

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF081723\  
 Data File : BF134818.D  
 Acq On : 17 Aug 2023 11:43  
 Operator : CG\JU  
 Sample : PB154866BL  
 Misc :  
 ALS Vial : 3 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 PB154866BL

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: BF134818.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         | 2.146       | 5             | 10          | 15           | rVB      | 64138          | 89856         | 1.58%           | 0.241%        |
| 2         | 5.445       | 565           | 571         | 574          | rBV      | 4267177        | 4856459       | 85.23%          | 13.035%       |
| 3         | 6.445       | 734           | 741         | 743          | rBV      | 3780110        | 4795856       | 84.17%          | 12.872%       |
| 4         | 6.798       | 798           | 801         | 805          | rVB      | 1202493        | 914815        | 16.05%          | 2.455%        |
| 5         | 7.363       | 891           | 897         | 900          | rBV      | 2953255        | 3267798       | 57.35%          | 8.771%        |
| 6         | 8.075       | 1013          | 1018        | 1022         | rBV      | 1380831        | 1235624       | 21.68%          | 3.316%        |
| 7         | 9.157       | 1196          | 1202        | 1205         | rBV      | 5185933        | 5611790       | 98.48%          | 15.062%       |
| 8         | 9.833       | 1311          | 1317        | 1320         | rBV      | 1655655        | 1403538       | 24.63%          | 3.767%        |
| 9         | 10.628      | 1446          | 1452        | 1455         | rBV      | 3592838        | 3722204       | 65.32%          | 9.990%        |
| 10        | 11.322      | 1566          | 1570        | 1574         | rBV      | 1741327        | 1461236       | 25.64%          | 3.922%        |
| 11        | 11.851      | 1655          | 1660        | 1671         | rBV      | 256596         | 370696        | 6.51%           | 0.995%        |
| 12        | 12.645      | 1789          | 1795        | 1807         | rBV      | 99598          | 144489        | 2.54%           | 0.388%        |
| 13        | 12.921      | 1837          | 1842        | 1845         | rBV      | 5075298        | 5698154       | 100.00%         | 15.294%       |
| 14        | 13.321      | 1885          | 1910        | 1911         | rBV2     | 267474         | 943415        | 16.56%          | 2.532%        |
| 15        | 13.827      | 1991          | 1996        | 2001         | rBV      | 74906          | 85984         | 1.51%           | 0.231%        |
| 16        | 13.968      | 2016          | 2020        | 2028         | rBV      | 903487         | 943159        | 16.55%          | 2.531%        |
| 17        | 14.145      | 2046          | 2050        | 2059         | rVB      | 98464          | 113630        | 1.99%           | 0.305%        |
| 18        | 14.351      | 2075          | 2085        | 2086         | rBV      | 157727         | 362340        | 6.36%           | 0.973%        |
| 19        | 14.451      | 2099          | 2102        | 2107         | rVB      | 123450         | 143376        | 2.52%           | 0.385%        |
| 20        | 14.763      | 2151          | 2155        | 2162         | rVB      | 81528          | 92518         | 1.62%           | 0.248%        |
| 21        | 15.104      | 2210          | 2213        | 2220         | rBV2     | 54069          | 68217         | 1.20%           | 0.183%        |
| 22        | 15.445      | 2266          | 2271        | 2277         | rBV      | 677870         | 932959        | 16.37%          | 2.504%        |

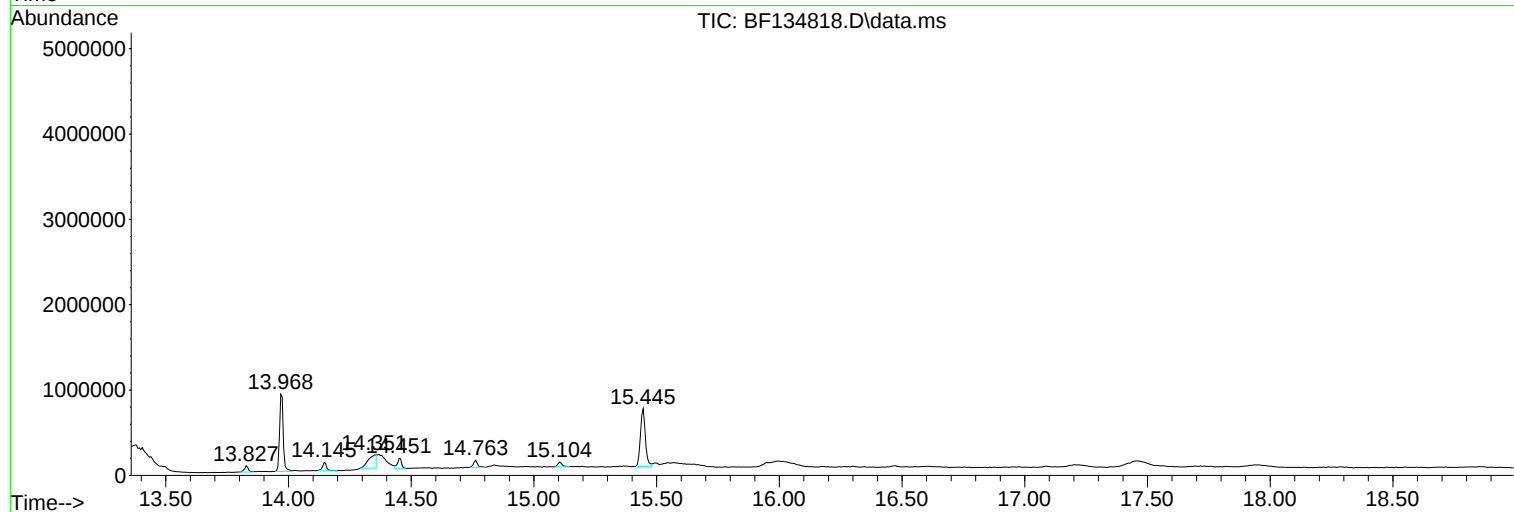
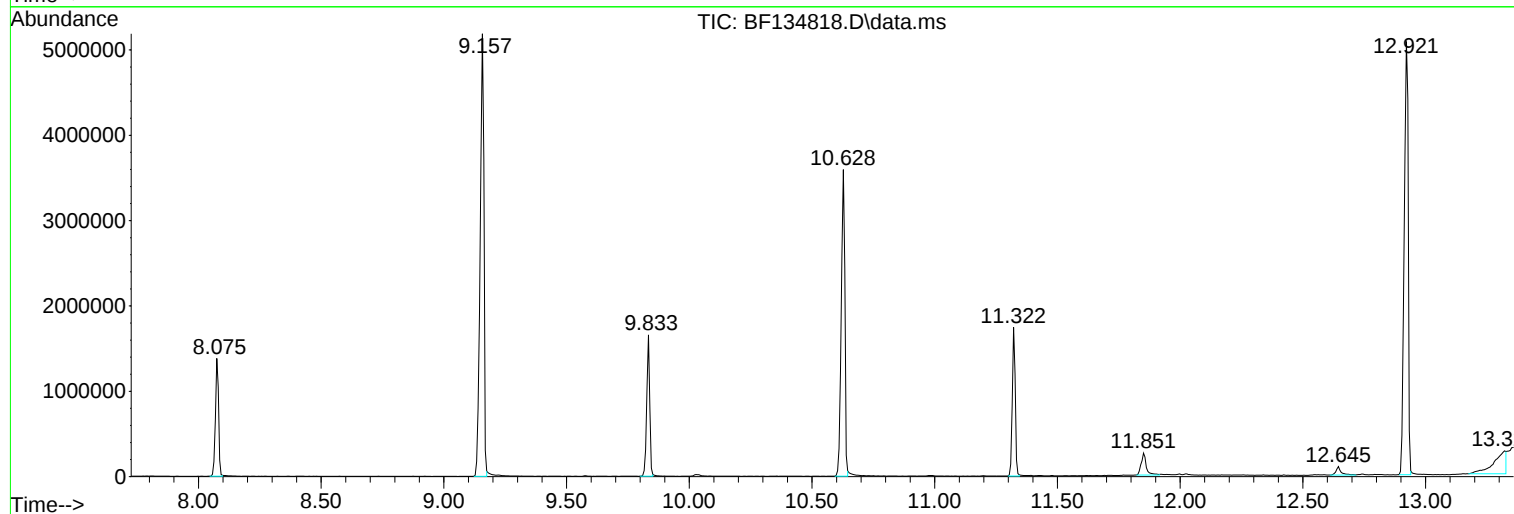
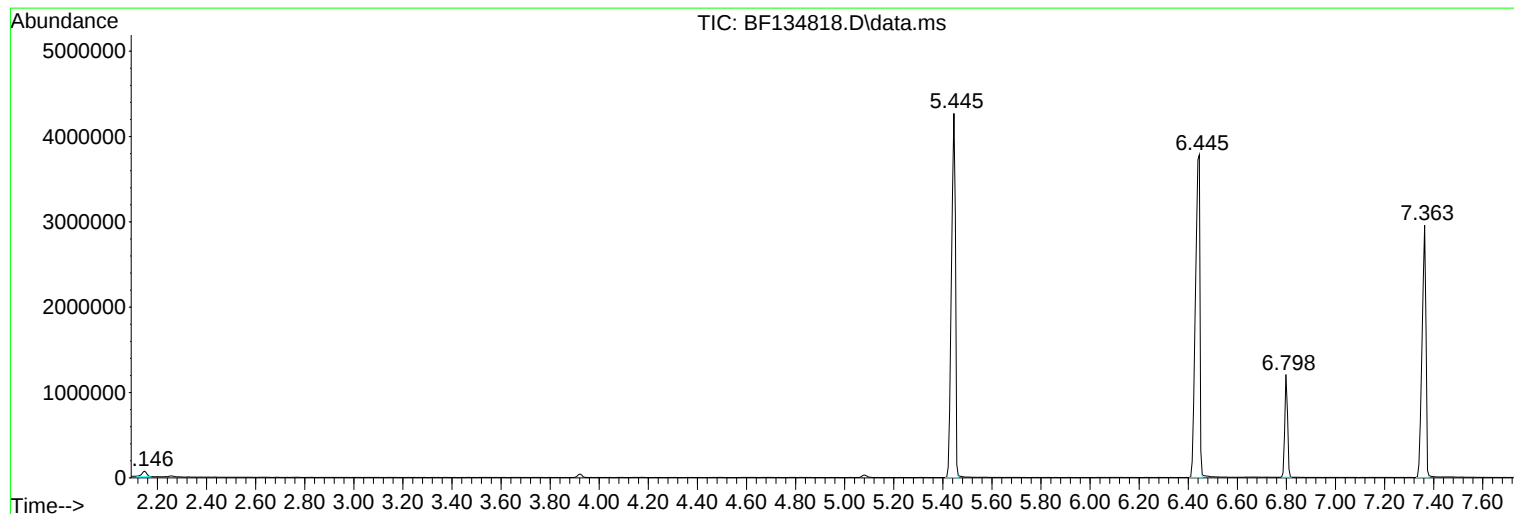
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Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PB154866BL

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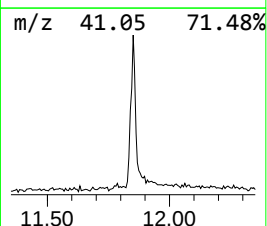
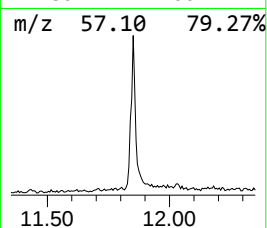
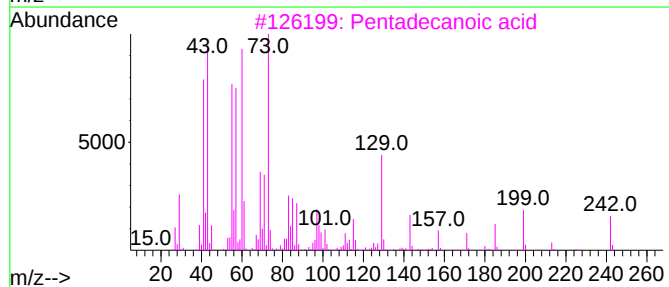
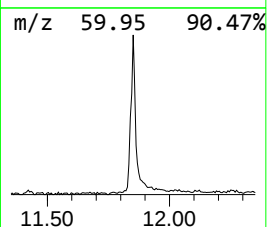
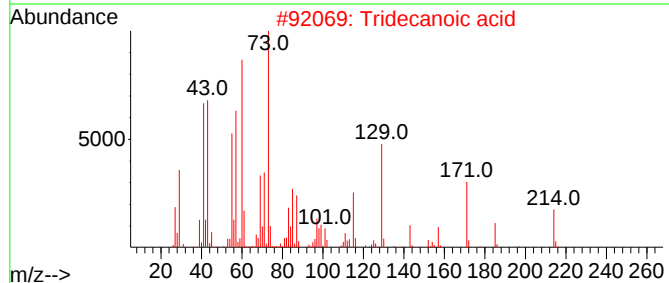
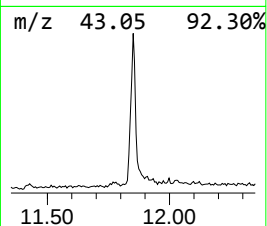
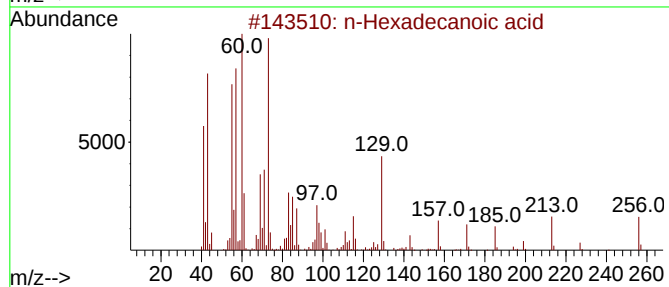
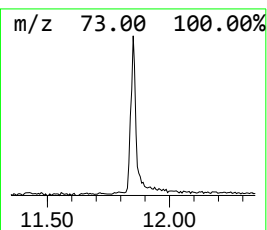
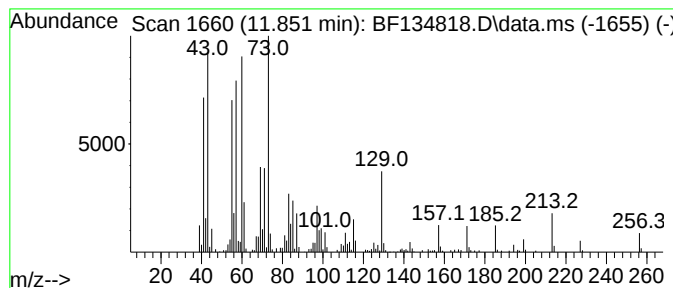
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF080123.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 n-Hexadecanoic acid Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 11.851 | 5.07 ng | 370696 | Phenanthrene-d10 | 11.322 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 99   |
| 2    |    |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 93   |
| 3    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 90   |
| 4    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 80   |
| 5    |    |   | Octanoic acid       | 144 | C8H16O2  | 000124-07-2 | 49   |



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ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PB154866BL

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

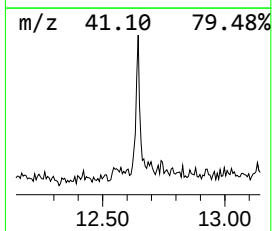
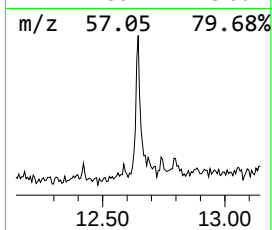
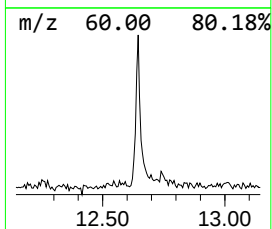
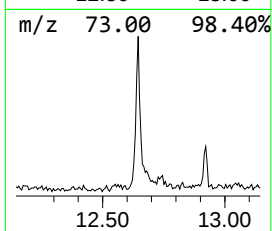
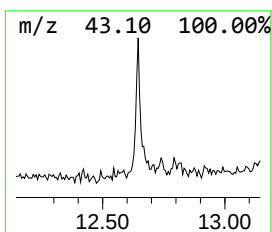
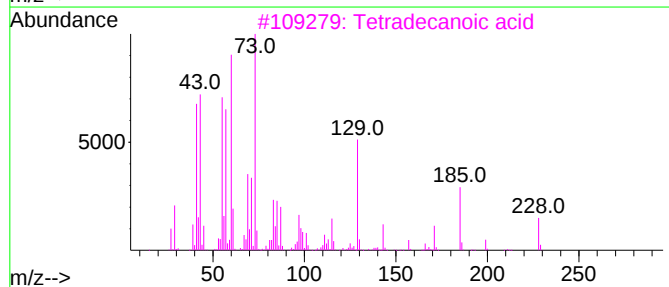
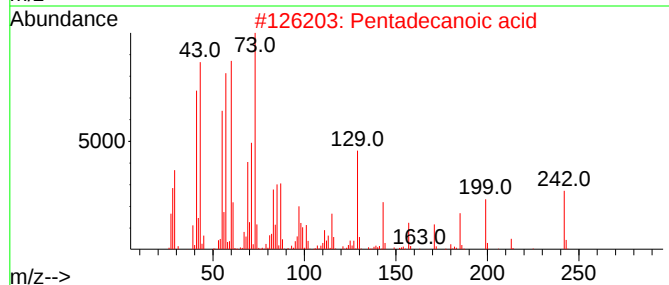
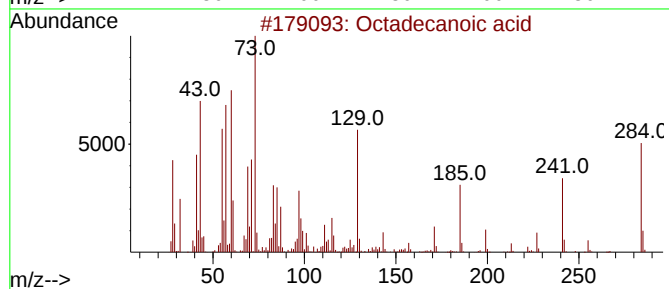
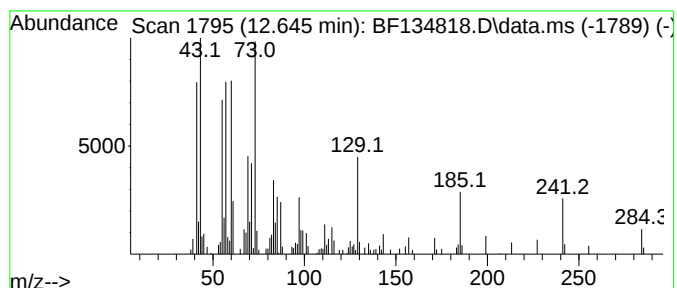
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 Octadecanoic acid Concentration Rank 4

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 12.645 | 3.06 ng | 144489 | Chrysene-d12     | 13.969 |

| Hit# | of | 5 | Tentative ID          | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-----------------------|-----|----------|-------------|------|
| 1    |    |   | Octadecanoic acid     | 284 | C18H36O2 | 000057-11-4 | 99   |
| 2    |    |   | Pentadecanoic acid    | 242 | C15H30O2 | 001002-84-2 | 93   |
| 3    |    |   | Tetradecanoic acid    | 228 | C14H28O2 | 000544-63-8 | 83   |
| 4    |    |   | n-Decanoic acid       | 172 | C10H20O2 | 000334-48-5 | 70   |
| 5    |    |   | 8-Methylnonanoic acid | 172 | C10H20O2 | 005963-14-4 | 55   |



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ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PB154866BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF080123.M  
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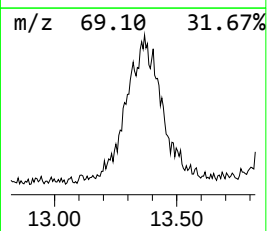
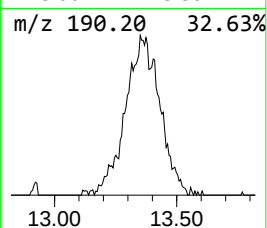
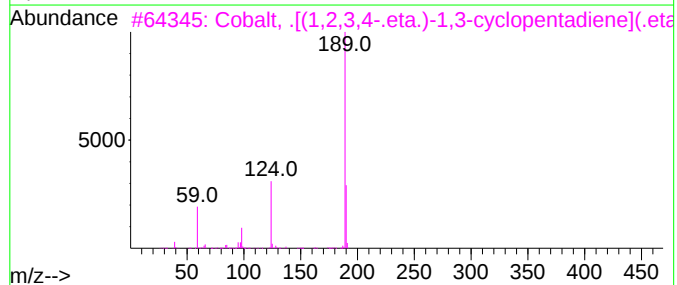
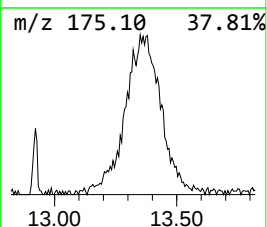
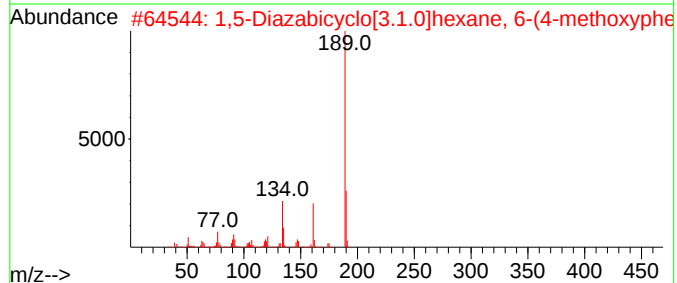
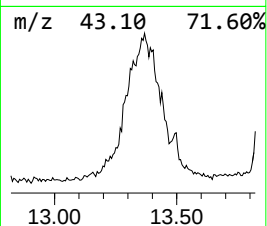
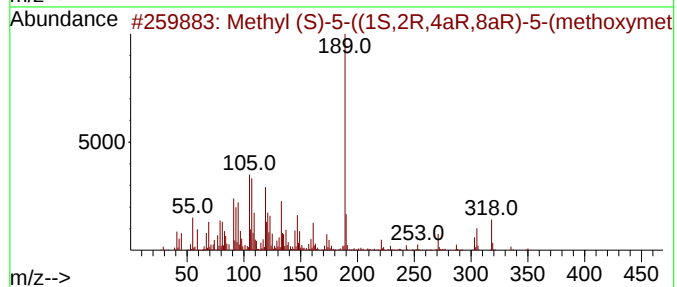
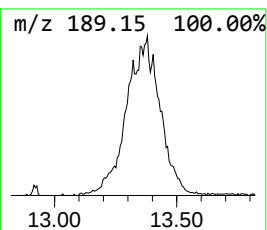
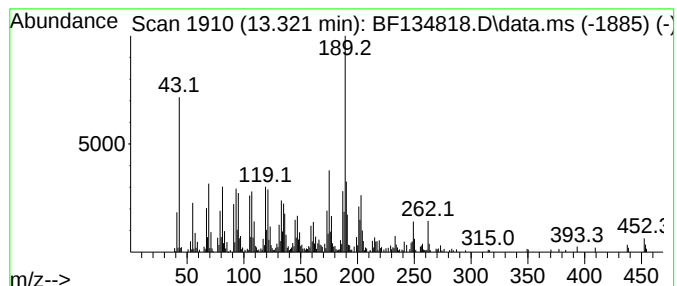
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 Methyl (S)-5-((1S,2R,4aR,8a... Concentration Rank 1

| R.T.   | EstConc  | Area   | Relative to ISTD | R.T.   |
|--------|----------|--------|------------------|--------|
| 13.321 | 20.01 ng | 943415 | Chrysene-d12     | 13.969 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm     | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|-------------|--------------|------|
| 1    |    |   | Methyl (S)-5-((1S,2R,4aR,8aR)-5-... | 350 | C22H38O3    | 1010495-83-9 | 94   |
| 2    |    |   | 1,5-Diazabicyclo[3.1.0]hexane, 6... | 190 | C11H14N2O   | 1000337-54-5 | 43   |
| 3    |    |   | Cobalt, .[(1,2,3,4-.eta.)-1,3-cy... | 190 | C10H11Co    | 033032-03-0  | 43   |
| 4    |    |   | Cyclopenta[b]pyridine, 3-cyano-2... | 262 | C13H14N2O2S | 166113-76-4  | 43   |
| 5    |    |   | 6-(4-Fluorophenyl)-2-hydroxypyri... | 189 | C11H8FNO    | 1010509-20-5 | 43   |



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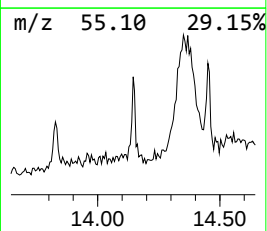
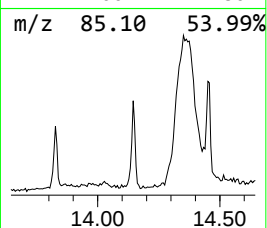
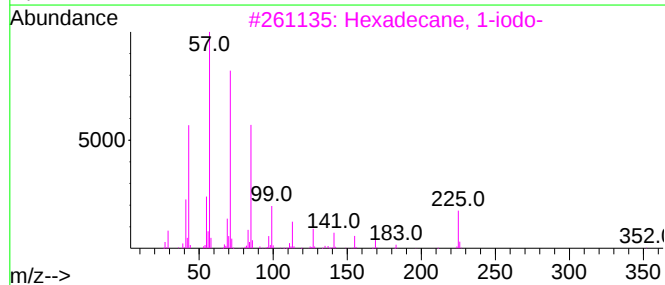
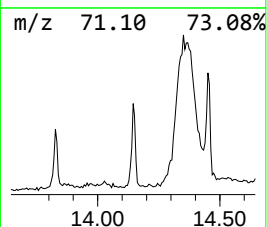
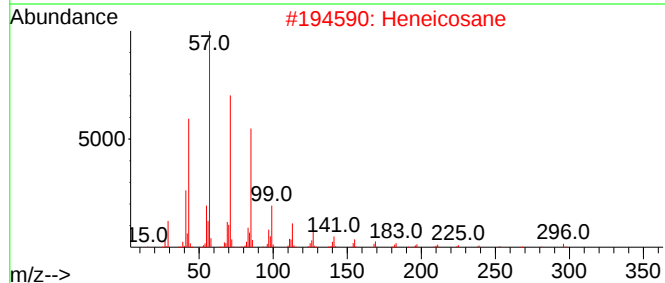
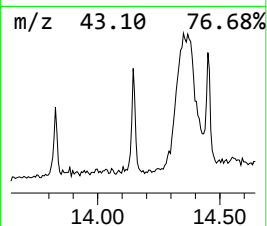
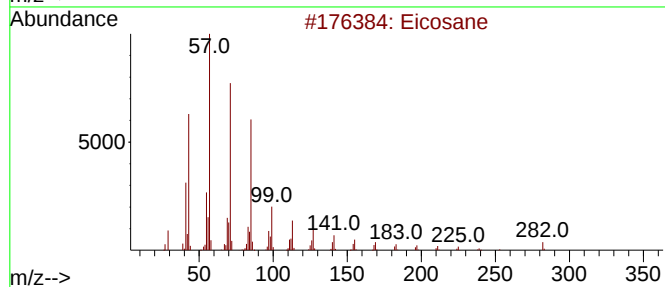
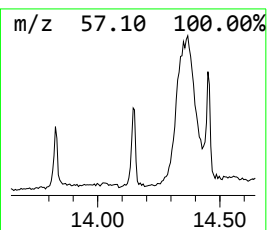
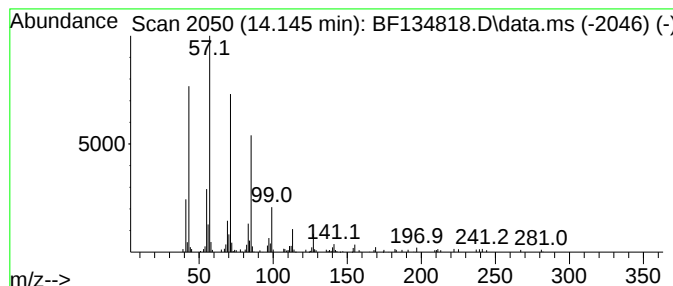
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF080123.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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\*\*\*\*\*  
Peak Number 4 Eicosane Concentration Rank 6

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 14.145 | 2.41 ng | 113630 | Chrysene-d12     | 13.969 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm | CAS#        | Qual |
|------|----|---|---------------------|-----|---------|-------------|------|
| 1    |    |   | Eicosane            | 282 | C20H42  | 000112-95-8 | 95   |
| 2    |    |   | Heneicosane         | 296 | C21H44  | 000629-94-7 | 87   |
| 3    |    |   | Hexadecane, 1-iodo- | 352 | C16H33I | 000544-77-4 | 80   |
| 4    |    |   | Tridecane, 1-iodo-  | 310 | C13H27I | 035599-77-0 | 80   |
| 5    |    |   | Octadecane          | 254 | C18H38  | 000593-45-3 | 80   |



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

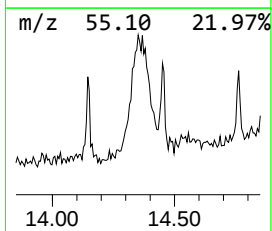
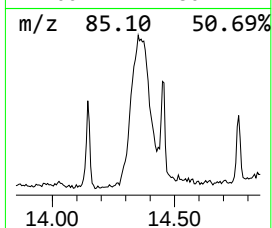
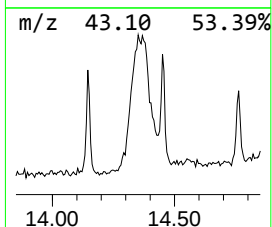
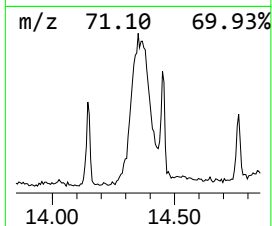
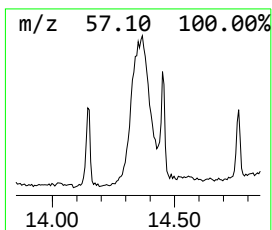
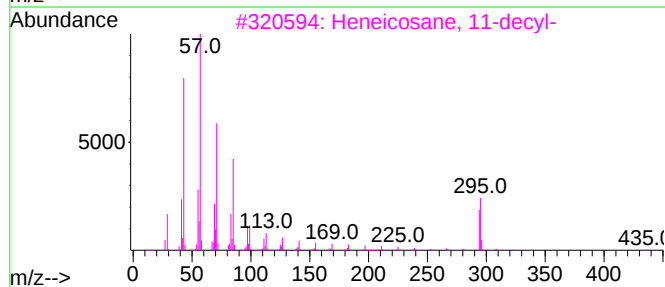
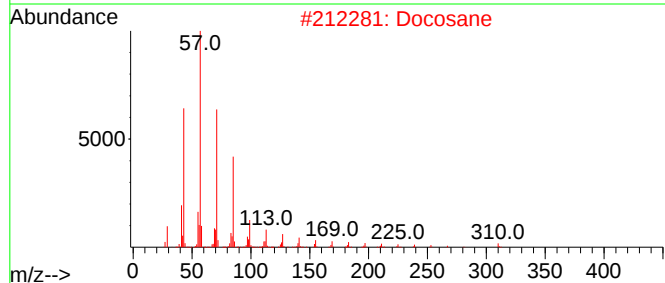
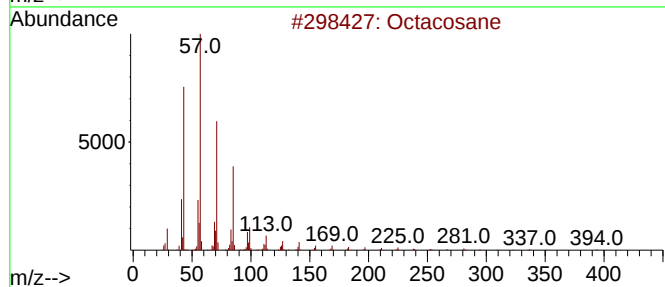
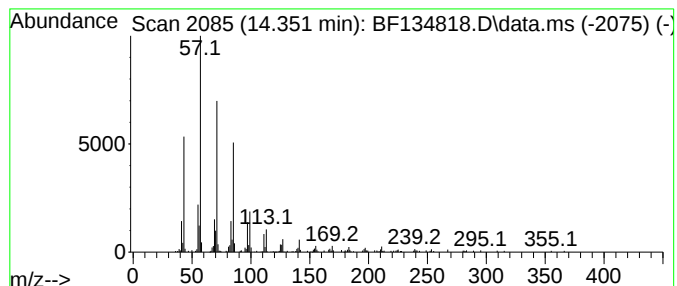
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 Octacosane Concentration Rank 2

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 14.351 | 7.68 ng | 362340 | Chrysene-d12     | 13.969 |

| Hit# | of | 5 | Tentative ID           | MW  | MolForm | CAS#        | Qual |
|------|----|---|------------------------|-----|---------|-------------|------|
| 1    |    |   | Octacosane             | 394 | C28H58  | 000630-02-4 | 90   |
| 2    |    |   | Docosane               | 310 | C22H46  | 000629-97-0 | 87   |
| 3    |    |   | Heneicosane, 11-decyl- | 437 | C31H64  | 055320-06-4 | 87   |
| 4    |    |   | Tetracosane            | 338 | C24H50  | 000646-31-1 | 87   |
| 5    |    |   | Octacosane, 2-methyl-  | 408 | C29H60  | 001560-98-1 | 87   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF081723\  
Data File : BF134818.D  
Acq On : 17 Aug 2023 11:43  
Operator : CG\JU  
Sample : PB154866BL  
Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PB154866BL

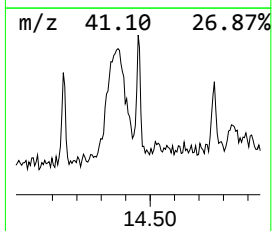
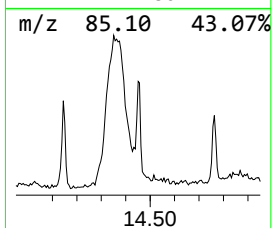
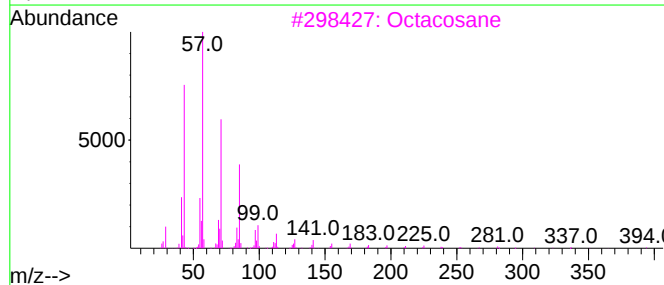
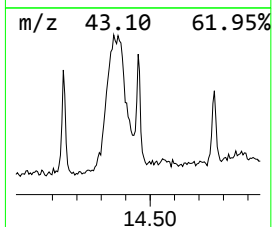
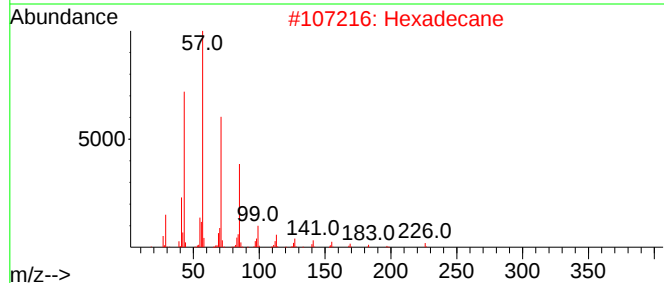
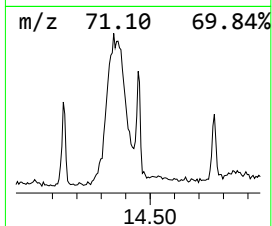
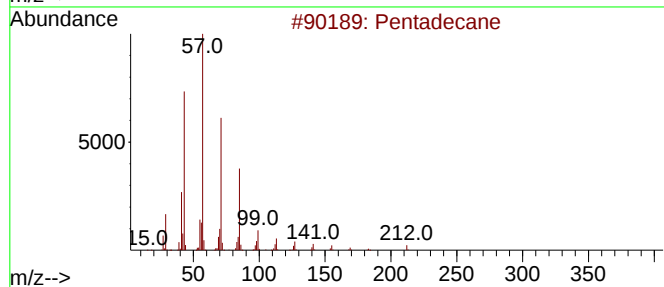
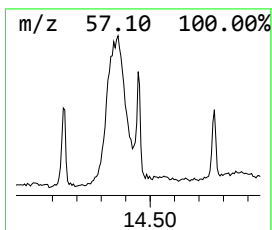
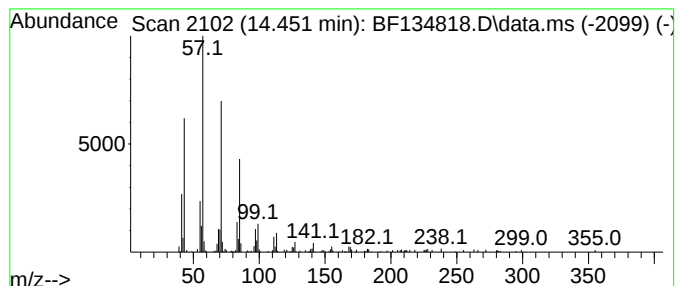
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 6 Pentadecane Concentration Rank 5

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 14.451 | 3.04 ng | 143376 | Chrysene-d12     | 13.969 |

| Hit# | of 5 | Tentative ID                       | MW  | MolForm | CAS#        | Qual |
|------|------|------------------------------------|-----|---------|-------------|------|
| 1    |      | Pentadecane                        | 212 | C15H32  | 000629-62-9 | 95   |
| 2    |      | Hexadecane                         | 226 | C16H34  | 000544-76-3 | 94   |
| 3    |      | Octacosane                         | 394 | C28H58  | 000630-02-4 | 90   |
| 4    |      | Tetracosane                        | 338 | C24H50  | 000646-31-1 | 87   |
| 5    |      | Hexadecane, 2,6,10,14-tetramethyl- | 282 | C20H42  | 000638-36-8 | 87   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF081723\  
Data File : BF134818.D  
Acq On : 17 Aug 2023 11:43  
Operator : CG\JU  
Sample : PB154866BL  
Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PB154866BL

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 ... | 11.851 | 5.1     | ng    | 370696   | 4                     | 11.322 | 1461240 | 20.0 |
| Octadecanoic acid  | 12.645 | 3.1     | ng    | 144489   | 5                     | 13.969 | 943159  | 20.0 |
| Methyl (S)-5-((... | 13.321 | 20.0    | ng    | 943415   | 5                     | 13.969 | 943159  | 20.0 |
| Eicosane           | 14.145 | 2.4     | ng    | 113630   | 5                     | 13.969 | 943159  | 20.0 |
| Octacosane         | 14.351 | 7.7     | ng    | 362340   | 5                     | 13.969 | 943159  | 20.0 |
| Pentadecane        | 14.451 | 3.0     | ng    | 143376   | 5                     | 13.969 | 943159  | 20.0 |