

Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG072722\  
 Data File : BG054414.D  
 Acq On : 27 Jul 2022 13:31  
 Operator : CG/JU  
 Sample : N3861-07  
 Misc :  
 ALS Vial : 7 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 MW-2

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\_G\Methods\8270-BG071522.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG054414.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         | 3.028       | 3             | 7           | 16           | rVV      | 25833          | 51650         | 2.96%           | 0.861%        |
| 2         | 3.111       | 16            | 21          | 34           | rVB      | 201961         | 330745        | 18.95%          | 5.511%        |
| 3         | 5.561       | 431           | 438         | 452          | rVB      | 83272          | 141218        | 8.09%           | 2.353%        |
| 4         | 7.170       | 705           | 712         | 721          | rBV      | 50816          | 92369         | 5.29%           | 1.539%        |
| 5         | 7.987       | 843           | 851         | 857          | rBB      | 43643          | 75111         | 4.30%           | 1.252%        |
| 6         | 9.151       | 1041          | 1049        | 1057         | rBV      | 154650         | 282113        | 16.17%          | 4.701%        |
| 7         | 10.796      | 1321          | 1329        | 1336         | rBV      | 59836          | 109595        | 6.28%           | 1.826%        |
| 8         | 13.246      | 1738          | 1746        | 1754         | rBV      | 506257         | 825950        | 47.33%          | 13.763%       |
| 9         | 14.621      | 1974          | 1980        | 1987         | rBB      | 123163         | 190595        | 10.92%          | 3.176%        |
| 10        | 16.113      | 2227          | 2234        | 2247         | rBV      | 585833         | 895634        | 51.32%          | 14.925%       |
| 11        | 17.364      | 2441          | 2447        | 2454         | rVB      | 182559         | 284305        | 16.29%          | 4.738%        |
| 12        | 18.022      | 2555          | 2559        | 2564         | rVB      | 30606          | 37601         | 2.15%           | 0.627%        |
| 13        | 18.252      | 2592          | 2598        | 2608         | rBV3     | 29864          | 51277         | 2.94%           | 0.854%        |
| 14        | 19.527      | 2808          | 2815        | 2820         | rBV3     | 22198          | 40159         | 2.30%           | 0.669%        |
| 15        | 19.973      | 2885          | 2891        | 2897         | rBV      | 1225576        | 1745158       | 100.00%         | 29.081%       |
| 16        | 21.266      | 3106          | 3111        | 3120         | rBV3     | 40416          | 74248         | 4.25%           | 1.237%        |
| 17        | 21.630      | 3167          | 3173        | 3180         | rVB      | 208585         | 353276        | 20.24%          | 5.887%        |
| 18        | 23.281      | 3450          | 3454        | 3461         | rVB3     | 15313          | 28678         | 1.64%           | 0.478%        |
| 19        | 24.826      | 3708          | 3717        | 3731         | rVB3     | 129555         | 391407        | 22.43%          | 6.522%        |

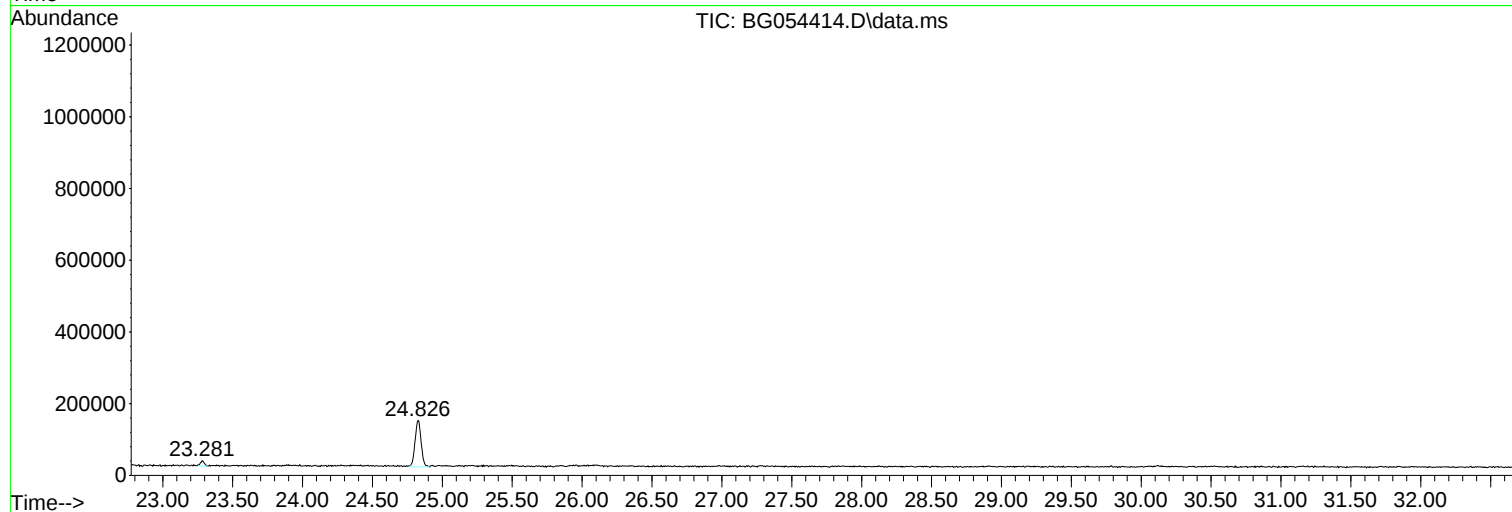
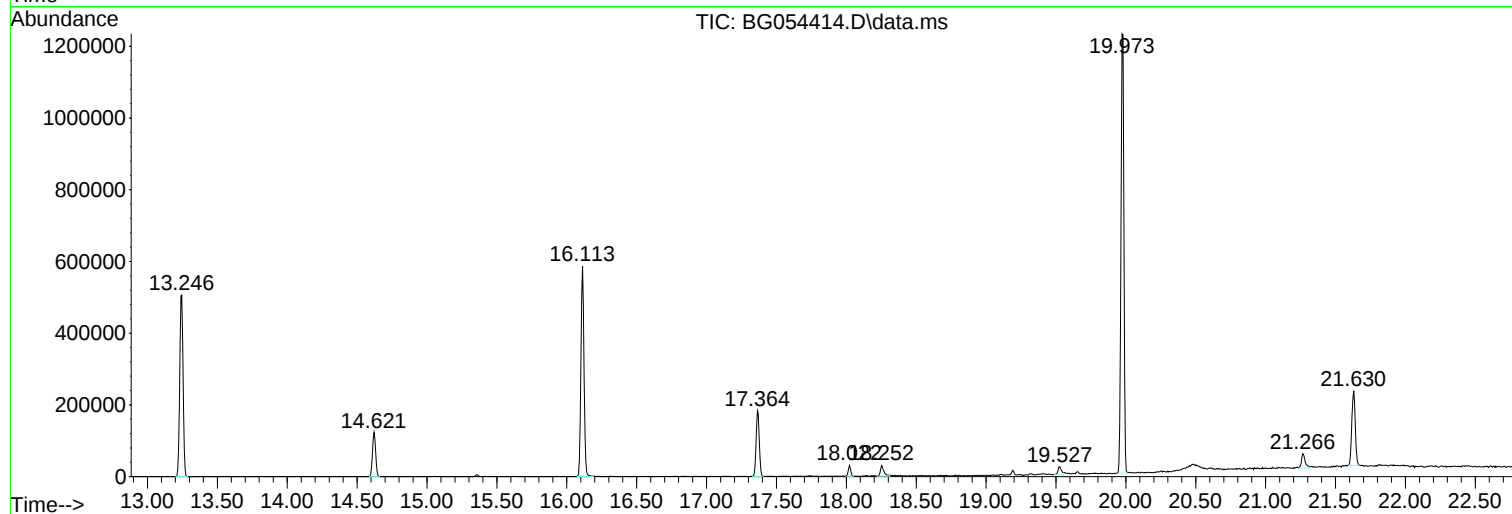
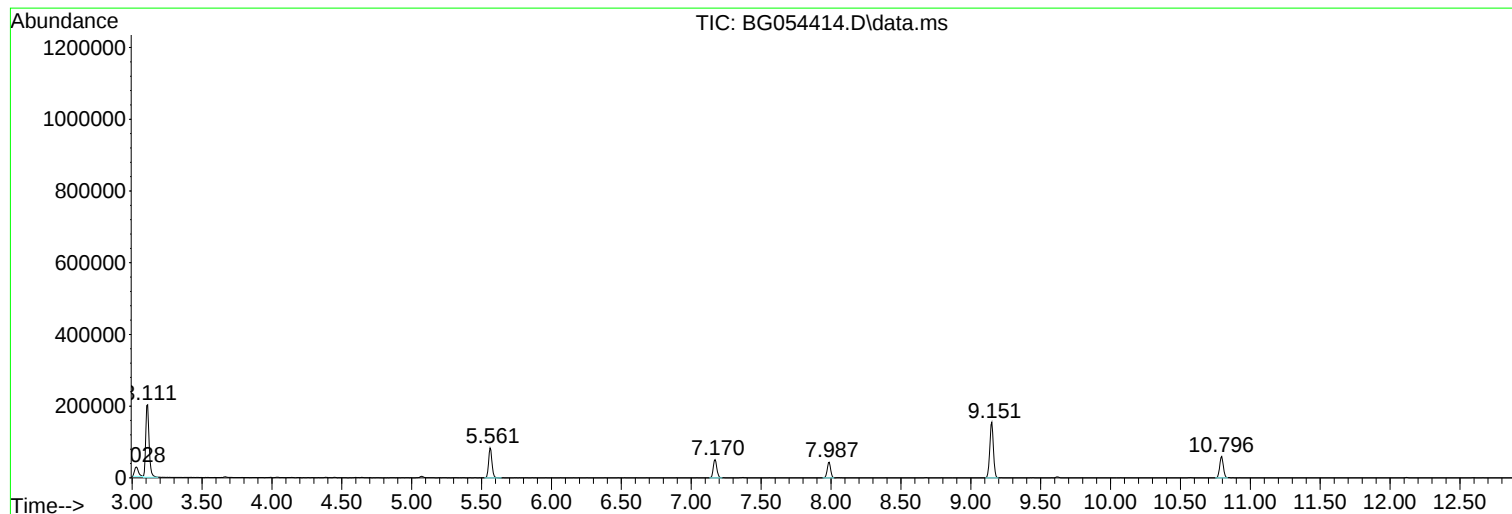
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Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG072722\  
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Misc :  
ALS Vial : 7 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
MW-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG071522.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\_G\Data\BG072722\  
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Instrument :  
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ClientSampleId :  
MW-2

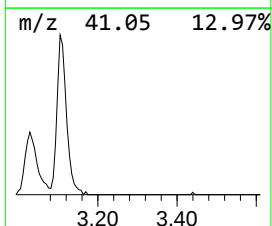
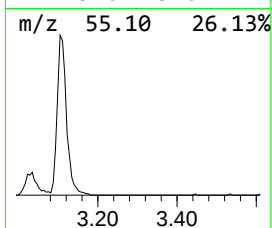
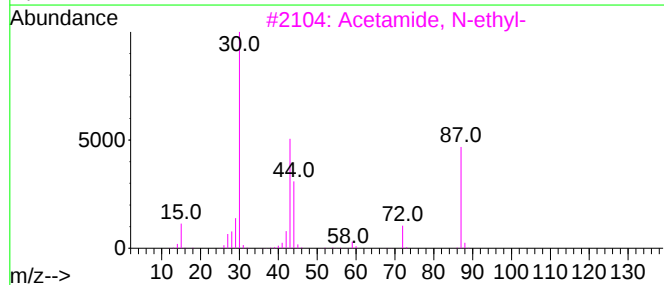
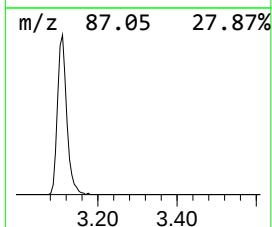
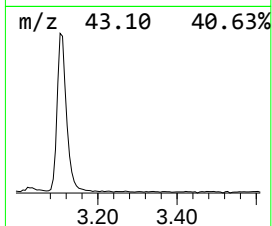
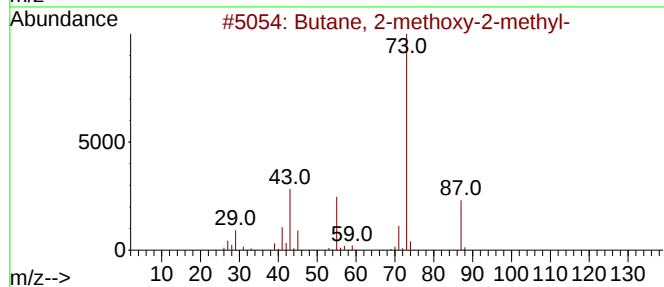
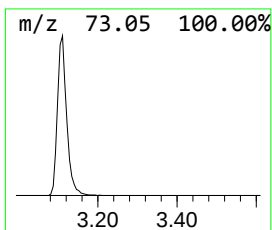
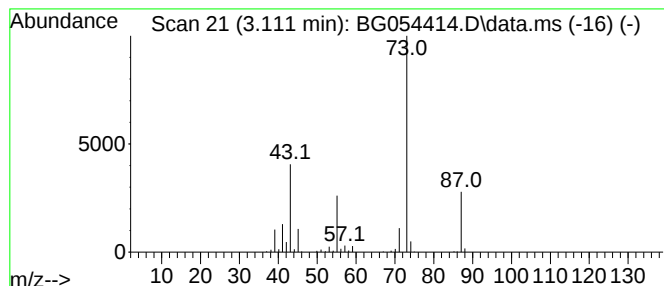
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 1

| R.T.  | EstConc  | Area   | Relative to ISTD       | R.T.  |
|-------|----------|--------|------------------------|-------|
| 3.111 | 88.07 ng | 330745 | 1,4-Dichlorobenzene-d4 | 7.987 |

| Hit# | of | 5 | Tentative ID                | MW  | MolForm | CAS#        | Qual |
|------|----|---|-----------------------------|-----|---------|-------------|------|
| 1    |    |   | Butane, 2-methoxy-2-methyl- | 102 | C6H14O  | 000994-05-8 | 78   |
| 2    |    |   | 2,2,4-Trimethyl-3-pentanol  | 130 | C8H18O  | 005162-48-1 | 39   |
| 3    |    |   | Acetamide, N-ethyl-         | 87  | C4H9NO  | 000625-50-3 | 35   |
| 4    |    |   | Silane, tetramethyl-        | 88  | C4H12Si | 000075-76-3 | 9    |
| 5    |    |   | N-Ethylformamide            | 73  | C3H7NO  | 000627-45-2 | 9    |



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Sample : N3861-07  
Misc :  
ALS Vial : 7 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
MW-2

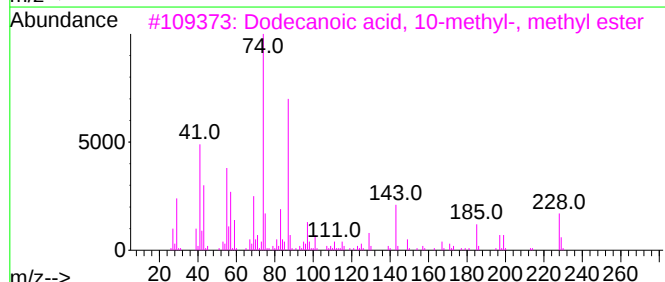
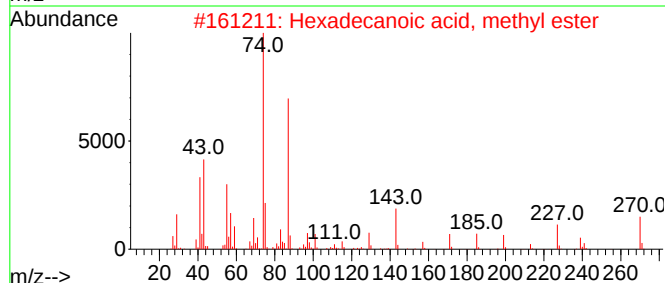
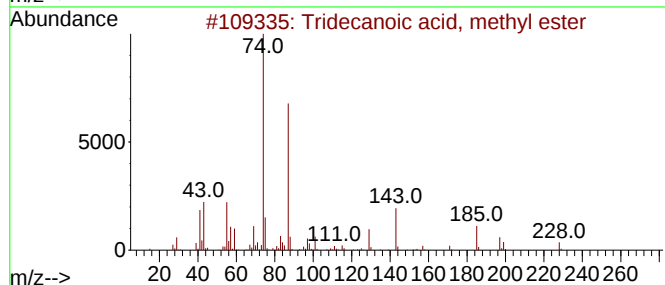
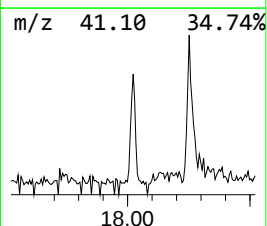
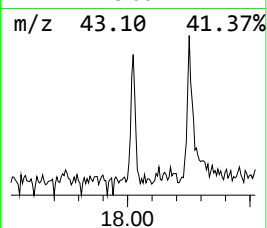
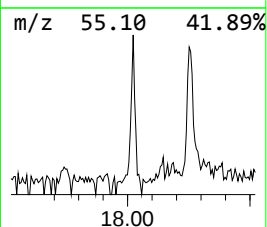
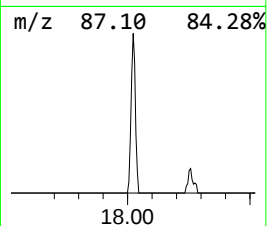
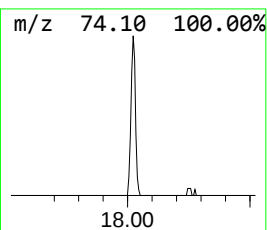
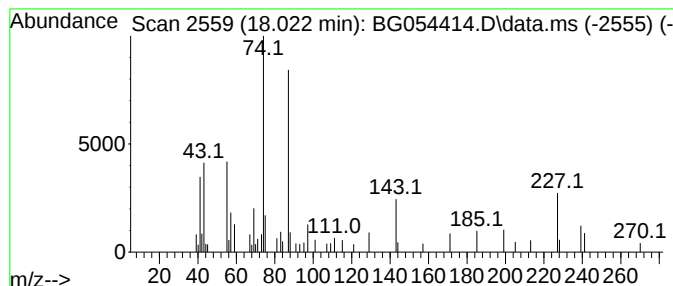
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG071522.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 3 Tridecanoic acid, methyl ester Concentration Rank 5

| R.T.      | EstConc                             | Area  | Relative to ISTD | R.T.        |      |
|-----------|-------------------------------------|-------|------------------|-------------|------|
| 18.023    | 2.65 ng                             | 37601 | Phenanthrene-d10 | 17.364      |      |
| Hit# of 5 | Tentative ID                        | MW    | MolForm          | CAS#        | Qual |
| 1         | Tridecanoic acid, methyl ester      | 228   | C14H28O2         | 001731-88-0 | 93   |
| 2         | Hexadecanoic acid, methyl ester     | 270   | C17H34O2         | 000112-39-0 | 90   |
| 3         | Dodecanoic acid, 10-methyl-, met... | 228   | C14H28O2         | 005129-65-7 | 87   |
| 4         | Methyl 9-methyltetradecanoate       | 256   | C16H32O2         | 213617-69-7 | 80   |
| 5         | Tridecanoic acid, 12-methyl-, me... | 242   | C15H30O2         | 005129-58-8 | 72   |



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Misc :  
ALS Vial : 7 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
MW-2

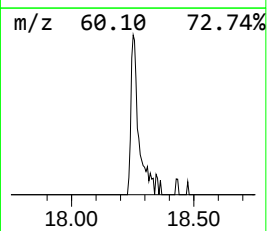
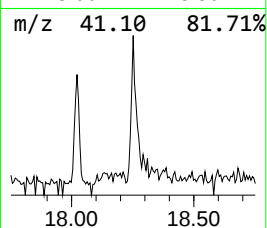
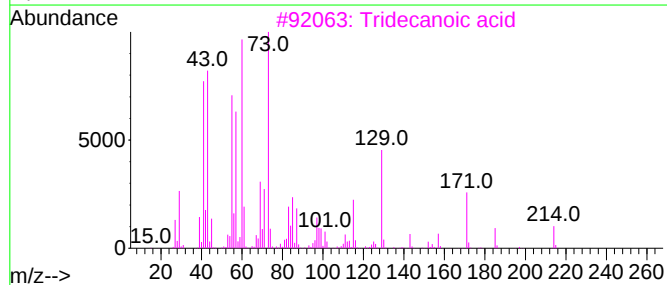
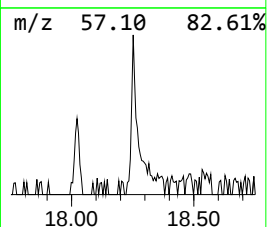
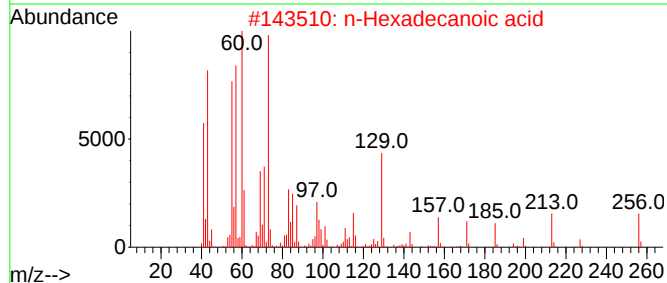
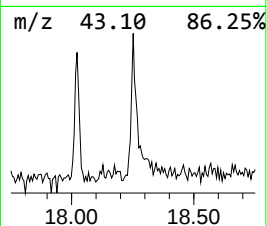
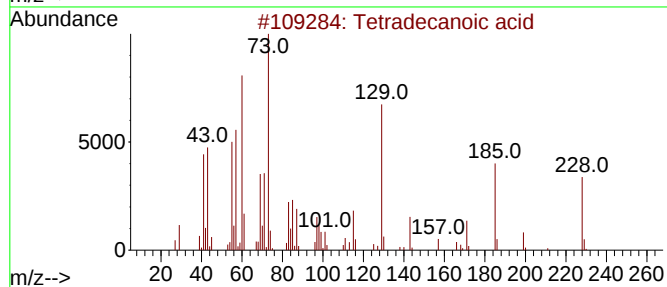
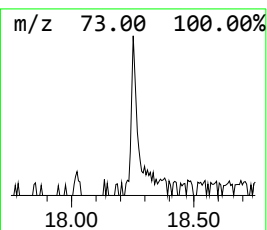
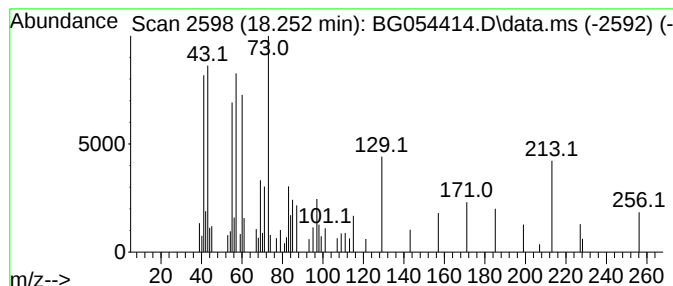
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG071522.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 4 Tetradecanoic acid Concentration Rank 4

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 18.252 | 3.61 ng | 51277 | Phenanthrene-d10 | 17.364 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 94   |
| 2    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 64   |
| 3    |    |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 52   |
| 4    |    |   | Dodecanoic acid     | 200 | C12H24O2 | 000143-07-7 | 47   |
| 5    |    |   | n-Decanoic acid     | 172 | C10H20O2 | 000334-48-5 | 38   |



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Sample : N3861-07  
Misc :  
ALS Vial : 7 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
MW-2

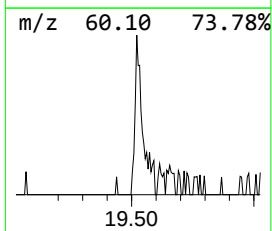
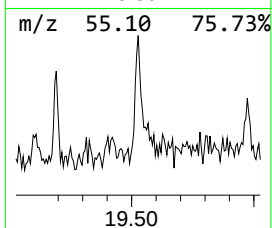
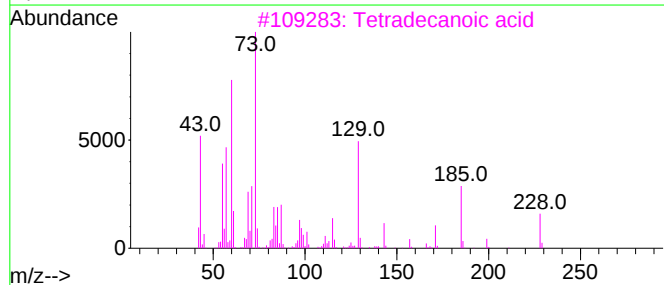
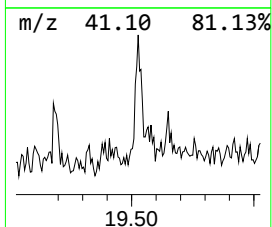
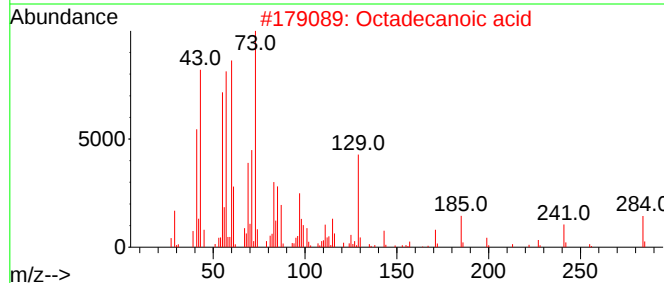
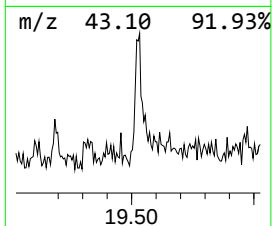
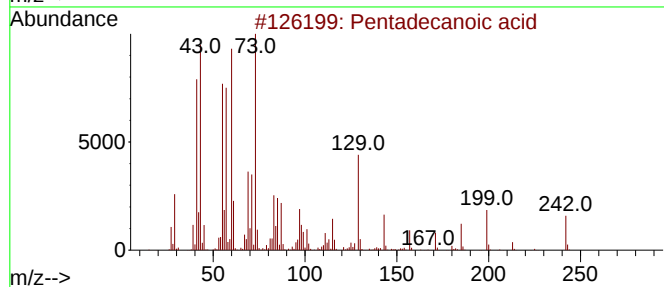
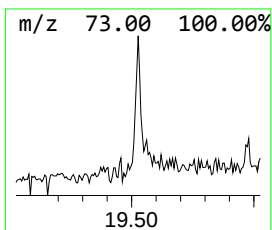
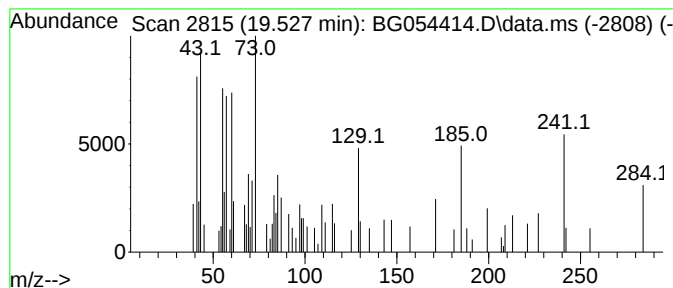
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 5 Pentadecanoic acid Concentration Rank 6

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 19.527 | 2.27 ng | 40159 | Chrysene-d12     | 21.630 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 93   |
| 2    |    |   | Octadecanoic acid   | 284 | C18H36O2 | 000057-11-4 | 92   |
| 3    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 43   |
| 4    |    |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 43   |
| 5    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 41   |



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BNA\_G  
ClientSampleId :  
MW-2

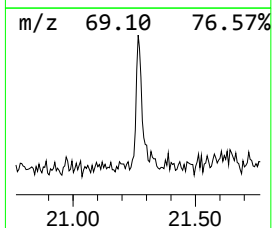
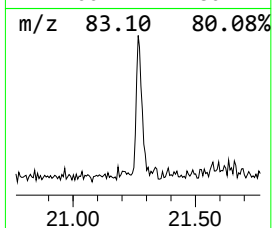
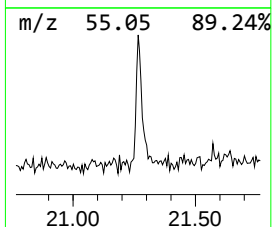
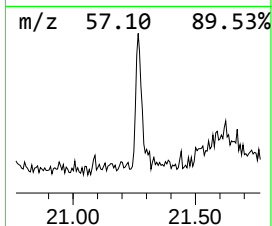
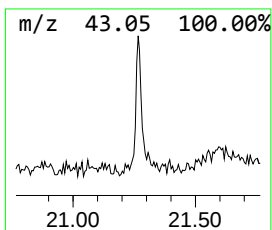
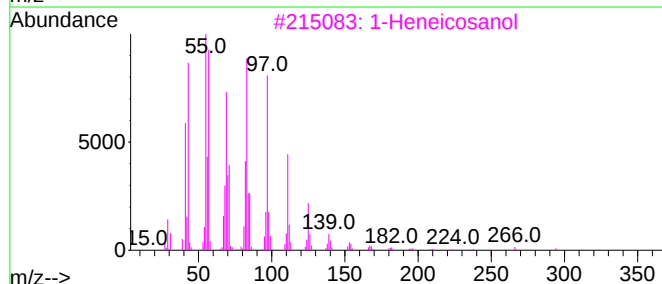
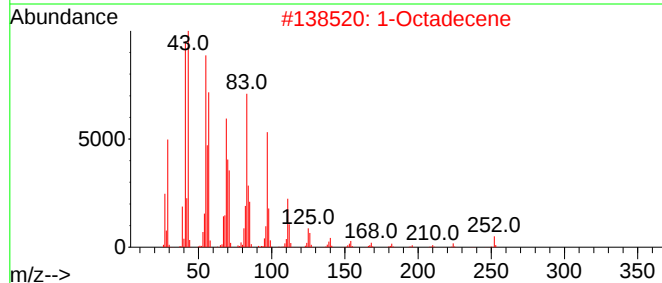
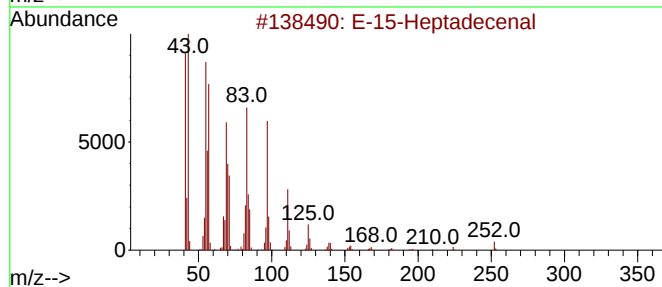
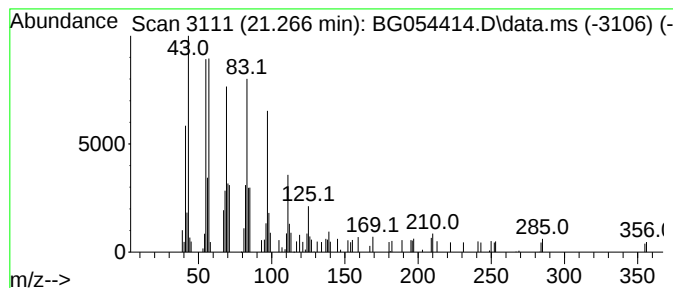
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 6 E-15-Heptadecenal Concentration Rank 3

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 21.266 | 4.20 ng | 74248 | Chrysene-d12     | 21.630 |

| Hit# | of 5 | Tentative ID                | MW  | MolForm    | CAS#         | Qual |
|------|------|-----------------------------|-----|------------|--------------|------|
| 1    |      | E-15-Heptadecenal           | 252 | C17H32O    | 1000130-97-9 | 95   |
| 2    |      | 1-Octadecene                | 252 | C18H36     | 000112-88-9  | 95   |
| 3    |      | 1-Heneicosanol              | 312 | C21H44O    | 015594-90-8  | 94   |
| 4    |      | Trifluoroacetoxy hexadecane | 338 | C18H33F3O2 | 006222-03-3  | 94   |
| 5    |      | Tetradecyl trifluoroacetate | 310 | C16H29F3O2 | 006222-02-2  | 93   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG072722\  
Data File : BG054414.D  
Acq On : 27 Jul 2022 13:31  
Operator : CG/JU  
Sample : N3861-07  
Misc :  
ALS Vial : 7 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
MW-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG071522.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 |
| Butane, 2-metho... | 3.111  | 88.1    | ng    | 330745   | 1                     | 7.987  | 75111  | 20.0 |
| Tridecanoic aci... | 18.023 | 2.6     | ng    | 37601    | 4                     | 17.364 | 284305 | 20.0 |
| Tetradecanoic acid | 18.252 | 3.6     | ng    | 51277    | 4                     | 17.364 | 284305 | 20.0 |
| Pentadecanoic acid | 19.527 | 2.3     | ng    | 40159    | 5                     | 21.630 | 353276 | 20.0 |
| E-15-Heptadecenal  | 21.266 | 4.2     | ng    | 74248    | 5                     | 21.630 | 353276 | 20.0 |