

Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG062923\  
 Data File : BG057916.D  
 Acq On : 29 Jun 2023 23:02  
 Operator : CG/JU  
 Sample : 03366-03  
 Misc :  
 ALS Vial : 17 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 SB38

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-BG062723.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057916.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         | 5.022       | 323           | 329         | 338          | rVB      | 63458          | 97526         | 5.23%           | 0.718%        |
| 2         | 5.492       | 402           | 409         | 426          | rBV      | 756508         | 1192706       | 63.95%          | 8.783%        |
| 3         | 7.084       | 672           | 680         | 690          | rBV      | 738771         | 1254426       | 67.26%          | 9.237%        |
| 4         | 7.912       | 814           | 821         | 829          | rBV      | 232554         | 388898        | 20.85%          | 2.864%        |
| 5         | 9.076       | 1011          | 1019        | 1027         | rBV      | 450637         | 775856        | 41.60%          | 5.713%        |
| 6         | 10.721      | 1291          | 1299        | 1306         | rBV      | 304886         | 563287        | 30.20%          | 4.148%        |
| 7         | 13.171      | 1709          | 1716        | 1724         | rBV      | 1037443        | 1618748       | 86.79%          | 11.920%       |
| 8         | 14.552      | 1945          | 1951        | 1959         | rBV      | 475544         | 724294        | 38.83%          | 5.333%        |
| 9         | 15.903      | 2176          | 2181        | 2187         | rVB      | 111852         | 159055        | 8.53%           | 1.171%        |
| 10        | 16.038      | 2197          | 2204        | 2217         | rBV      | 784319         | 1203631       | 64.54%          | 8.863%        |
| 11        | 17.295      | 2412          | 2418        | 2423         | rBV      | 554922         | 820498        | 43.99%          | 6.042%        |
| 12        | 17.336      | 2423          | 2425        | 2431         | rVB      | 38604          | 46182         | 2.48%           | 0.340%        |
| 13        | 18.059      | 2543          | 2548        | 2552         | rBV6     | 14267          | 29060         | 1.56%           | 0.214%        |
| 14        | 18.183      | 2564          | 2569        | 2580         | rBV      | 267475         | 431010        | 23.11%          | 3.174%        |
| 15        | 19.346      | 2763          | 2767        | 2774         | rVB      | 141063         | 216770        | 11.62%          | 1.596%        |
| 16        | 19.458      | 2782          | 2786        | 2791         | rBV      | 79610          | 126260        | 6.77%           | 0.930%        |
| 17        | 19.710      | 2825          | 2829        | 2833         | rVB      | 107456         | 144324        | 7.74%           | 1.063%        |
| 18        | 19.910      | 2858          | 2863        | 2868         | rVB      | 1460412        | 1865060       | 100.00%         | 13.734%       |
| 19        | 21.197      | 3079          | 3082        | 3092         | rVB3     | 137612         | 240111        | 12.87%          | 1.768%        |
| 20        | 21.549      | 3136          | 3142        | 3147         | rVB2     | 449470         | 748707        | 40.14%          | 5.513%        |
| 21        | 24.704      | 3672          | 3679        | 3695         | rVB      | 294416         | 933707        | 50.06%          | 6.876%        |

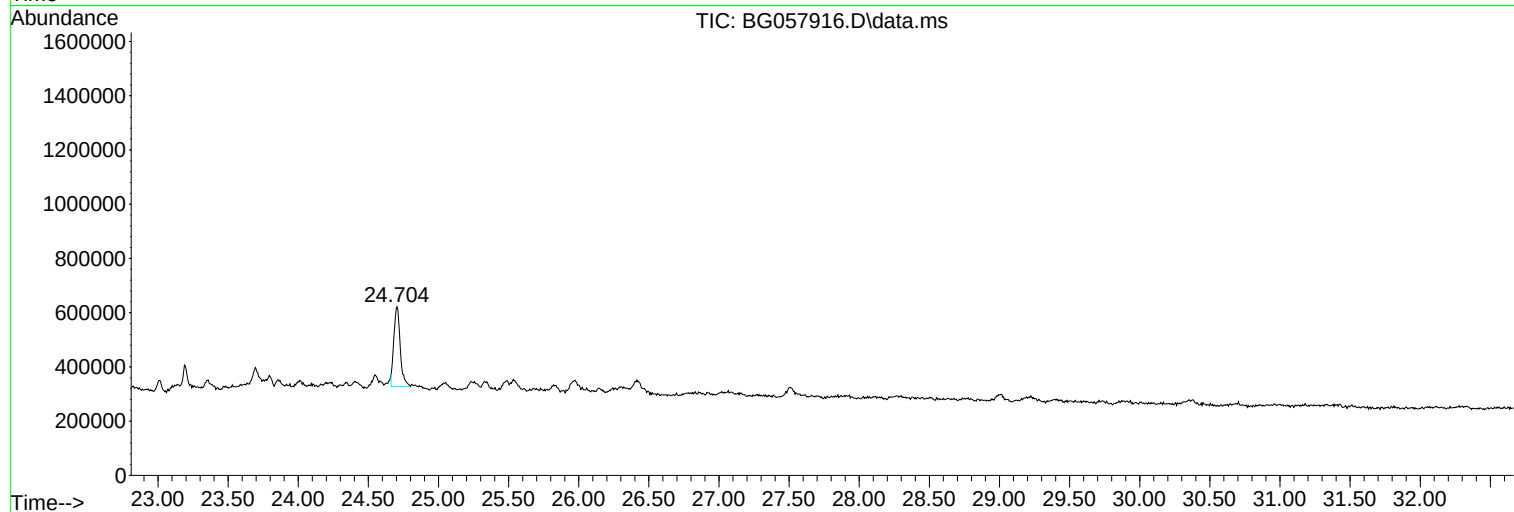
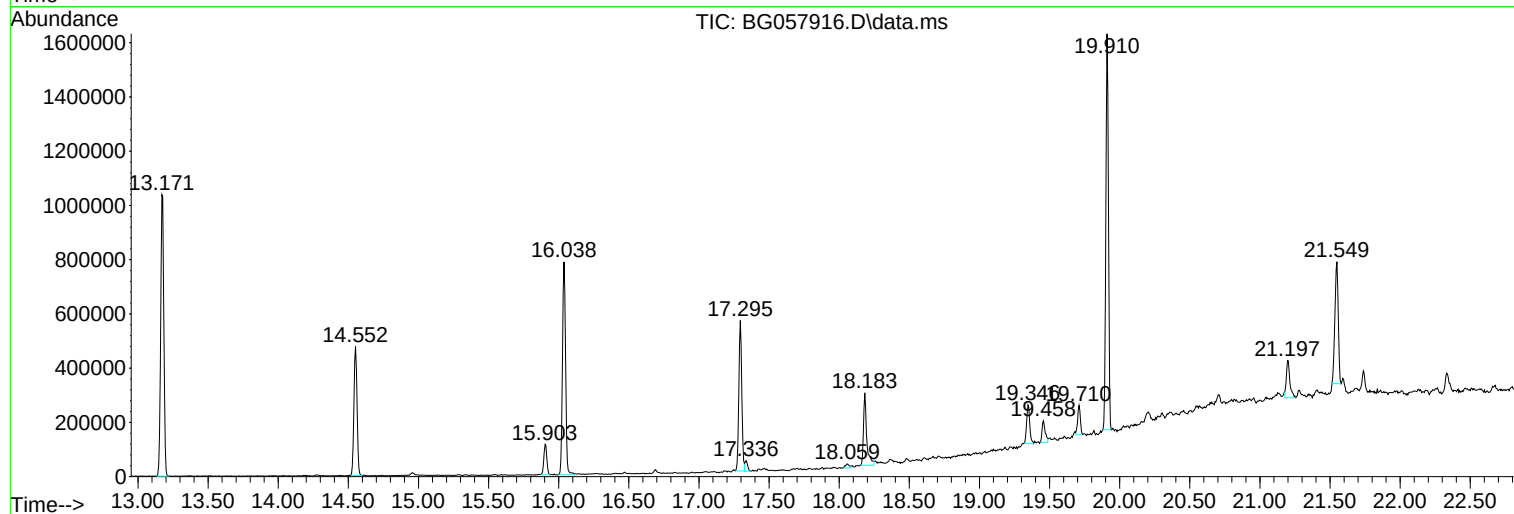
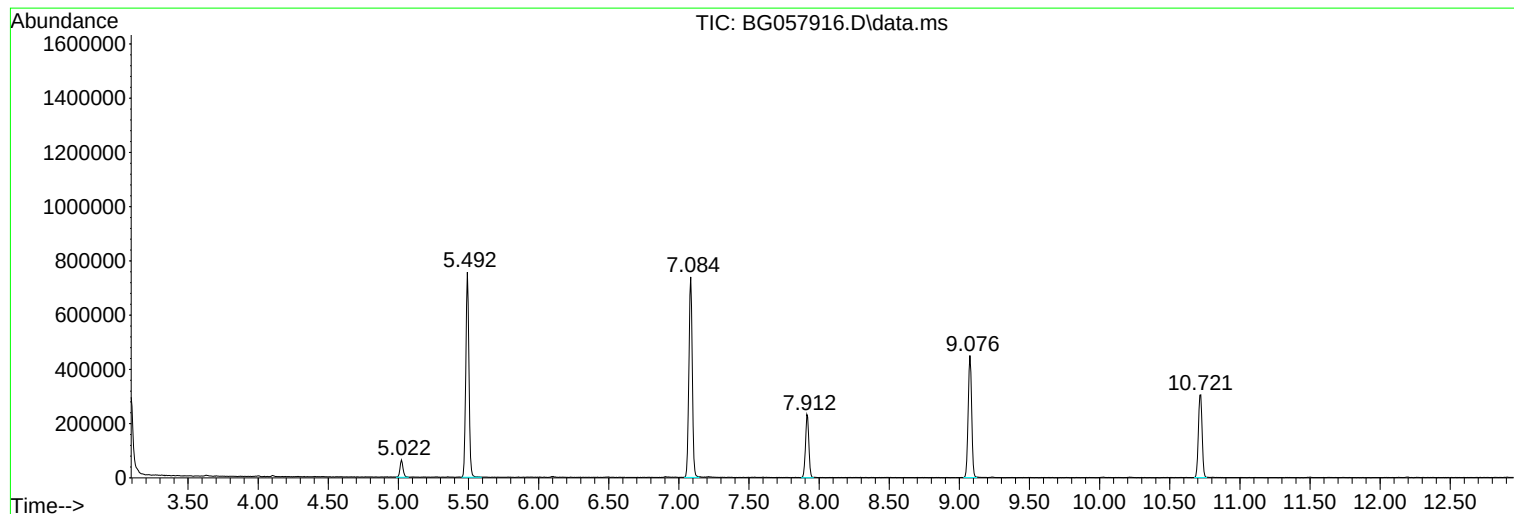
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ALS Vial : 17 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
SB38

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG062723.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\BG062923\  
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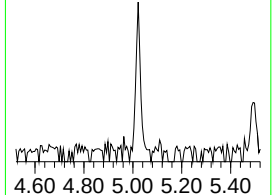
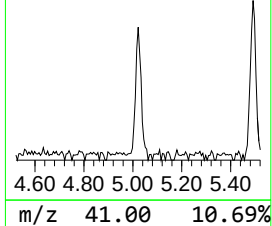
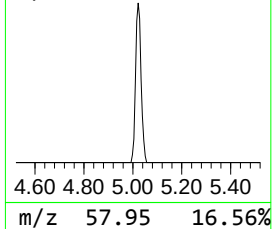
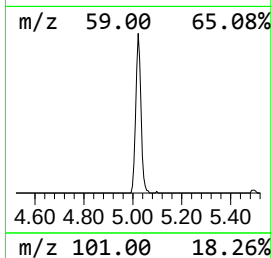
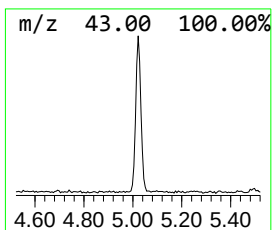
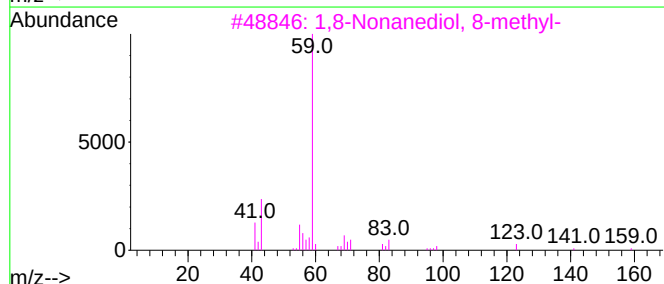
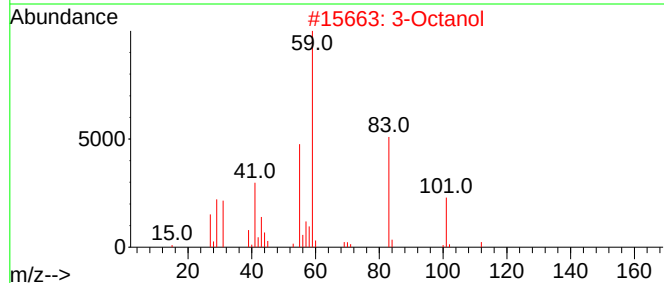
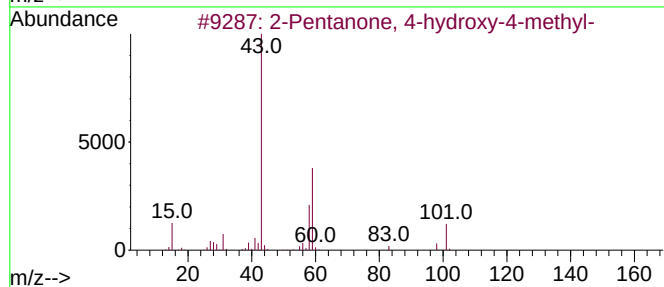
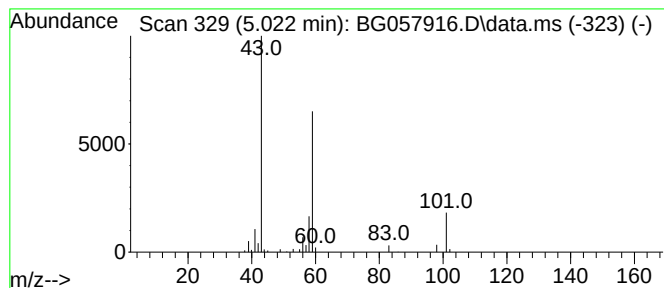
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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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.  |
|-------|---------|-------|------------------------|-------|
| 5.022 | 5.02 ng | 97526 | 1,4-Dichlorobenzene-d4 | 7.912 |

| Hit# | of 5                             | Tentative ID | MW       | MolForm     | CAS# | Qual |
|------|----------------------------------|--------------|----------|-------------|------|------|
| 1    | 2-Pentanone, 4-hydroxy-4-methyl- | 116          | C6H12O2  | 000123-42-2 | 50   |      |
| 2    | 3-Octanol                        | 130          | C8H18O   | 000589-98-0 | 33   |      |
| 3    | 1,8-Nonanediol, 8-methyl-        | 174          | C10H22O2 | 054725-73-4 | 25   |      |
| 4    | Butane, 1-ethoxy-                | 102          | C6H14O   | 000628-81-9 | 9    |      |
| 5    | Morpholine, 4-methyl-            | 101          | C5H11NO  | 000109-02-4 | 9    |      |



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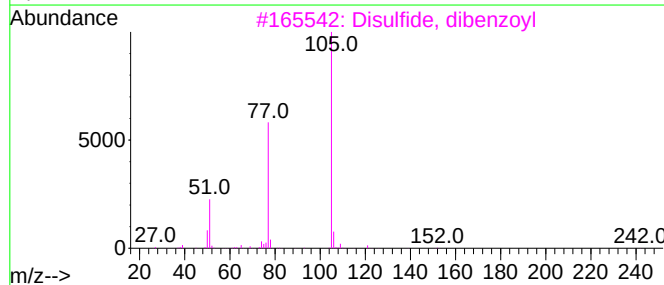
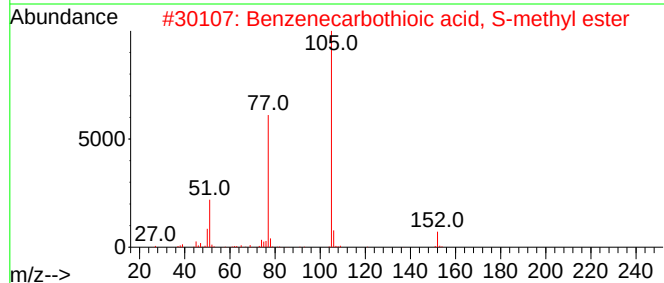
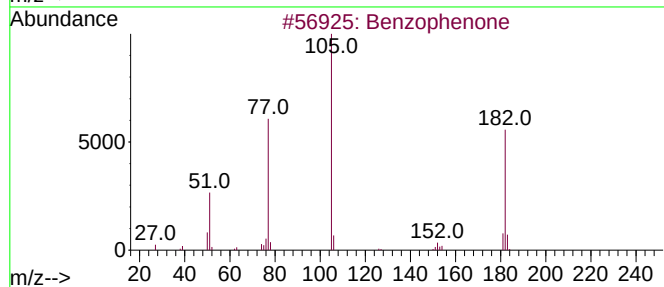
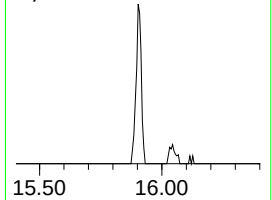
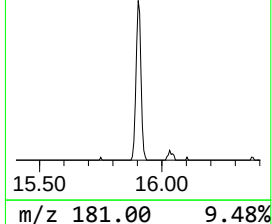
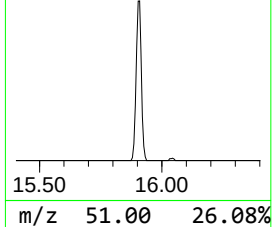
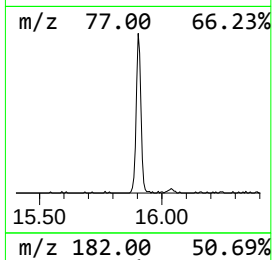
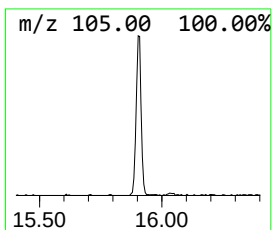
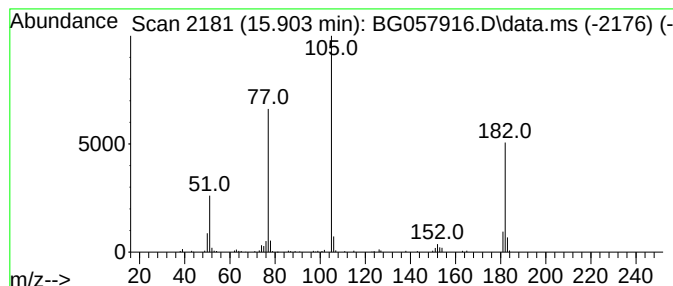
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 2 Benzophenone Concentration Rank 4

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 15.903 | 4.39 ng | 159055 | Acenaphthene-d10 | 14.552 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|------------|--------------|------|
| 1    |    |   | Benzophenone                        | 182 | C13H10O    | 000119-61-9  | 96   |
| 2    |    |   | Benzenecarbothioic acid, S-methy... | 152 | C8H8OS     | 005925-68-8  | 53   |
| 3    |    |   | Disulfide, dibenzoyl                | 274 | C14H10O2S2 | 000644-32-6  | 49   |
| 4    |    |   | 2-Benzoyl-4-bromo-5-methyl-1,2-o... | 281 | C11H8BrNO3 | 1000444-92-3 | 47   |
| 5    |    |   | 2-(2-Oxo-2-phenyl-ethyl)-malonon... | 184 | C11H8N2O   | 1000296-76-9 | 47   |



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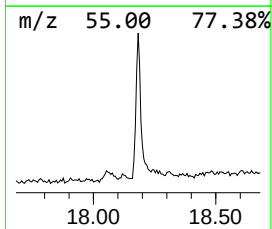
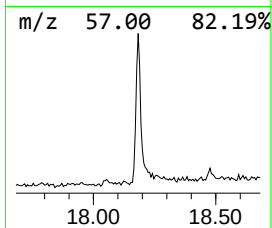
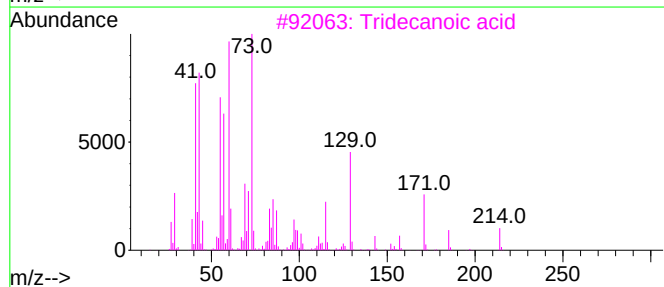
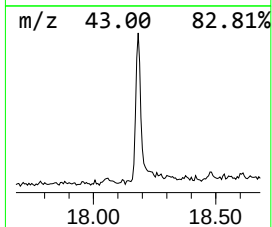
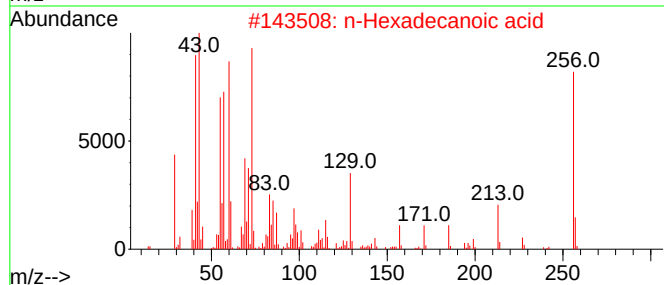
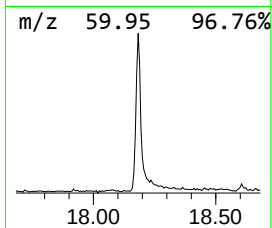
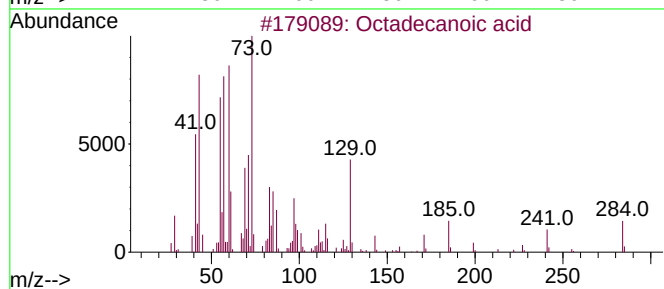
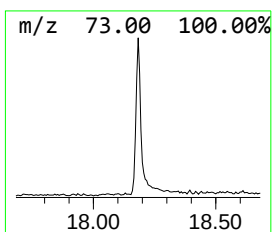
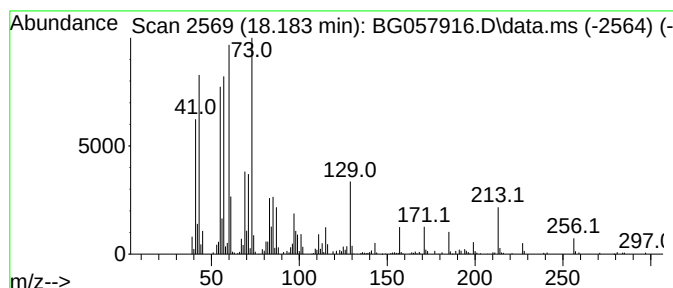
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG062723.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 3 Octadecanoic acid Concentration Rank 1

| R.T.      | EstConc             | Area   | Relative to ISTD | R.T.        |      |
|-----------|---------------------|--------|------------------|-------------|------|
| 18.183    | 10.51 ng            | 431010 | Phenanthrene-d10 | 17.295      |      |
| 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 | 98   |
| 3         | Tridecanoic acid    | 214    | C13H26O2         | 000638-53-9 | 86   |
| 4         | Pentadecanoic acid  | 242    | C15H30O2         | 001002-84-2 | 81   |
| 5         | Tetradecanoic acid  | 228    | C14H28O2         | 000544-63-8 | 62   |



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SB38

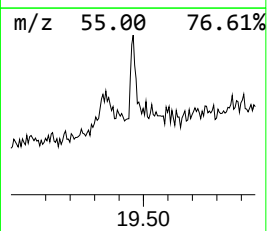
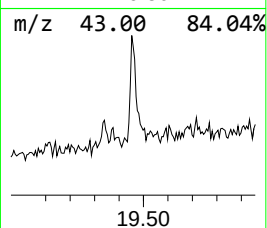
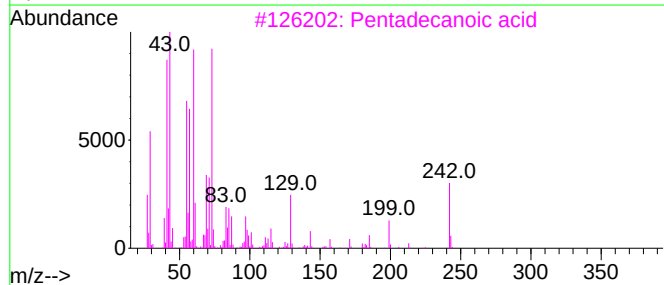
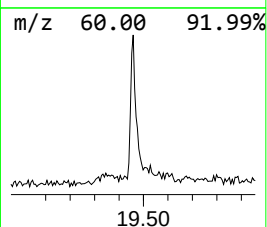
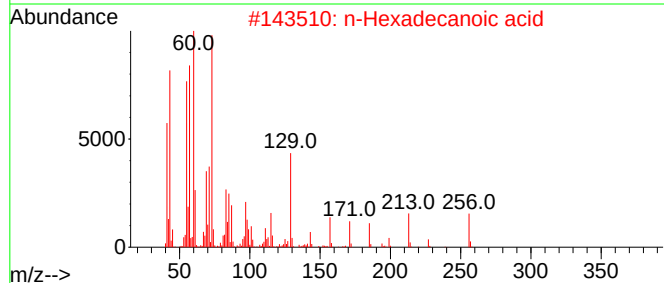
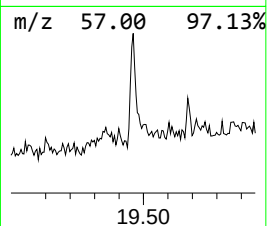
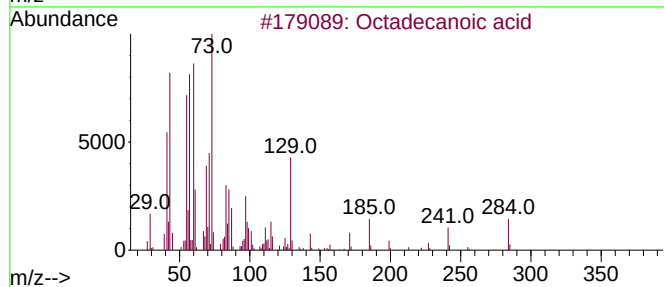
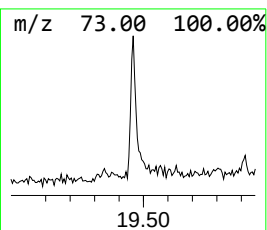
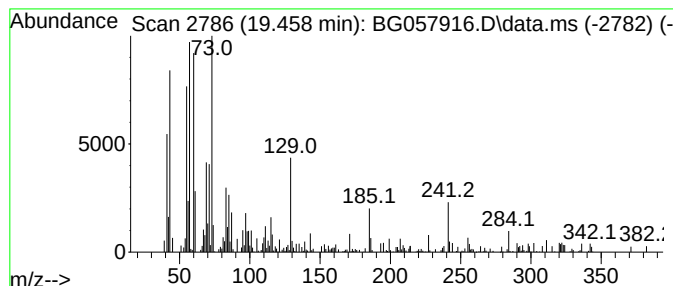
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG062723.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 19.458 | 3.37 ng | 126260 | Chrysene-d12     | 21.549 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | Octadecanoic acid   | 284 | C18H36O2 | 000057-11-4 | 98   |
| 2    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 94   |
| 3    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 90   |
| 4    |    |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 89   |
| 5    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 72   |



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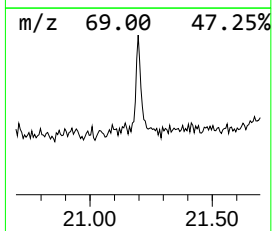
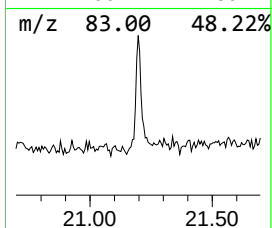
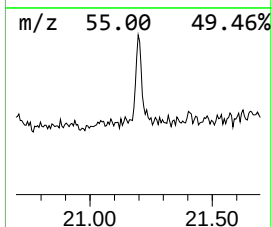
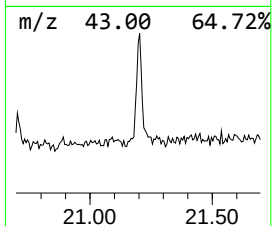
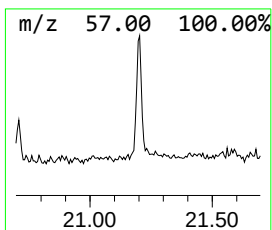
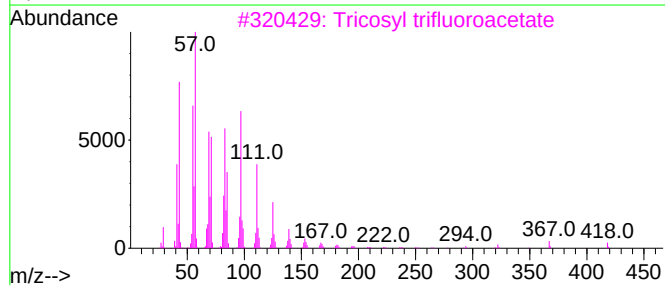
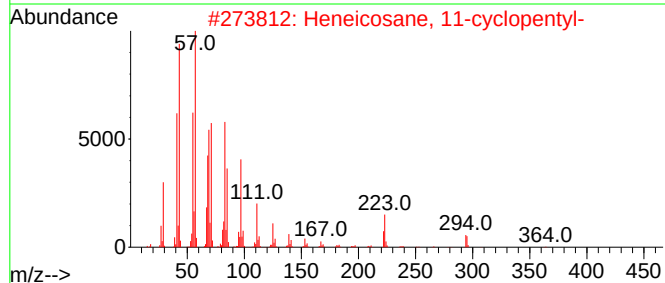
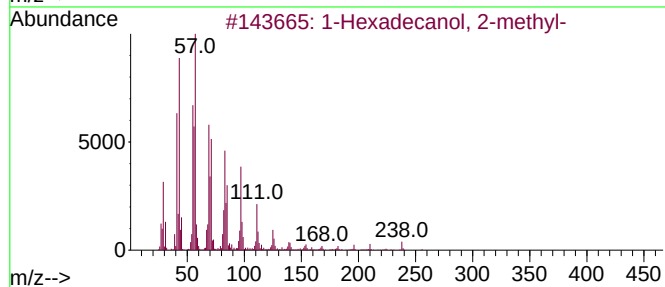
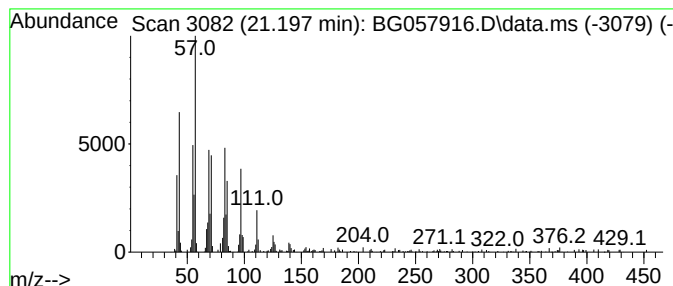
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 5 1-Hexadecanol, 2-methyl- Concentration Rank 2

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 21.197 | 6.41 ng | 240111 | Chrysene-d12     | 21.549 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|------------|--------------|------|
| 1    |    |   | 1-Hexadecanol, 2-methyl-            | 256 | C17H36O    | 002490-48-4  | 93   |
| 2    |    |   | Heneicosane, 11-cyclopentyl-        | 364 | C26H52     | 006703-81-7  | 93   |
| 3    |    |   | Tricosyl trifluoroacetate           | 436 | C25H47F3O2 | 1000351-75-1 | 87   |
| 4    |    |   | Oxalic acid, isobutyl hexadecyl ... | 370 | C22H42O4   | 1000309-38-1 | 87   |
| 5    |    |   | Nonadecyl trifluoroacetate          | 380 | C21H39F3O2 | 1000351-76-3 | 87   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG062923\  
Data File : BG057916.D  
Acq On : 29 Jun 2023 23:02  
Operator : CG/JU  
Sample : 03366-03  
Misc :  
ALS Vial : 17 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
SB38

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG062723.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-... | 5.022  | 5.0     | ng    | 97526    | 1                     | 7.912  | 388898 | 20.0 |
| Benzophenone       | 15.903 | 4.4     | ng    | 159055   | 3                     | 14.552 | 724294 | 20.0 |
| Octadecanoic acid  | 18.183 | 10.5    | ng    | 431010   | 4                     | 17.295 | 820498 | 20.0 |
| n-Hexadecanoic ... | 19.458 | 3.4     | ng    | 126260   | 5                     | 21.549 | 748707 | 20.0 |
| 1-Hexadecanol, ... | 21.197 | 6.4     | ng    | 240111   | 5                     | 21.549 | 748707 | 20.0 |