

Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM092023\  
 Data File : BM041941.D  
 Acq On : 20 Sep 2023 16:48  
 Operator : MA/JU  
 Sample : 04436-14  
 Misc :  
 ALS Vial : 12 Sample Multiplier: 1

Instrument :  
 BNA\_M  
 ClientSampleId :  
 CPT102-23

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\_M\Methods\8270-BM091823.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM041941.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         | 5.057       | 314           | 318         | 324          | rVB      | 145221         | 203092        | 1.88%           | 0.344%        |
| 2         | 5.498       | 386           | 393         | 403          | rBV      | 3776881        | 5368757       | 49.72%          | 9.100%        |
| 3         | 7.104       | 658           | 666         | 678          | rBV      | 3791058        | 6004194       | 55.60%          | 10.177%       |
| 4         | 7.957       | 805           | 811         | 820          | rBV      | 933573         | 1482436       | 13.73%          | 2.513%        |
| 5         | 9.151       | 1002          | 1014        | 1025         | rBV      | 2284061        | 3725255       | 34.50%          | 6.314%        |
| 6         | 10.775      | 1281          | 1290        | 1299         | rBV      | 1254232        | 2138000       | 19.80%          | 3.624%        |
| 7         | 13.221      | 1699          | 1706        | 1714         | rBV      | 5315389        | 7787203       | 72.11%          | 13.199%       |
| 8         | 14.604      | 1933          | 1941        | 1950         | rBV      | 1956778        | 2907320       | 26.92%          | 4.928%        |
| 9         | 16.098      | 2188          | 2195        | 2209         | rBV      | 4756939        | 6831441       | 63.26%          | 11.579%       |
| 10        | 17.356      | 2403          | 2409        | 2415         | rBV      | 2519237        | 3502909       | 32.44%          | 5.937%        |
| 11        | 18.203      | 2547          | 2553        | 2562         | rBV2     | 359815         | 578083        | 5.35%           | 0.980%        |
| 12        | 19.474      | 2765          | 2769        | 2777         | rBV      | 99192          | 149411        | 1.38%           | 0.253%        |
| 13        | 19.968      | 2847          | 2853        | 2862         | rBV      | 8750638        | 10798761      | 100.00%         | 18.303%       |
| 14        | 20.633      | 2963          | 2966        | 2975         | rVB      | 199434         | 255427        | 2.37%           | 0.433%        |
| 15        | 21.191      | 3057          | 3061        | 3071         | rBV      | 599427         | 868590        | 8.04%           | 1.472%        |
| 16        | 21.527      | 3113          | 3118        | 3123         | rBV      | 2636560        | 3440960       | 31.86%          | 5.832%        |
| 17        | 23.944      | 3522          | 3529        | 3540         | rVB      | 1443415        | 2957266       | 27.39%          | 5.012%        |

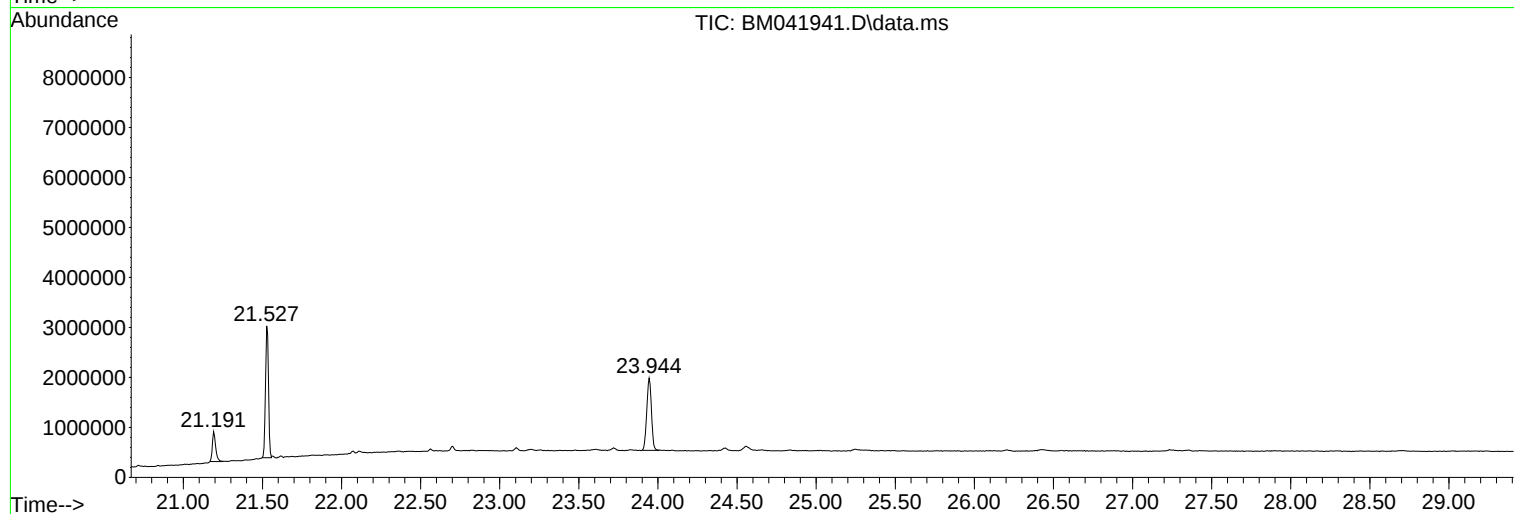
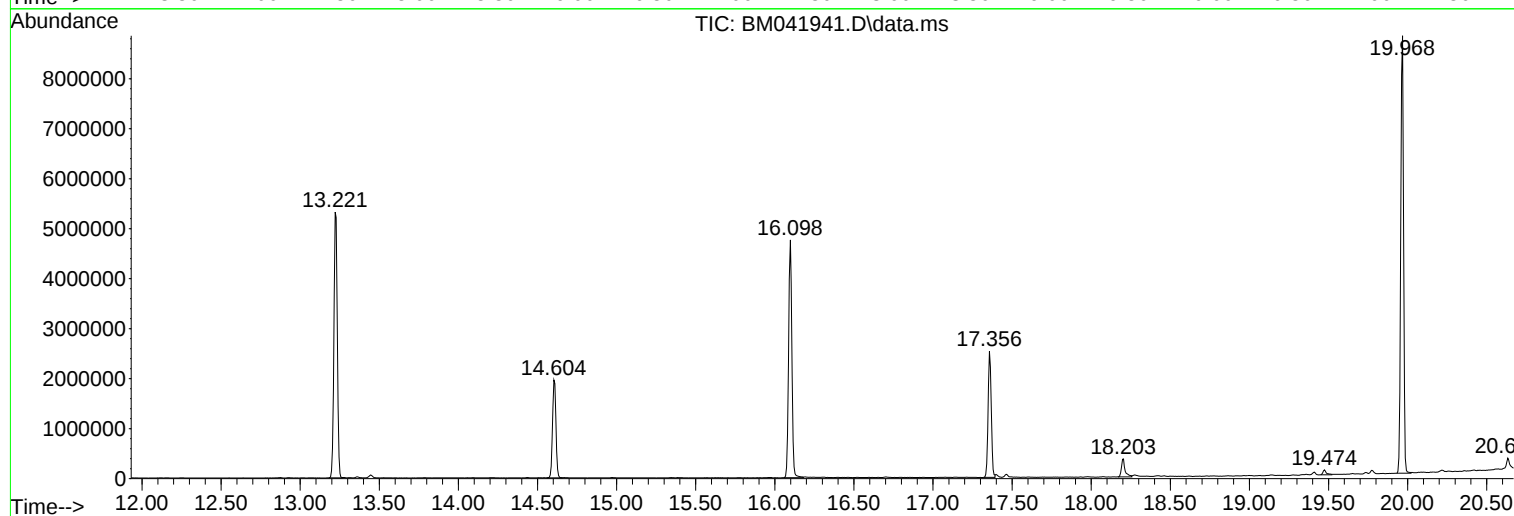
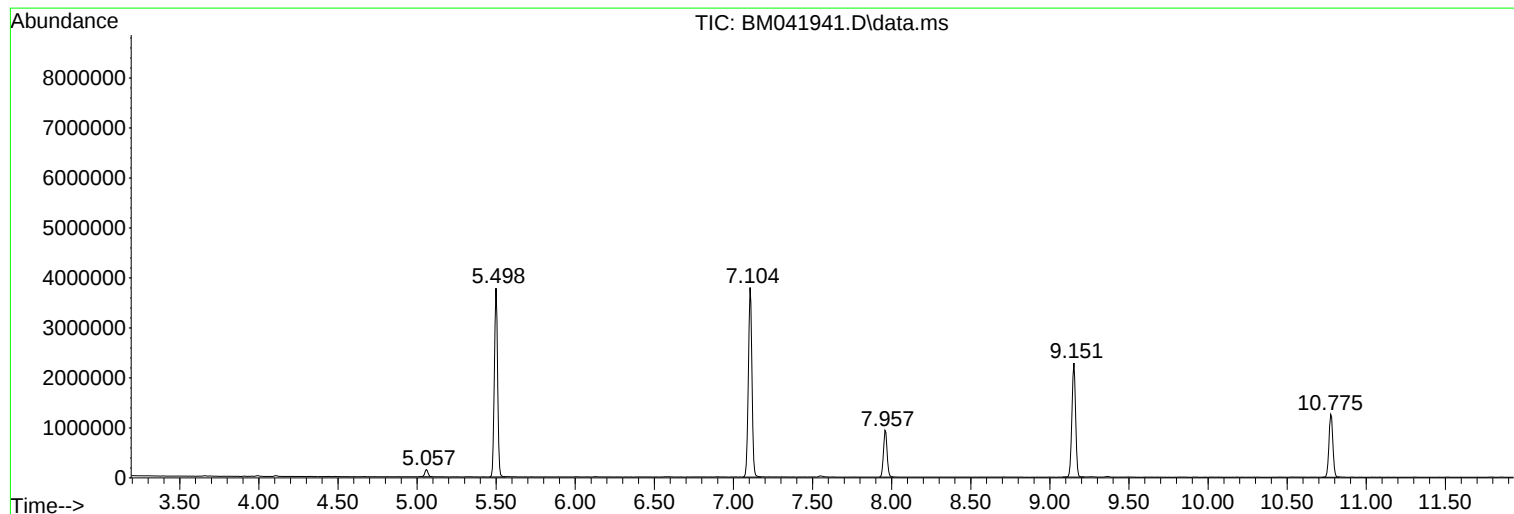
Sum of corrected areas: 58999105

Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM092023\  
Data File : BM041941.D  
Acq On : 20 Sep 2023 16:48  
Operator : MA/JU  
Sample : 04436-14  
Misc :  
ALS Vial : 12 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
CPT102-23

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM091823.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM092023\  
Data File : BM041941.D  
Acq On : 20 Sep 2023 16:48  
Operator : MA/JU  
Sample : 04436-14  
Misc :  
ALS Vial : 12 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
CPT102-23

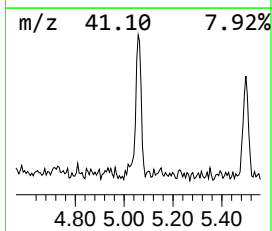
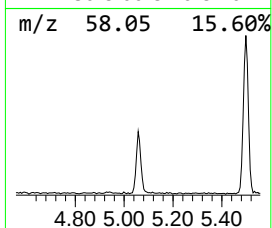
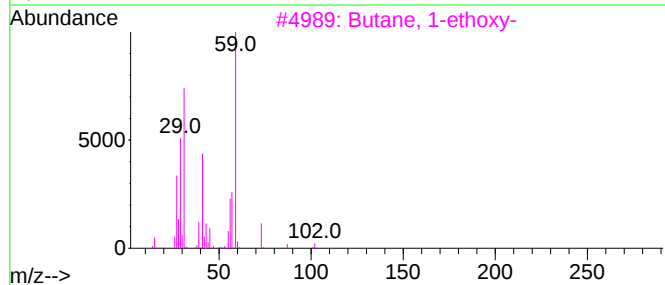
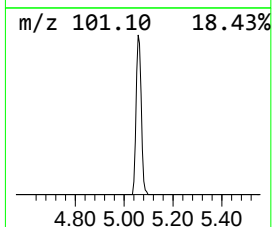
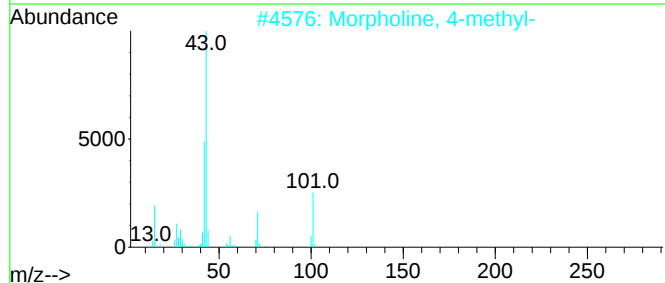
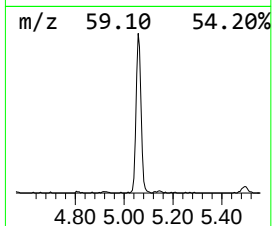
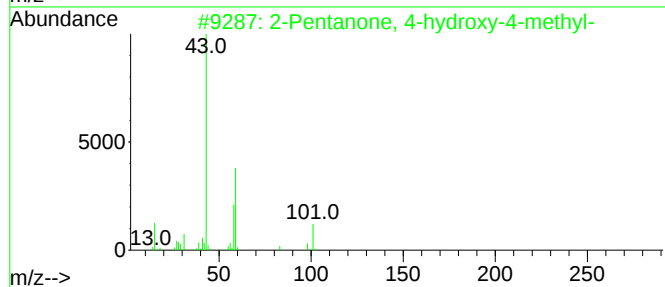
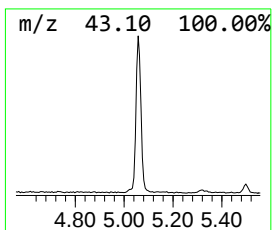
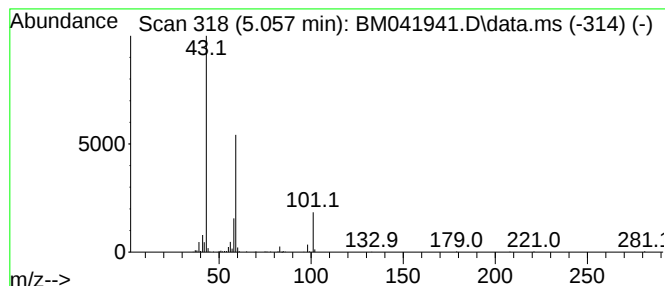
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM091823.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T.  | EstConc | Area   | Relative to ISTD       | R.T.  |
|-------|---------|--------|------------------------|-------|
| 5.057 | 2.74 ng | 203092 | 1,4-Dichlorobenzene-d4 | 7.957 |

| Hit# | of                               | 5   | Tentative ID | MW          | MolForm | CAS# | Qual |
|------|----------------------------------|-----|--------------|-------------|---------|------|------|
| 1    | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2      | 000123-42-2 | 56      |      |      |
| 2    | Morpholine, 4-methyl-            | 101 | C5H11NO      | 000109-02-4 | 9       |      |      |
| 3    | Butane, 1-ethoxy-                | 102 | C6H14O       | 000628-81-9 | 9       |      |      |
| 4    | Acetamide, N-(aminocarbonyl)-    | 102 | C3H6N2O2     | 000591-07-1 | 9       |      |      |
| 5    | Guanidine                        | 59  | CH5N3        | 000113-00-8 | 9       |      |      |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM092023\  
Data File : BM041941.D  
Acq On : 20 Sep 2023 16:48  
Operator : MA/JU  
Sample : 04436-14  
Misc :  
ALS Vial : 12 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
CPT102-23

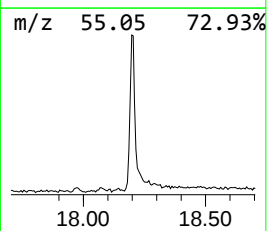
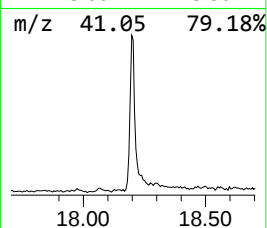
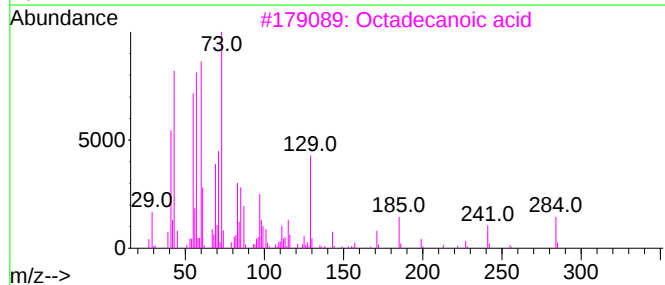
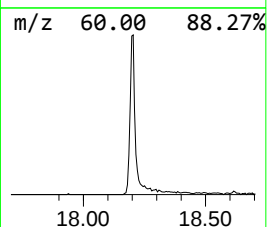
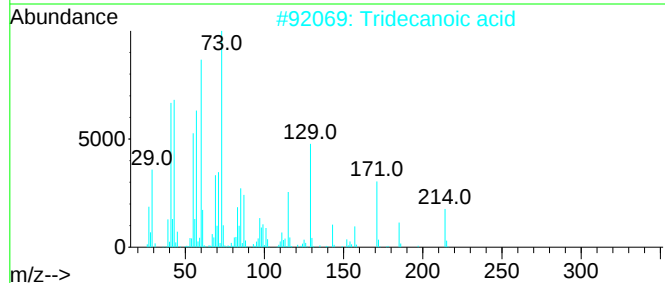
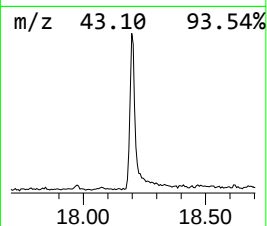
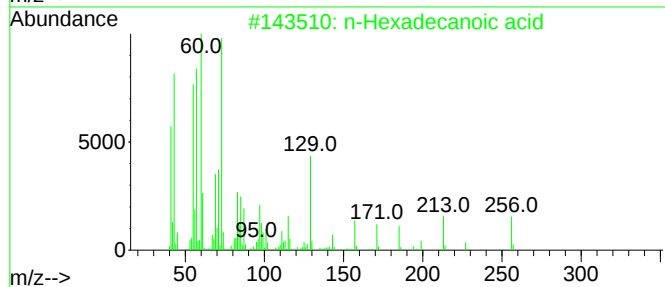
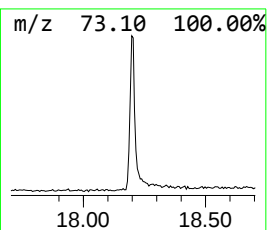
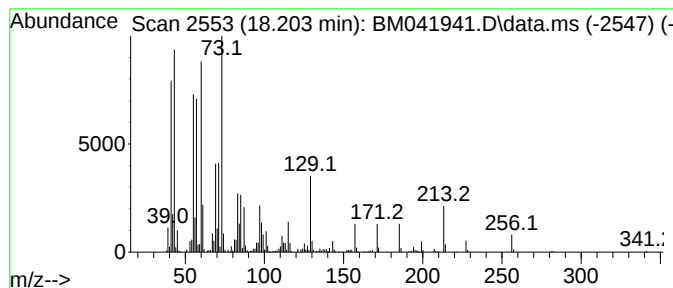
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM091823.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 18.203 | 3.30 ng | 578083 | Phenanthrene-d10 | 17.356 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 98   |
| 2    |    |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 92   |
| 3    |    |   | Octadecanoic acid   | 284 | C18H36O2 | 000057-11-4 | 90   |
| 4    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 90   |
| 5    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 90   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM092023\  
Data File : BM041941.D  
Acq On : 20 Sep 2023 16:48  
Operator : MA/JU  
Sample : 04436-14  
Misc :  
ALS Vial : 12 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
CPT102-23

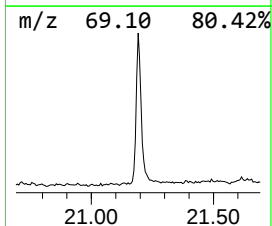
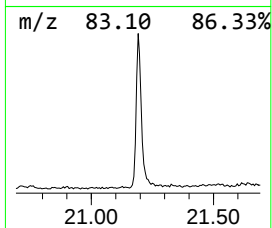
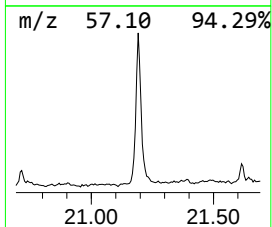
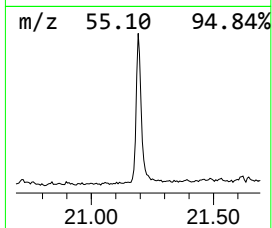
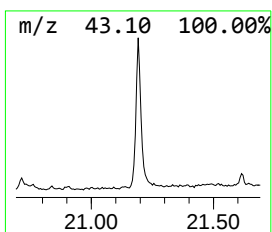
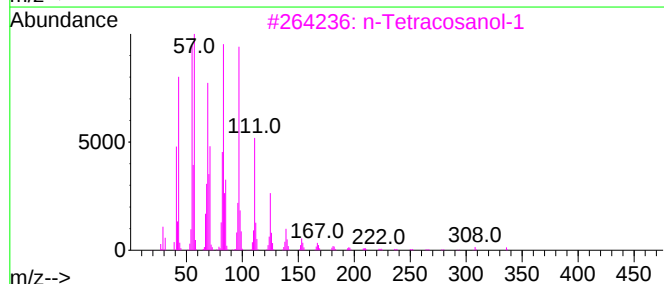
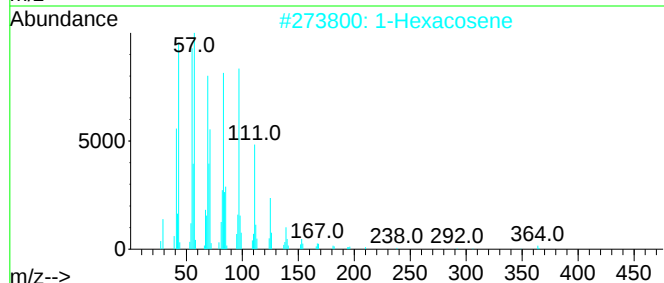
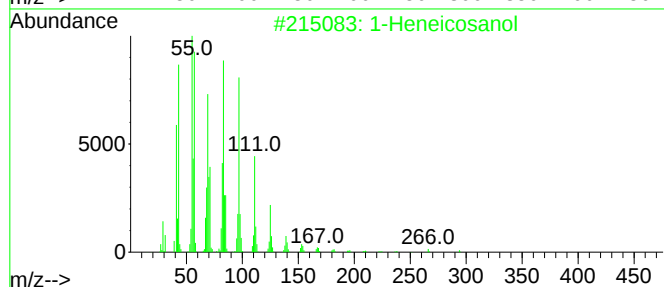
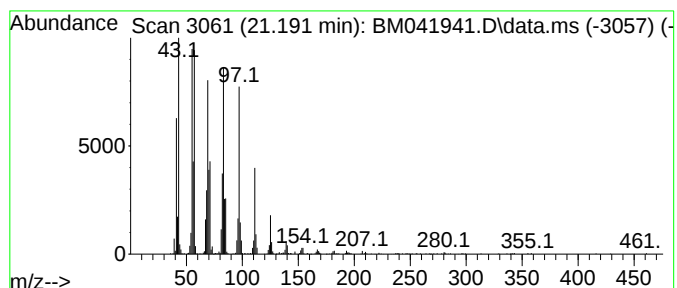
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM091823.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*

Peak Number 3 1-Heneicosanol Concentration Rank 1

| R.T.      | EstConc          | Area   | Relative to ISTD | R.T.        |      |
|-----------|------------------|--------|------------------|-------------|------|
| 21.192    | 5.05 ng          | 868590 | Chrysene-d12     | 21.527      |      |
| Hit# of 5 | Tentative ID     | MW     | MolForm          | CAS#        | Qual |
| 1         | 1-Heneicosanol   | 312    | C21H44O          | 015594-90-8 | 95   |
| 2         | 1-Hexacosene     | 364    | C26H52           | 018835-33-1 | 94   |
| 3         | n-Tetracosanol-1 | 354    | C24H50O          | 000506-51-4 | 94   |
| 4         | 1-Tetracosene    | 336    | C24H48           | 010192-32-2 | 94   |
| 5         | Pentacos-1-ene   | 350    | C25H50           | 016980-85-1 | 94   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM092023\  
Data File : BM041941.D  
Acq On : 20 Sep 2023 16:48  
Operator : MA/JU  
Sample : 04436-14  
Misc :  
ALS Vial : 12 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
CPT102-23

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM091823.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 |
| 2-Pentanone, 4-... | 5.057  | 2.7     | ng    | 203092   | 1                     | 7.957  | 1482440 | 20.0 |
| n-Hexadecanoic ... | 18.203 | 3.3     | ng    | 578083   | 4                     | 17.356 | 3502910 | 20.0 |
| 1-Heneicosanol     | 21.192 | 5.0     | ng    | 868590   | 5                     | 21.527 | 3440960 | 20.0 |