

Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG062923\  
 Data File : BG057908.D  
 Acq On : 29 Jun 2023 17:26  
 Operator : CG/JU  
 Sample : 03358-05  
 Misc :  
 ALS Vial : 9 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 SB-4-(8-10)

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: BG057908.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         | 5.016       | 323           | 328         | 337          | rVB      | 24423          | 37738         | 1.76%           | 0.306%        |
| 2         | 5.492       | 402           | 409         | 421          | rBV      | 628267         | 1013829       | 47.20%          | 8.231%        |
| 3         | 7.085       | 672           | 680         | 691          | rBV      | 625388         | 1085457       | 50.53%          | 8.813%        |
| 4         | 7.913       | 815           | 821         | 828          | rBV      | 152131         | 249759        | 11.63%          | 2.028%        |
| 5         | 9.076       | 1011          | 1019        | 1029         | rBV      | 348177         | 616919        | 28.72%          | 5.009%        |
| 6         | 10.716      | 1288          | 1298        | 1306         | rBV      | 207210         | 365863        | 17.03%          | 2.970%        |
| 7         | 13.172      | 1709          | 1716        | 1724         | rVB      | 897096         | 1368194       | 63.69%          | 11.108%       |
| 8         | 14.552      | 1944          | 1951        | 1959         | rVB      | 326074         | 520833        | 24.25%          | 4.229%        |
| 9         | 15.904      | 2175          | 2181        | 2189         | rBV      | 209270         | 285206        | 13.28%          | 2.316%        |
| 10        | 16.039      | 2197          | 2204        | 2219         | rBV      | 752657         | 1192363       | 55.51%          | 9.681%        |
| 11        | 16.468      | 2272          | 2277        | 2283         | rVB2     | 29147          | 41650         | 1.94%           | 0.338%        |
| 12        | 17.296      | 2411          | 2418        | 2425         | rBV      | 444335         | 686087        | 31.94%          | 5.570%        |
| 13        | 19.911      | 2857          | 2863        | 2870         | rBV      | 1654744        | 2148079       | 100.00%         | 17.440%       |
| 14        | 20.704      | 2996          | 2998        | 3002         | rVB2     | 29755          | 33640         | 1.57%           | 0.273%        |
| 15        | 21.197      | 3078          | 3082        | 3093         | rVB2     | 204564         | 352096        | 16.39%          | 2.859%        |
| 16        | 21.544      | 3136          | 3141        | 3148         | rBV2     | 440876         | 715474        | 33.31%          | 5.809%        |
| 17        | 21.738      | 3170          | 3174        | 3181         | rVB      | 99380          | 139086        | 6.47%           | 1.129%        |
| 18        | 22.331      | 3271          | 3275        | 3283         | rVB2     | 86878          | 142625        | 6.64%           | 1.158%        |
| 19        | 22.989      | 3381          | 3387        | 3399         | rVB2     | 215711         | 498979        | 23.23%          | 4.051%        |
| 20        | 24.687      | 3668          | 3676        | 3690         | rVB      | 287112         | 822851        | 38.31%          | 6.681%        |

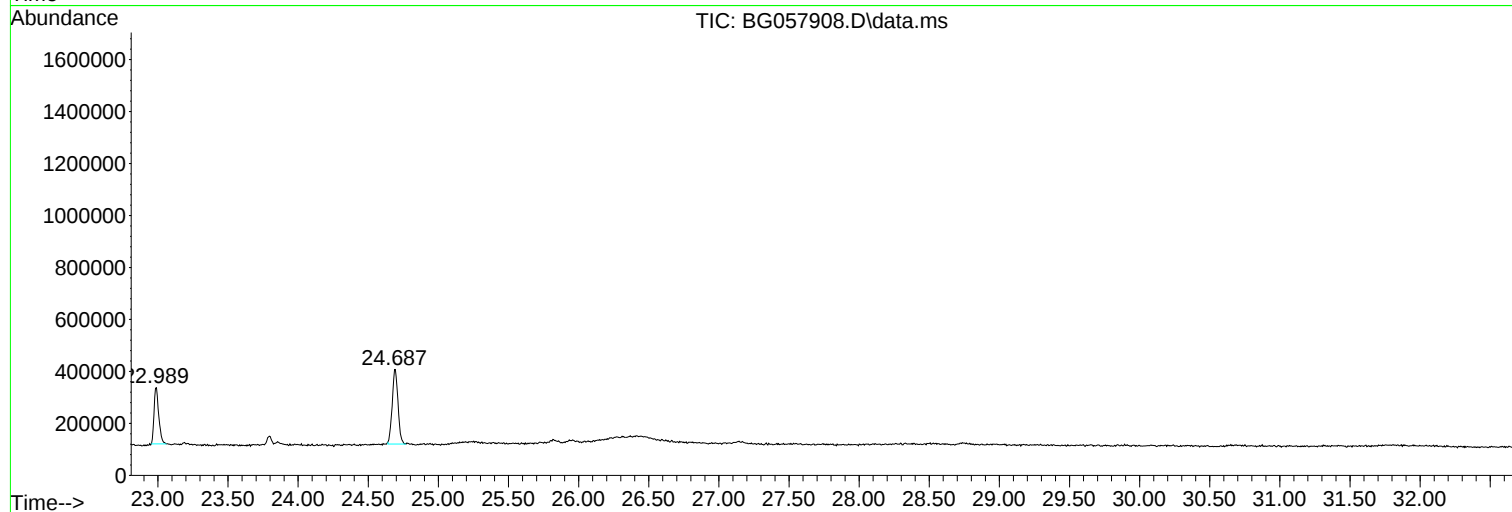
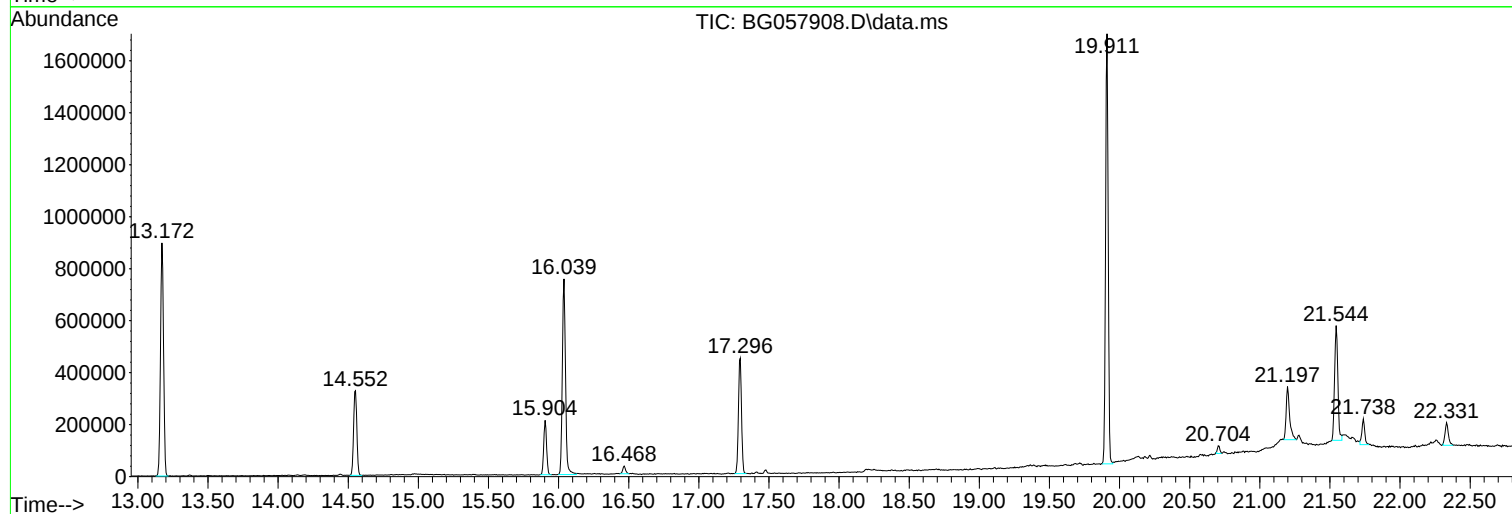
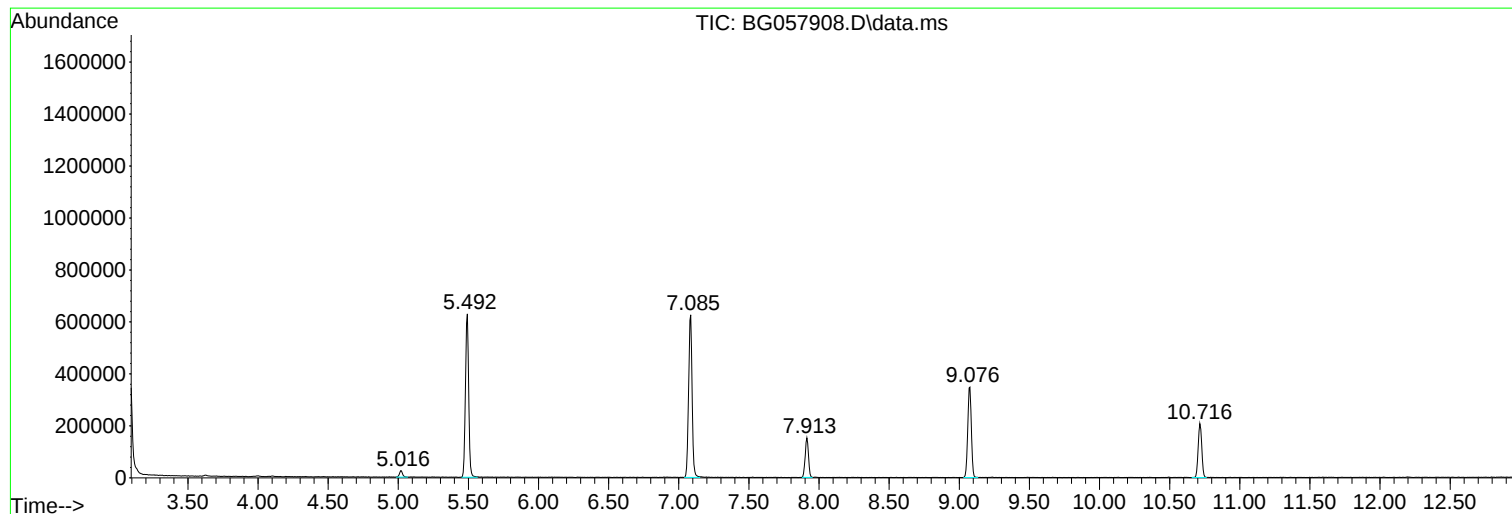
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Misc :  
ALS Vial : 9 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
SB-4-(8-10)

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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Instrument :  
BNA\_G  
ClientSampleId :  
SB-4-(8-10)

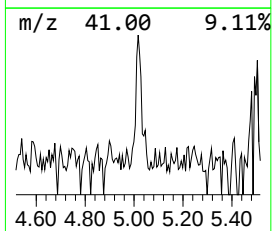
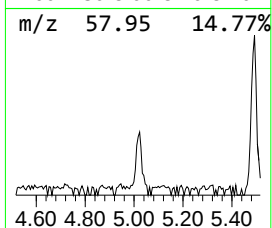
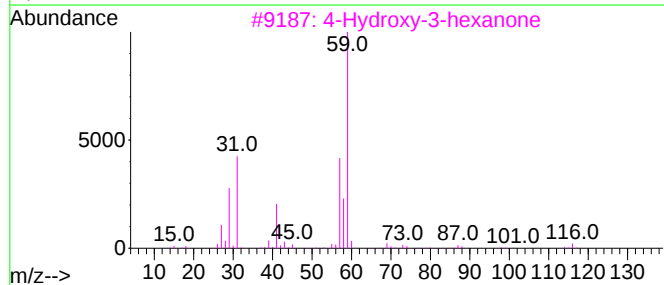
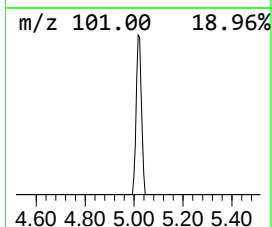
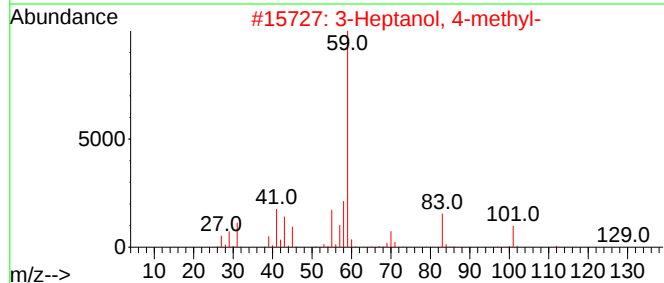
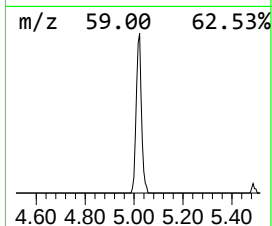
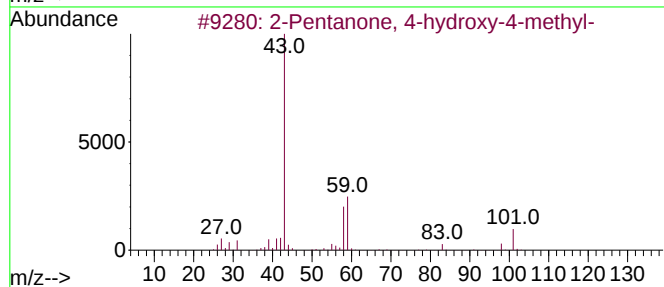
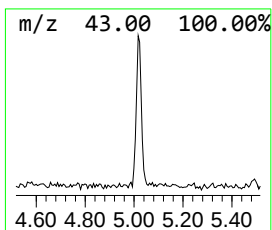
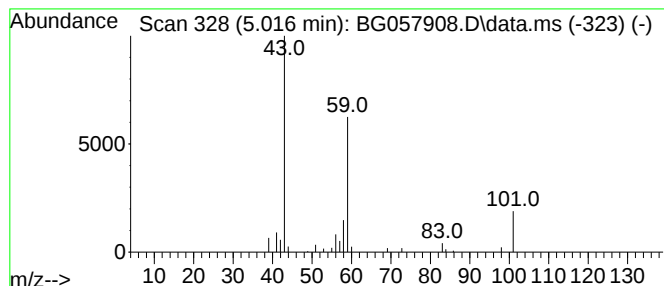
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG062723.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

| R.T.  | EstConc | Area  | Relative to ISTD       | R.T.  |
|-------|---------|-------|------------------------|-------|
| 5.016 | 3.02 ng | 37738 | 1,4-Dichlorobenzene-d4 | 7.913 |

| Hit# | of                               | 5   | Tentative ID | MW          | MolForm | CAS# | Qual |
|------|----------------------------------|-----|--------------|-------------|---------|------|------|
| 1    | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2      | 000123-42-2 | 45      |      |      |
| 2    | 3-Heptanol, 4-methyl-            | 130 | C8H18O       | 014979-39-6 | 36      |      |      |
| 3    | 4-Hydroxy-3-hexanone             | 116 | C6H12O2      | 004984-85-4 | 25      |      |      |
| 4    | 1,3-Dioxane, 4,4-dimethyl-       | 116 | C6H12O2      | 000766-15-4 | 23      |      |      |
| 5    | 1,8-Nonanediol, 8-methyl-        | 174 | C10H22O2     | 054725-73-4 | 23      |      |      |



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SB-4-(8-10)

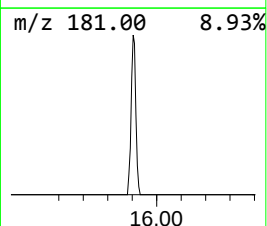
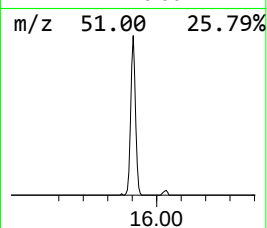
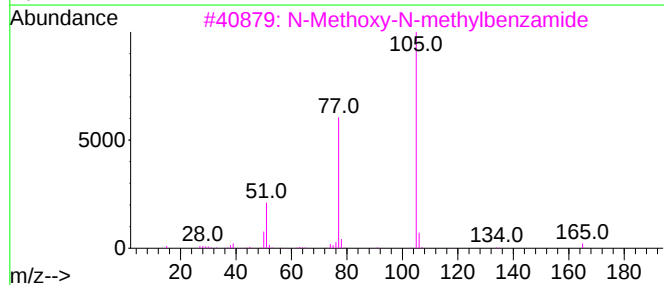
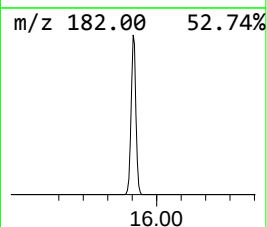
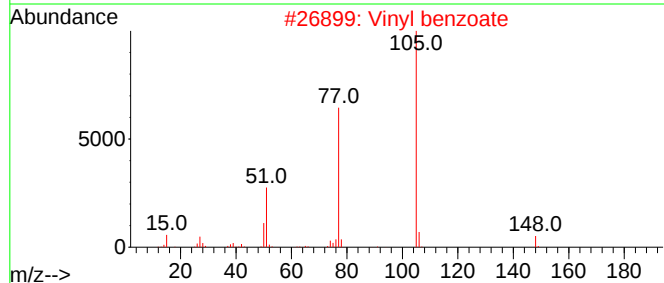
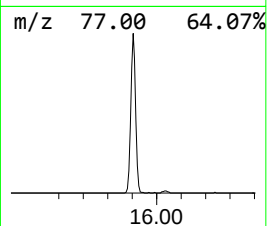
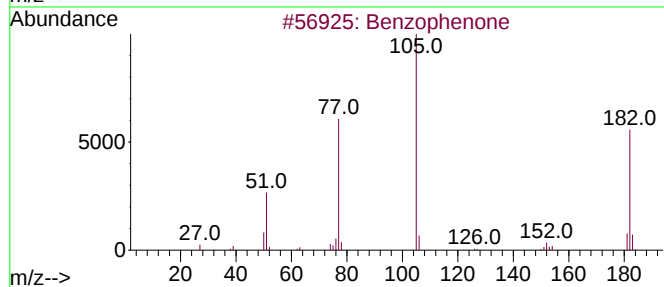
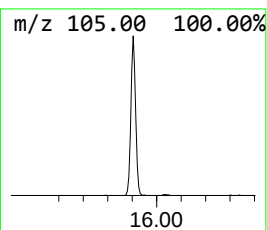
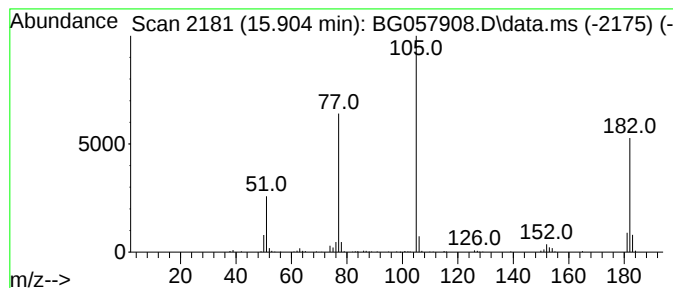
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG062723.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 2 Benzophenone Concentration Rank 2

| R.T.   | EstConc  | Area   | Relative to ISTD | R.T.   |
|--------|----------|--------|------------------|--------|
| 15.904 | 10.95 ng | 285206 | Acenaphthene-d10 | 14.552 |

| Hit# | of | 5 | Tentative ID                | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-----------------------------|-----|----------|-------------|------|
| 1    |    |   | Benzophenone                | 182 | C13H10O  | 000119-61-9 | 96   |
| 2    |    |   | Vinyl benzoate              | 148 | C9H8O2   | 000769-78-8 | 47   |
| 3    |    |   | N-Methoxy-N-methylbenzamide | 165 | C9H11NO2 | 006919-61-5 | 47   |
| 4    |    |   | Benzoyl isothiocyanate      | 163 | C8H5NOS  | 000532-55-8 | 47   |
| 5    |    |   | Benzoic acid, phenyl ester  | 198 | C13H10O2 | 000093-99-2 | 47   |



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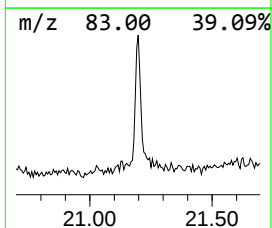
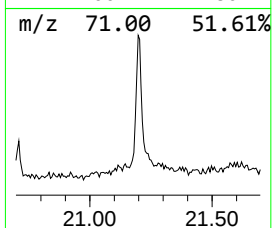
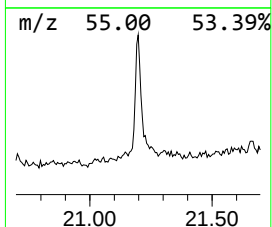
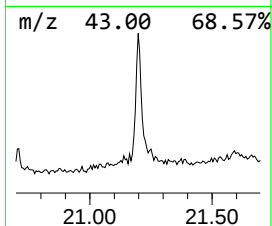
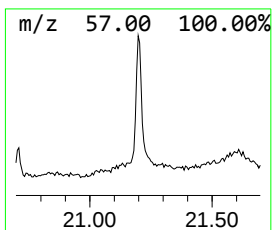
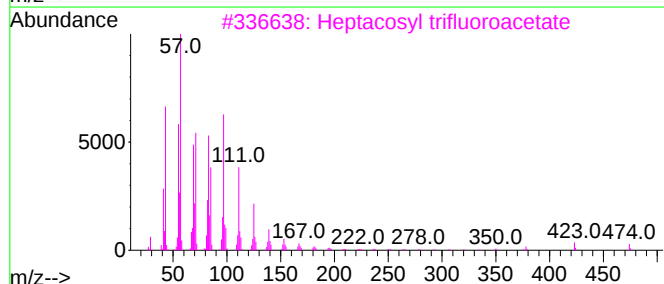
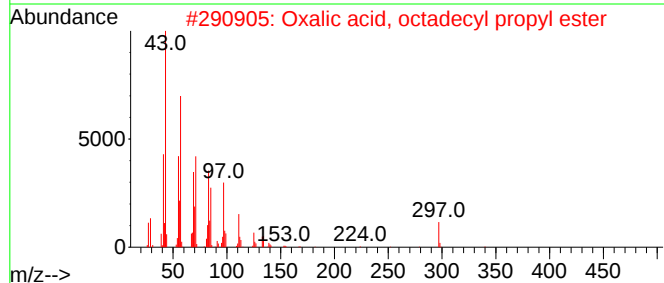
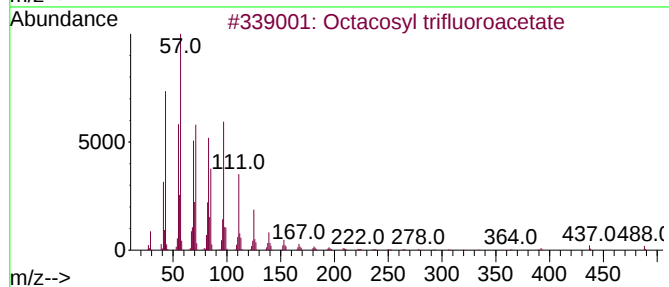
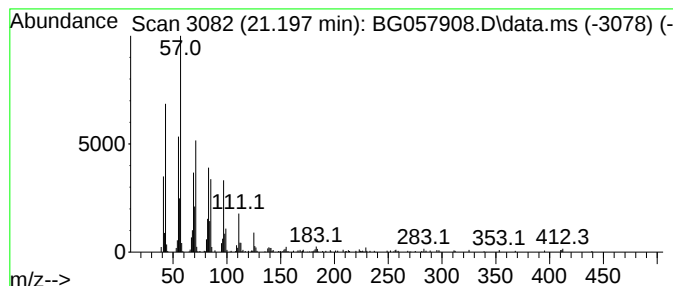
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG062723.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 3 Octacosyl trifluoroacetate Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 21.197 | 9.84 ng | 352096 | Chrysene-d12     | 21.544 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|------------|--------------|------|
| 1    |    |   | Octacosyl trifluoroacetate          | 506 | C30H57F3O2 | 1000351-74-9 | 91   |
| 2    |    |   | Oxalic acid, octadecyl propyl ester | 384 | C23H44O4   | 1000309-27-0 | 91   |
| 3    |    |   | Heptacosyl trifluoroacetate         | 492 | C29H55F3O2 | 1000351-75-8 | 91   |
| 4    |    |   | Oxalic acid, isobutyl hexadecyl ... | 370 | C22H42O4   | 1000309-38-1 | 91   |
| 5    |    |   | Heptacosyl pentafluoropropionate    | 542 | C30H55F5O2 | 1000351-81-6 | 91   |



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ClientSampleId :  
SB-4-(8-10)

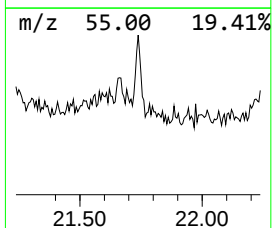
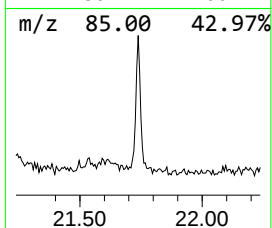
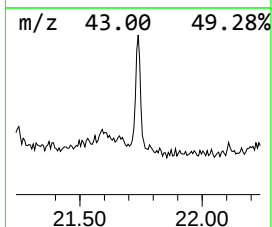
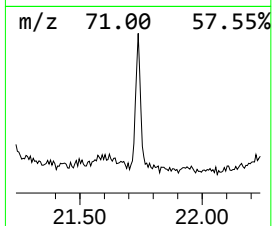
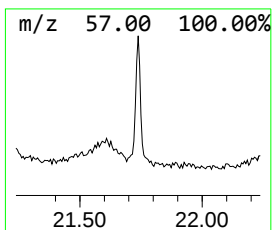
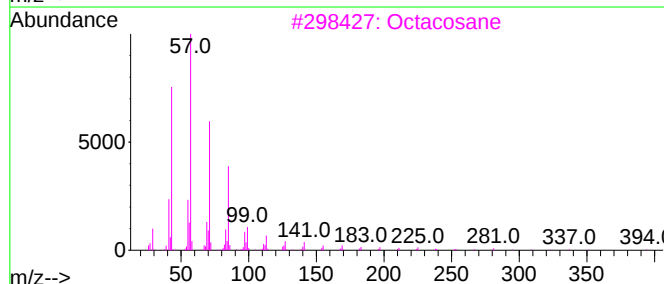
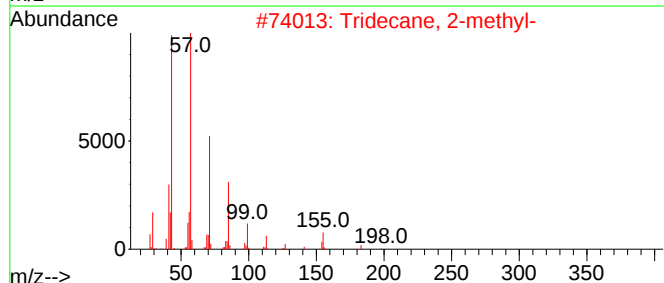
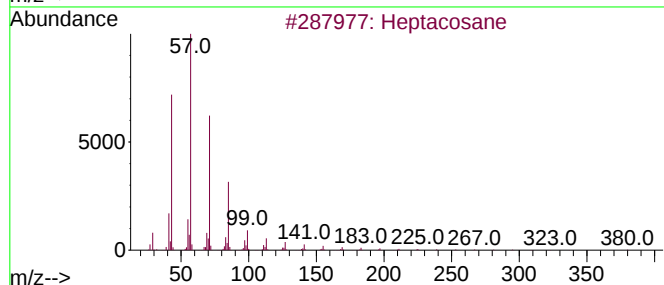
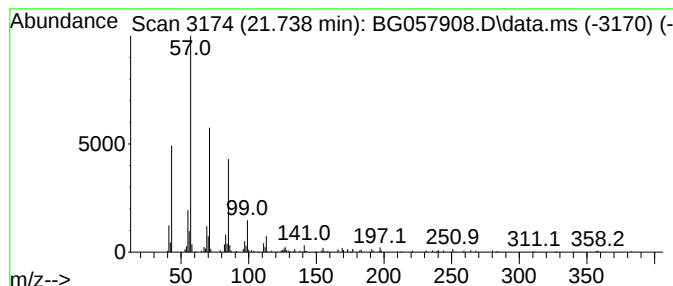
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG062723.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L  
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\*\*\*\*\*  
Peak Number 4 Heptacosane Concentration Rank 5

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 21.738 | 3.89 ng | 139086 | Chrysene-d12     | 21.544 |

| Hit# | of 5 | Tentative ID         | MW  | MolForm | CAS#        | Qual |
|------|------|----------------------|-----|---------|-------------|------|
| 1    |      | Heptacosane          | 380 | C27H56  | 000593-49-7 | 91   |
| 2    |      | Tridecane, 2-methyl- | 198 | C14H30  | 001560-96-9 | 87   |
| 3    |      | Octacosane           | 394 | C28H58  | 000630-02-4 | 80   |
| 4    |      | Heptadecane          | 240 | C17H36  | 000629-78-7 | 80   |
| 5    |      | Tridecane, 1-iodo-   | 310 | C13H27I | 035599-77-0 | 78   |



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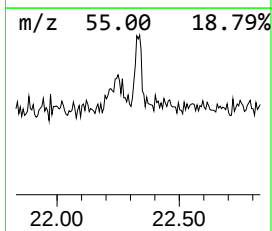
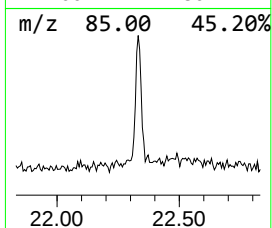
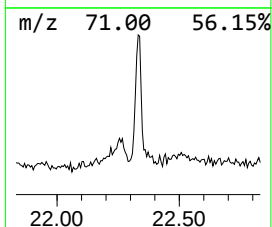
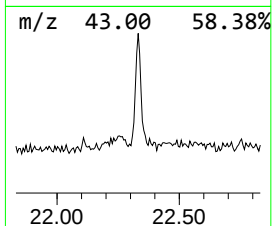
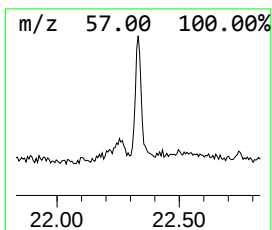
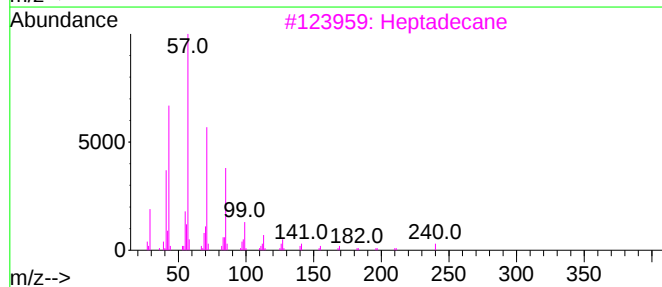
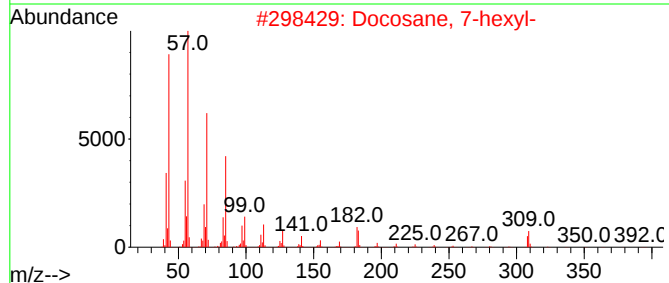
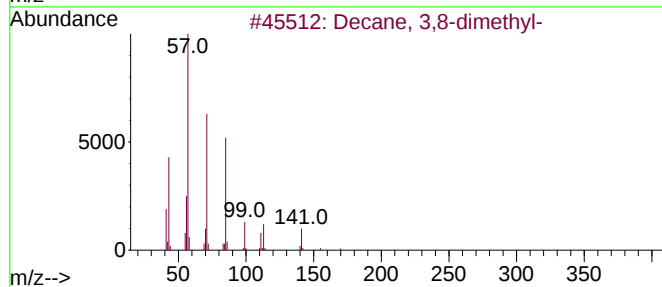
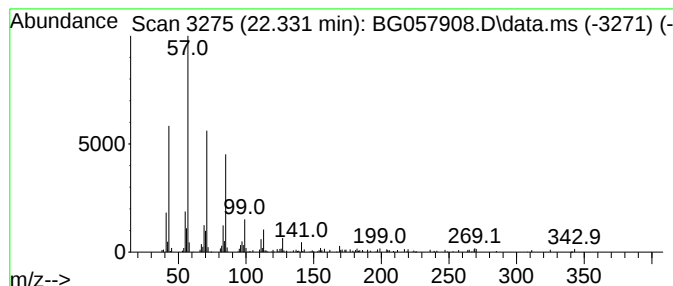
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\*\*\*\*\*  
Peak Number 5 Decane, 3,8-dimethyl- Concentration Rank 4

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 22.331 | 3.99 ng | 142625 | Chrysene-d12     | 21.544 |

| Hit# | of | 5 | Tentative ID          | MW  | MolForm | CAS#        | Qual |
|------|----|---|-----------------------|-----|---------|-------------|------|
| 1    |    |   | Decane, 3,8-dimethyl- | 170 | C12H26  | 017312-55-9 | 86   |
| 2    |    |   | Docosane, 7-hexyl-    | 394 | C28H58  | 055373-86-9 | 86   |
| 3    |    |   | Heptadecane           | 240 | C17H36  | 000629-78-7 | 86   |
| 4    |    |   | Hentriacontane        | 437 | C31H64  | 000630-04-6 | 86   |
| 5    |    |   | Dodecane, 2-methyl-   | 184 | C13H28  | 001560-97-0 | 72   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG062923\  
Data File : BG057908.D  
Acq On : 29 Jun 2023 17:26  
Operator : CG/JU  
Sample : 03358-05  
Misc :  
ALS Vial : 9 Sample Multiplier: 1

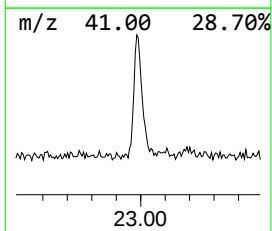
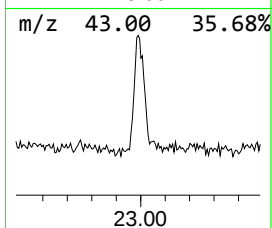
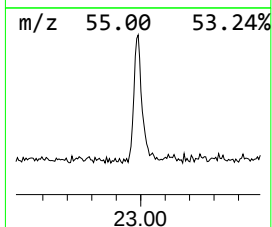
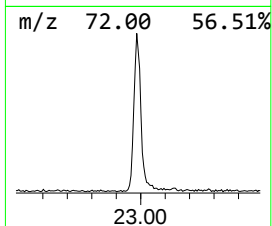
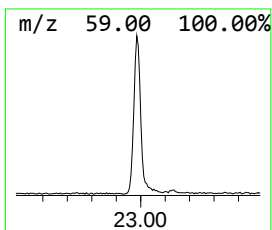
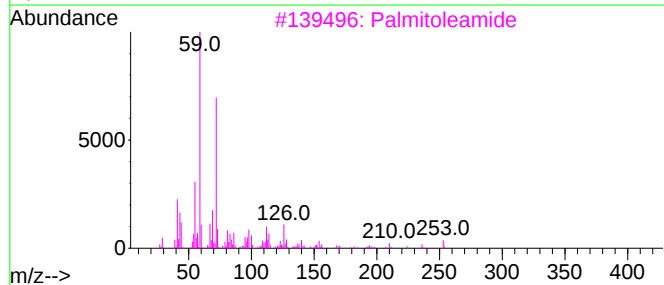
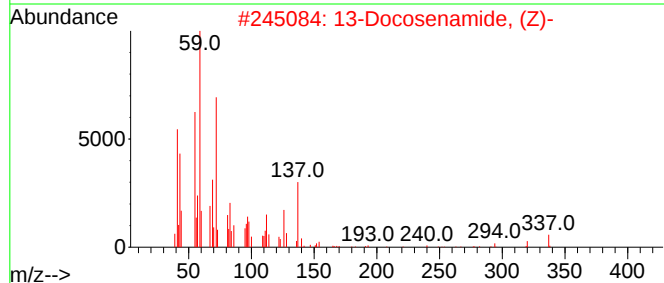
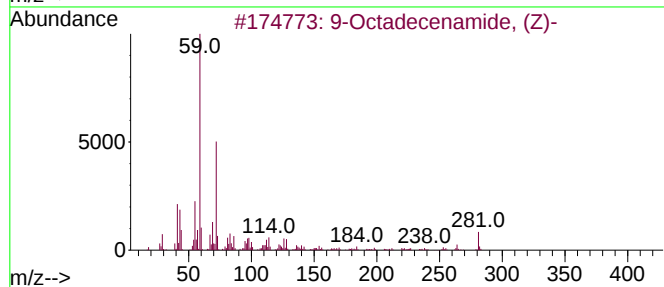
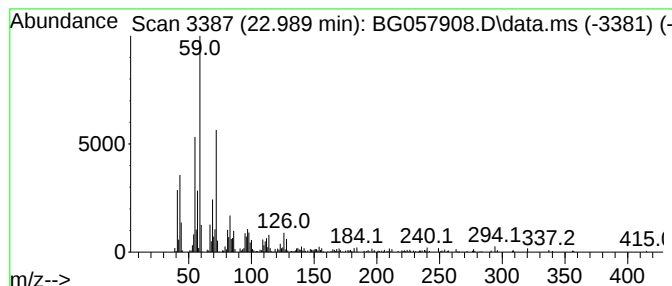
Instrument :  
BNA\_G  
ClientSampleId :  
SB-4-(8-10)

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

\*\*\*\*\*  
Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 1

| R.T.      | EstConc                        | Area   | Relative to ISTD |          | R.T.        |      |
|-----------|--------------------------------|--------|------------------|----------|-------------|------|
| 22.989    | 13.95 ng                       | 498979 | Chrysene-d12     |          | 21.544      |      |
| Hit# of 5 | Tentative ID                   |        | MW               | MolForm  | CAS#        | Qual |
| 1         | 9-Octadecenamide, (Z)-         |        | 281              | C18H35NO | 000301-02-0 | 91   |
| 2         | 13-Docosenamide, (Z)-          |        | 337              | C22H43NO | 000112-84-5 | 83   |
| 3         | Palmitoleamide                 |        | 253              | C16H31NO | 106010-22-4 | 72   |
| 4         | Heptanamide, 4-ethyl-5-methyl- |        | 171              | C10H21NO | 054789-40-1 | 64   |
| 5         | Hexadecanamide                 |        | 255              | C16H33NO | 000629-54-9 | 53   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG062923\  
Data File : BG057908.D  
Acq On : 29 Jun 2023 17:26  
Operator : CG/JU  
Sample : 03358-05  
Misc :  
ALS Vial : 9 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
SB-4-(8-10)

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

TIC Library : C:\Database\NIST0.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| 2-Pentanone, 4-... | 5.016  | 3.0     | ng    | 37738    | 1                     | 7.913  | 249759 | 20.0 |
| Benzophenone       | 15.904 | 10.9    | ng    | 285206   | 3                     | 14.552 | 520833 | 20.0 |
| Octacosyl trifl... | 21.197 | 9.8     | ng    | 352096   | 5                     | 21.544 | 715474 | 20.0 |
| Heptacosane        | 21.738 | 3.9     | ng    | 139086   | 5                     | 21.544 | 715474 | 20.0 |
| Decane, 3,8-dim... | 22.331 | 4.0     | ng    | 142625   | 5                     | 21.544 | 715474 | 20.0 |
| 9-Octadecenamid... | 22.989 | 13.9    | ng    | 498979   | 5                     | 21.544 | 715474 | 20.0 |