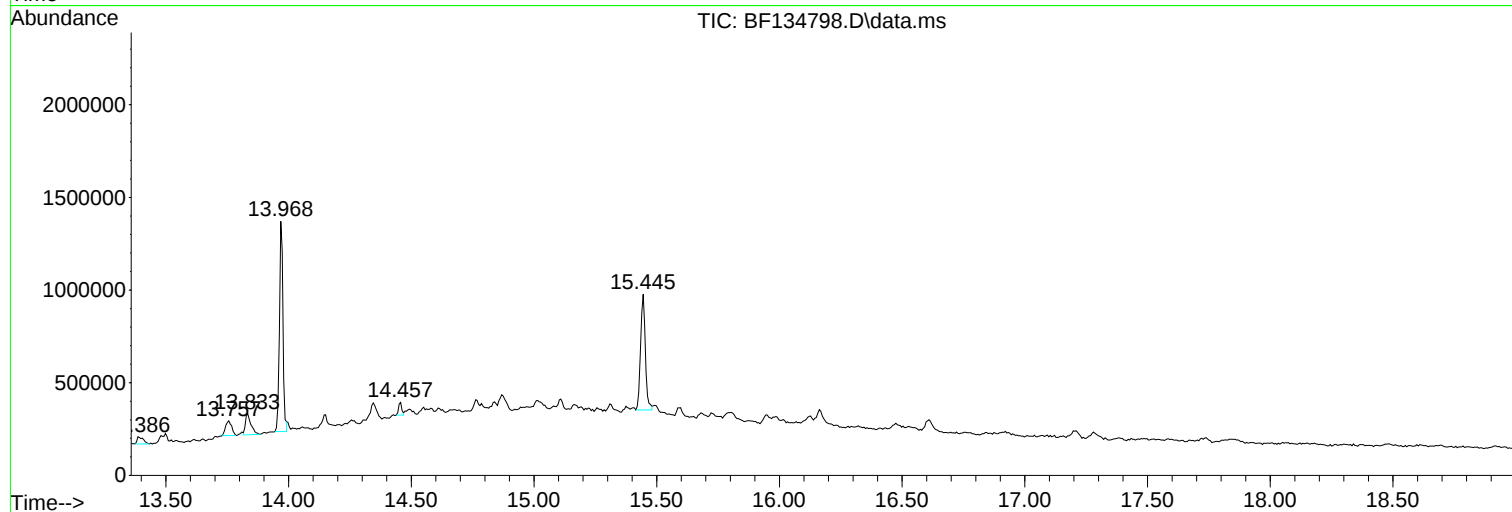
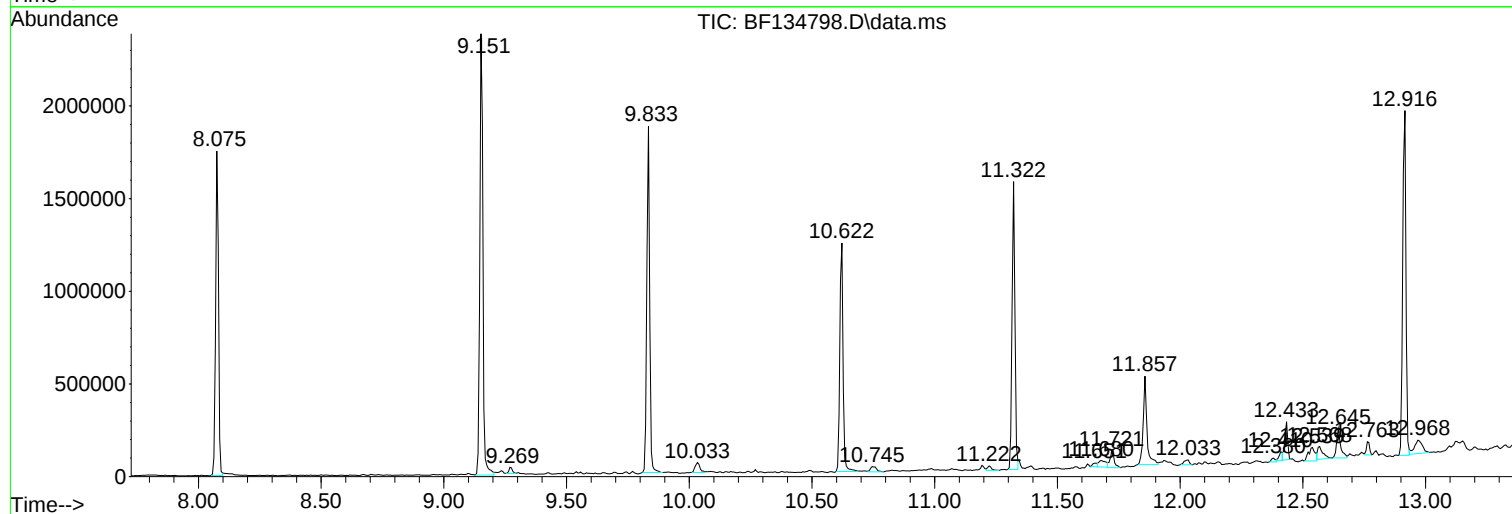
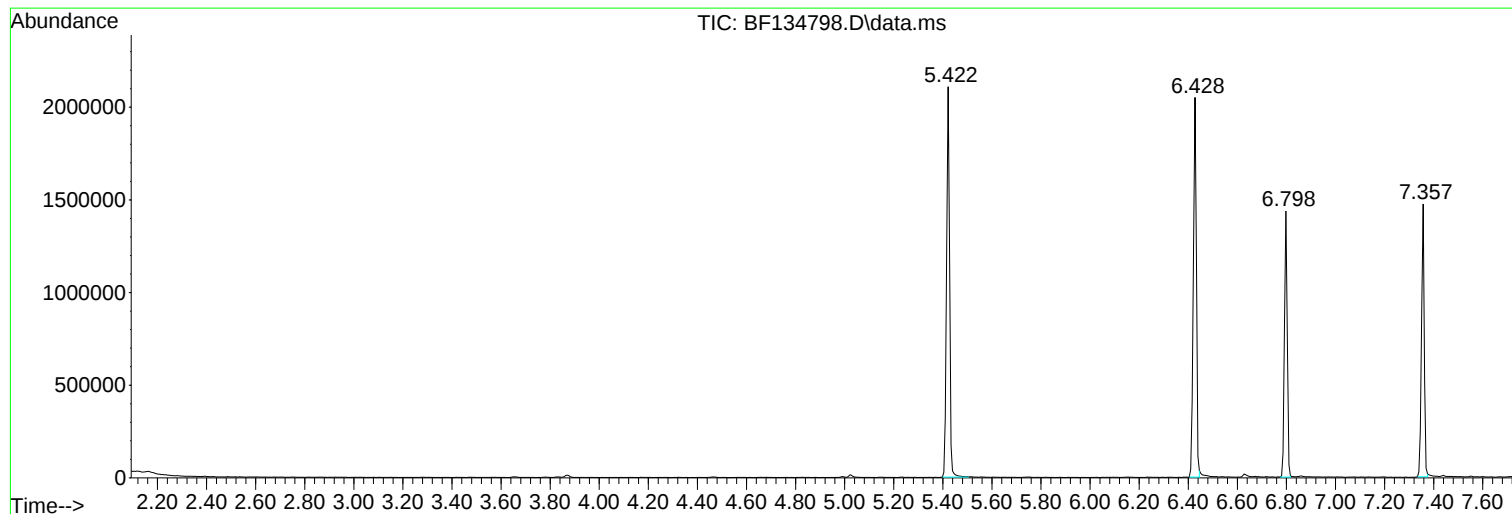
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ALS Vial : 4 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
JC-03-081423-B

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF080123.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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BNA\_F  
ClientSampleId :  
JC-03-081423-B

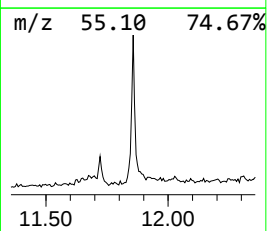
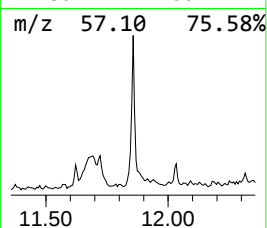
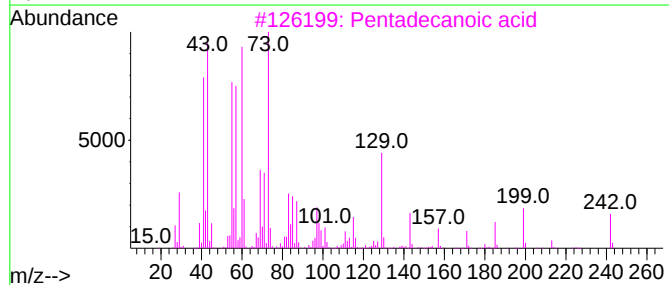
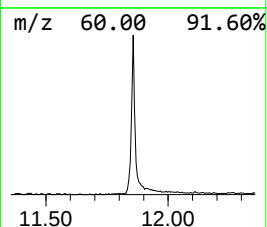
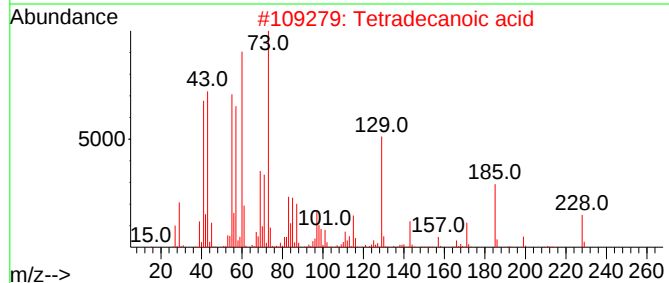
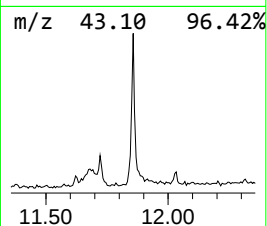
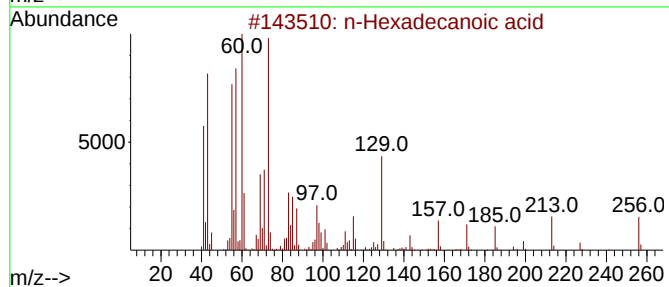
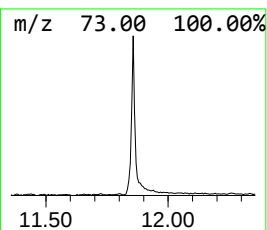
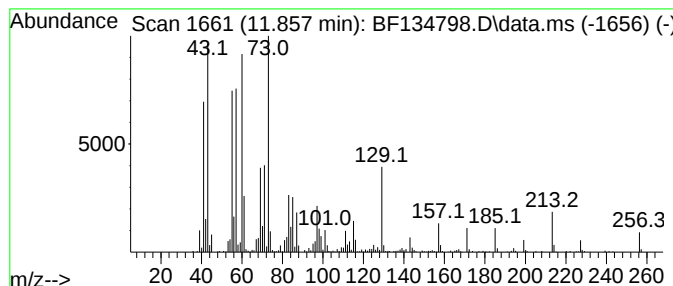
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 11.857 | 7.89 ng | 504348 | Phenanthrene-d10 | 11.322 |

| 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 | 93   |
| 3    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 93   |
| 4    |    |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 92   |
| 5    |    |   | Undecanoic acid     | 186 | C11H22O2 | 000112-37-8 | 81   |



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Instrument :  
BNA\_F  
ClientSampleId :  
JC-03-081423-B

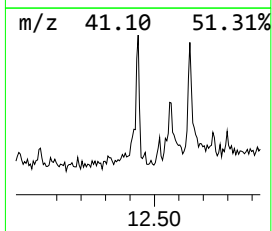
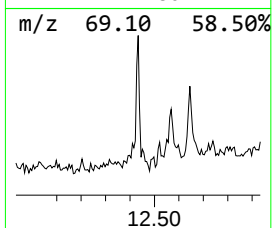
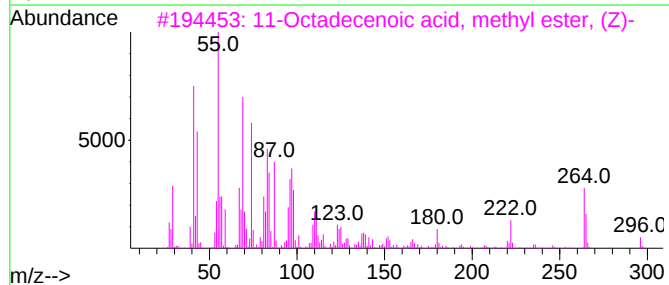
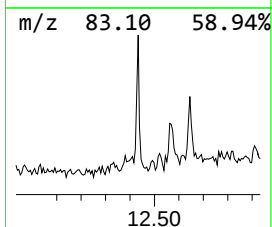
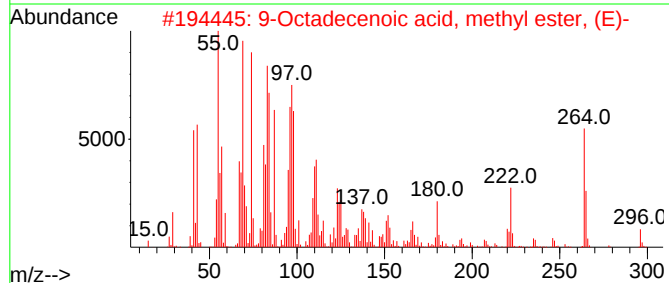
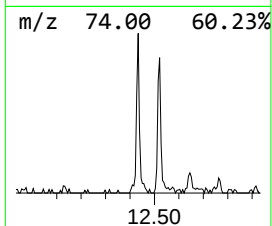
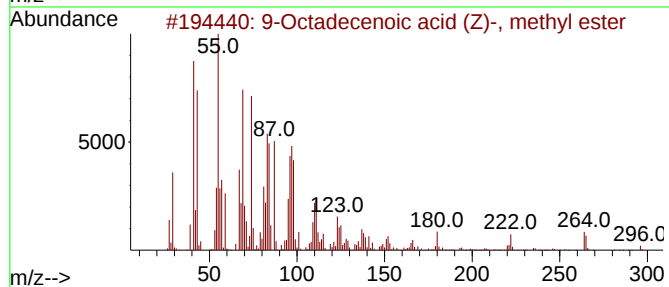
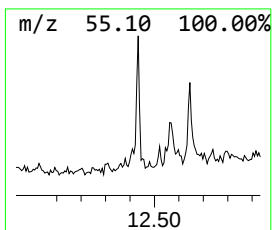
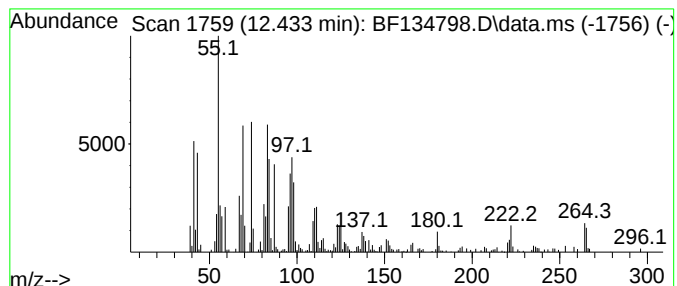
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF080123.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 2 9-Octadecenoic acid (Z)-, m... Concentration Rank 5

| R.T.      | EstConc                             | Area   | Relative to ISTD | R.T.         |      |
|-----------|-------------------------------------|--------|------------------|--------------|------|
| 12.433    | 2.63 ng                             | 168123 | Phenanthrene-d10 | 11.322       |      |
| Hit# of 5 | Tentative ID                        | MW     | MolForm          | CAS#         | Qual |
| 1         | 9-Octadecenoic acid (Z)-, methyl... | 296    | C19H36O2         | 000112-62-9  | 99   |
| 2         | 9-Octadecenoic acid, methyl este... | 296    | C19H36O2         | 001937-62-8  | 99   |
| 3         | 11-Octadecenoic acid, methyl est... | 296    | C19H36O2         | 001937-63-9  | 99   |
| 4         | cis-13-Octadecenoic acid, methyl... | 296    | C19H36O2         | 1010333-58-3 | 99   |
| 5         | 10-Octadecenoic acid, methyl ester  | 296    | C19H36O2         | 013481-95-3  | 99   |



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ALS Vial : 4 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
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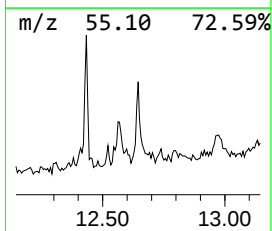
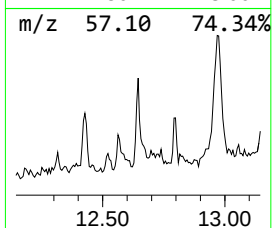
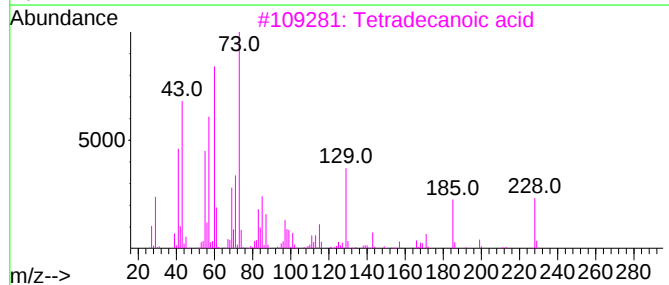
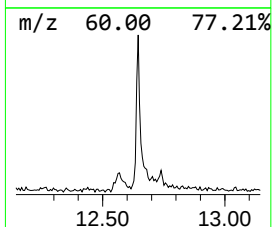
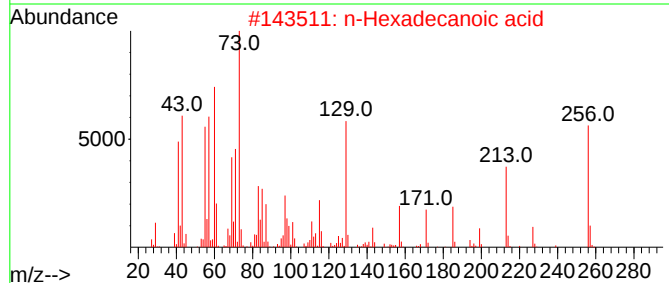
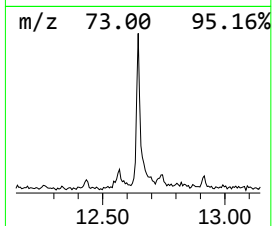
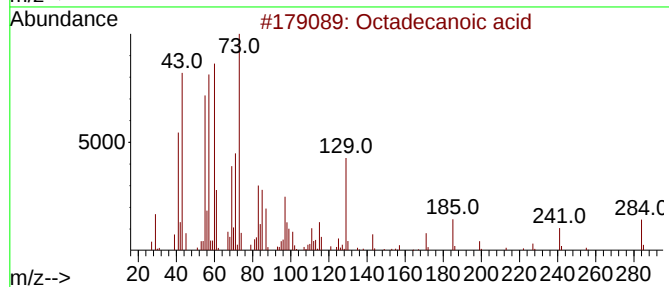
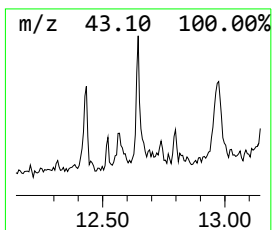
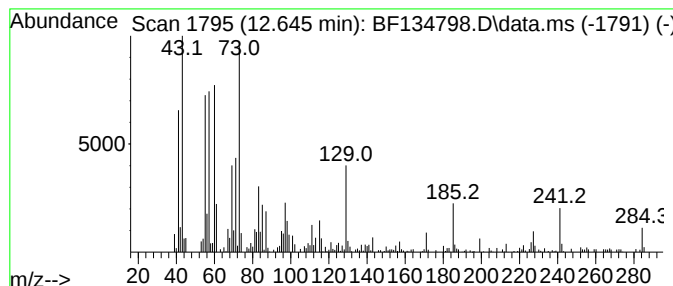
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 4 Octadecanoic acid Concentration Rank 2

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 12.645 | 3.23 ng | 182043 | Chrysene-d12     | 13.968 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | Octadecanoic acid   | 284 | C18H36O2 | 000057-11-4 | 99   |
| 2    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 93   |
| 3    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 87   |
| 4    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 68   |
| 5    |    |   | Undecanoic acid     | 186 | C11H22O2 | 000112-37-8 | 38   |



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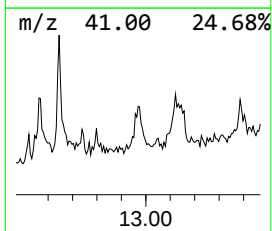
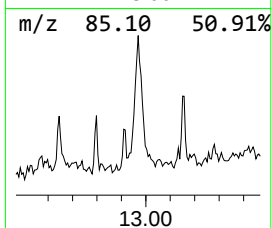
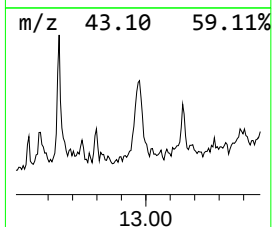
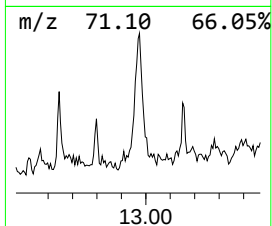
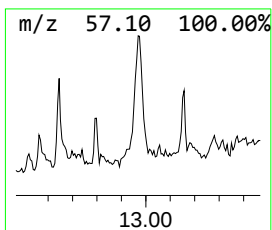
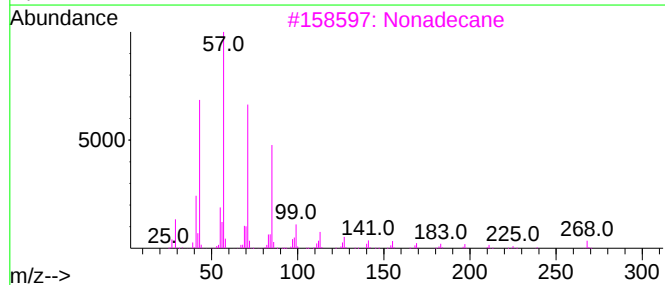
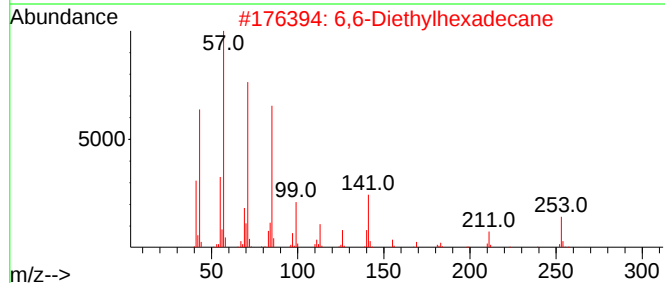
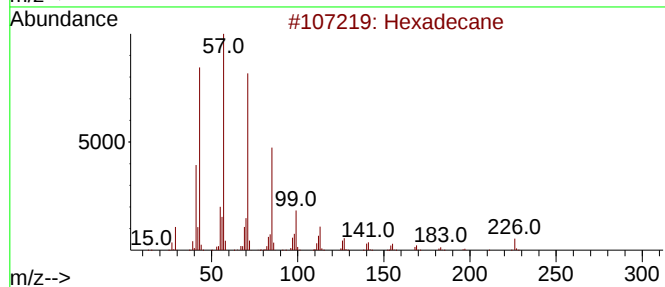
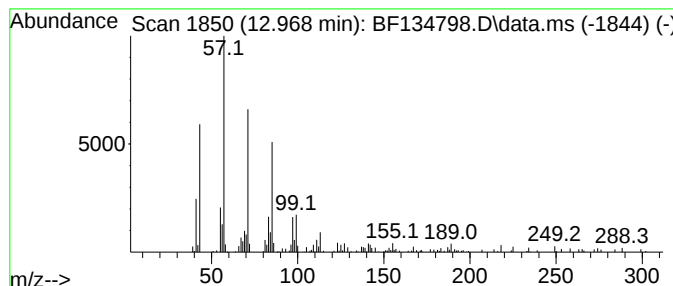
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF080123.M  
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TIC Library : C:\Database\NIST20.L  
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\*\*\*\*\*  
Peak Number 5 Hexadecane Concentration Rank 4

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 12.969 | 2.90 ng | 163675 | Chrysene-d12     | 13.968 |

| Hit# | of | 5 | Tentative ID               | MW  | MolForm | CAS#         | Qual |
|------|----|---|----------------------------|-----|---------|--------------|------|
| 1    |    |   | Hexadecane                 | 226 | C16H34  | 000544-76-3  | 86   |
| 2    |    |   | 6,6-Diethylhexadecane      | 282 | C20H42  | 1000360-41-4 | 86   |
| 3    |    |   | Nonadecane                 | 268 | C19H40  | 000629-92-5  | 86   |
| 4    |    |   | 5-Ethyl-5-methylnonadecane | 310 | C22H46  | 1000360-42-7 | 80   |
| 5    |    |   | Tetradecane, 1-iodo-       | 324 | C14H29I | 019218-94-1  | 72   |



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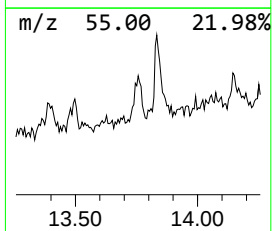
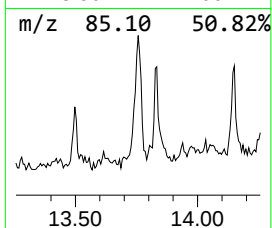
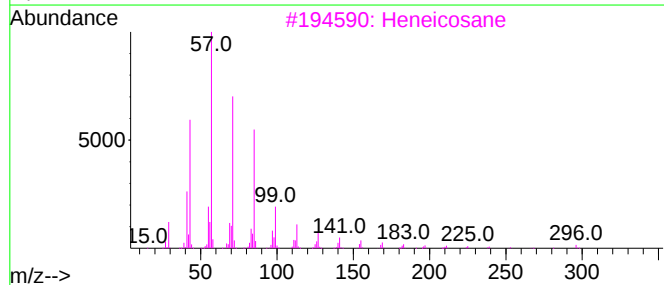
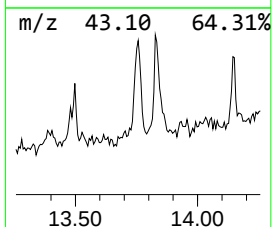
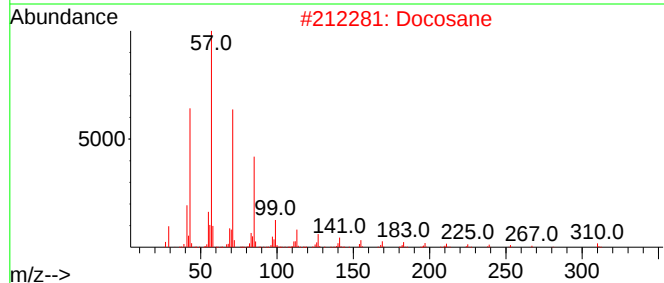
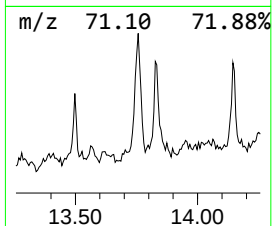
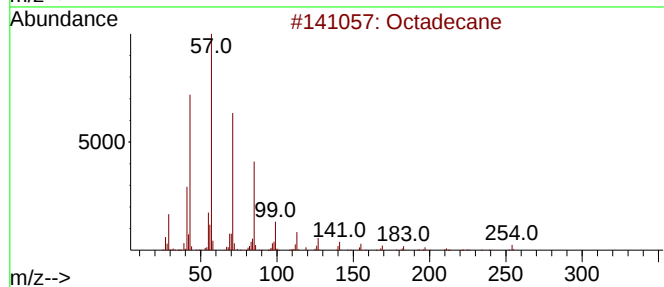
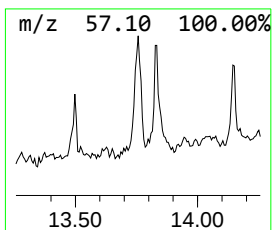
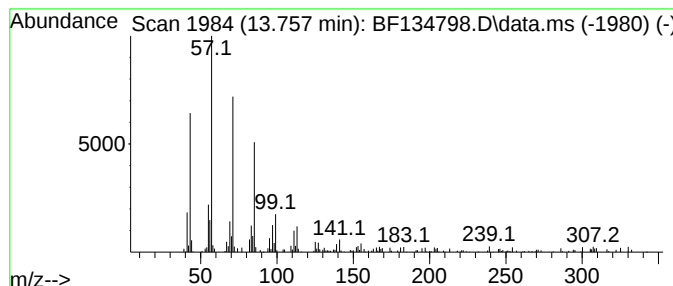
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 6 Octadecane Concentration Rank 6

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 13.757 | 2.40 ng | 135189 | Chrysene-d12     | 13.968 |

| Hit# | of 5 | Tentative ID          | MW  | MolForm | CAS#        | Qual |
|------|------|-----------------------|-----|---------|-------------|------|
| 1    |      | Octadecane            | 254 | C18H38  | 000593-45-3 | 91   |
| 2    |      | Docosane              | 310 | C22H46  | 000629-97-0 | 80   |
| 3    |      | Heneicosane           | 296 | C21H44  | 000629-94-7 | 80   |
| 4    |      | Tetradecane, 4-ethyl- | 226 | C16H34  | 055045-14-2 | 80   |
| 5    |      | Hentriacontane        | 437 | C31H64  | 000630-04-6 | 74   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF081623\  
Data File : BF134798.D  
Acq On : 16 Aug 2023 09:25  
Operator : CG\JU  
Sample : 04017-03  
Misc :  
ALS Vial : 4 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
JC-03-081423-B

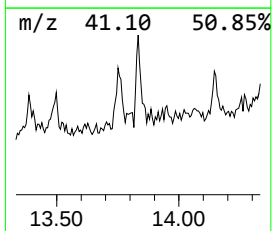
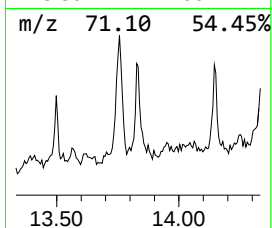
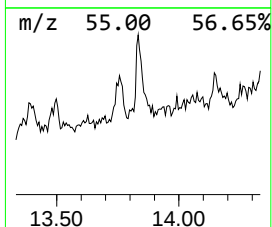
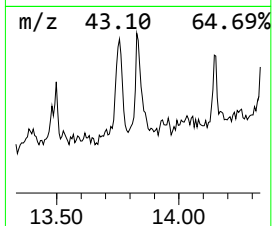
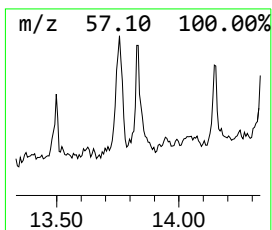
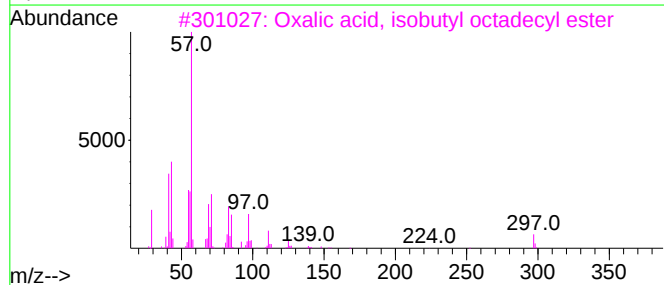
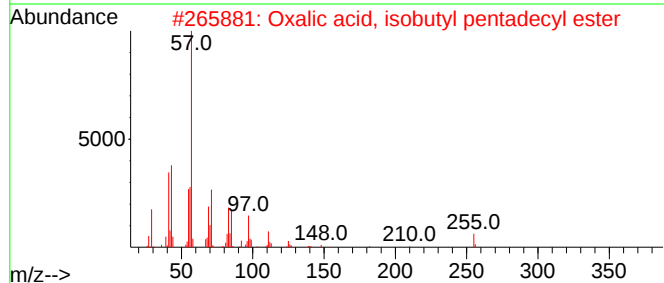
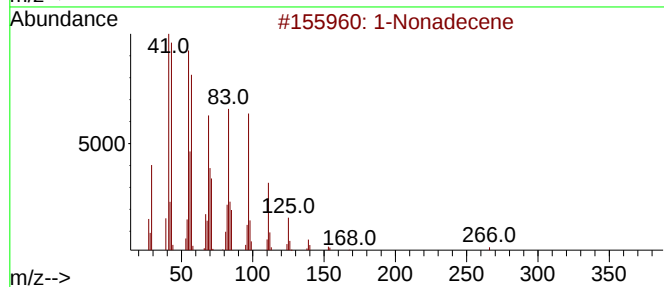
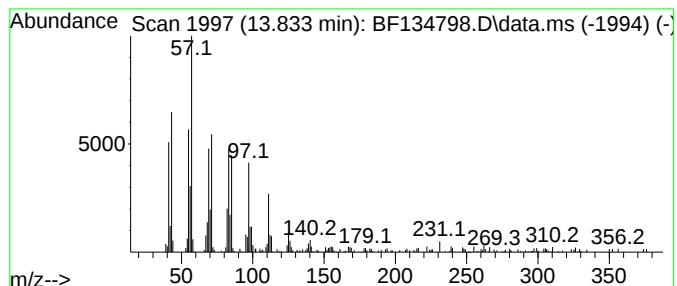
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF080123.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 7 1-Nonadecene Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 13.833 | 3.16 ng | 178031 | Chrysene-d12     | 13.968 |

| Hit# | of                                  | 5 | Tentative ID | MW  | MolForm  | CAS#         | Qual |
|------|-------------------------------------|---|--------------|-----|----------|--------------|------|
| 1    | 1-Nonadecene                        |   |              | 266 | C19H38   | 018435-45-5  | 95   |
| 2    | Oxalic acid, isobutyl pentadecyl... |   |              | 356 | C21H40O4 | 1000309-38-0 | 91   |
| 3    | Oxalic acid, isobutyl octadecyl ... |   |              | 398 | C24H46O4 | 1000309-38-3 | 91   |
| 4    | Oxalic acid, hexadecyl propyl ester |   |              | 356 | C21H40O4 | 1000309-26-9 | 91   |
| 5    | 9-Eicosene, (E)-                    |   |              | 280 | C20H40   | 074685-29-3  | 83   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF081623\  
Data File : BF134798.D  
Acq On : 16 Aug 2023 09:25  
Operator : CG\JU  
Sample : 04017-03  
Misc :  
ALS Vial : 4 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
JC-03-081423-B

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF080123.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 |
| n-Hexadecanoic ... | 11.857 | 7.9     | ng    | 504348   | 4                     | 11.322 | 1278420 | 20.0 |
| 9-Octadecenoic ... | 12.433 | 2.6     | ng    | 168123   | 4                     | 11.322 | 1278420 | 20.0 |
| Octadecanoic acid  | 12.645 | 3.2     | ng    | 182043   | 5                     | 13.968 | 1127360 | 20.0 |
| Hexadecane         | 12.969 | 2.9     | ng    | 163675   | 5                     | 13.968 | 1127360 | 20.0 |
| Octadecane         | 13.757 | 2.4     | ng    | 135189   | 5                     | 13.968 | 1127360 | 20.0 |
| 1-Nonadecene       | 13.833 | 3.2     | ng    | 178031   | 5                     | 13.968 | 1127360 | 20.0 |