

Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG062023\  
 Data File : BG057770.D  
 Acq On : 20 Jun 2023 10:45  
 Operator : CG/JU  
 Sample : 03289-05  
 Misc :  
 ALS Vial : 5 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 SB-02-12.0-14.0

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-BG061923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057770.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         | 5.033       | 324           | 331         | 341          | rVB      | 137597         | 202054        | 10.04%          | 1.890%        |
| 2         | 5.497       | 403           | 410         | 421          | rVB      | 541870         | 848801        | 42.16%          | 7.939%        |
| 3         | 7.083       | 672           | 680         | 687          | rBV      | 525861         | 874242        | 43.42%          | 8.177%        |
| 4         | 7.924       | 817           | 823         | 830          | rBV      | 117463         | 195893        | 9.73%           | 1.832%        |
| 5         | 9.081       | 1012          | 1020        | 1031         | rBV      | 305551         | 537862        | 26.72%          | 5.031%        |
| 6         | 10.726      | 1292          | 1300        | 1309         | rVB      | 162231         | 285426        | 14.18%          | 2.670%        |
| 7         | 13.182      | 1710          | 1718        | 1726         | rBV      | 694928         | 1105111       | 54.89%          | 10.336%       |
| 8         | 14.557      | 1945          | 1952        | 1961         | rBV2     | 248872         | 381224        | 18.94%          | 3.566%        |
| 9         | 15.914      | 2177          | 2183        | 2189         | rBV      | 129974         | 191935        | 9.53%           | 1.795%        |
| 10        | 16.044      | 2198          | 2205        | 2211         | rBV      | 632312         | 942103        | 46.79%          | 8.812%        |
| 11        | 17.301      | 2413          | 2419        | 2427         | rVB      | 345028         | 518282        | 25.74%          | 4.848%        |
| 12        | 18.194      | 2566          | 2571        | 2579         | rBV      | 207088         | 325745        | 16.18%          | 3.047%        |
| 13        | 18.458      | 2614          | 2616        | 2621         | rVB3     | 89882          | 118490        | 5.89%           | 1.108%        |
| 14        | 19.463      | 2783          | 2787        | 2798         | rVB2     | 94209          | 128856        | 6.40%           | 1.205%        |
| 15        | 19.921      | 2859          | 2865        | 2870         | rVB      | 1492266        | 2013263       | 100.00%         | 18.830%       |
| 16        | 21.173      | 3073          | 3078        | 3081         | rBV2     | 32170          | 65315         | 3.24%           | 0.611%        |
| 17        | 21.208      | 3081          | 3084        | 3092         | rVV2     | 178917         | 338724        | 16.82%          | 3.168%        |
| 18        | 21.290      | 3093          | 3098        | 3103         | rVB      | 241707         | 362286        | 17.99%          | 3.388%        |
| 19        | 21.555      | 3137          | 3143        | 3149         | rBV      | 383355         | 608929        | 30.25%          | 5.695%        |
| 20        | 24.704      | 3671          | 3679        | 3692         | rVB      | 239543         | 647184        | 32.15%          | 6.053%        |

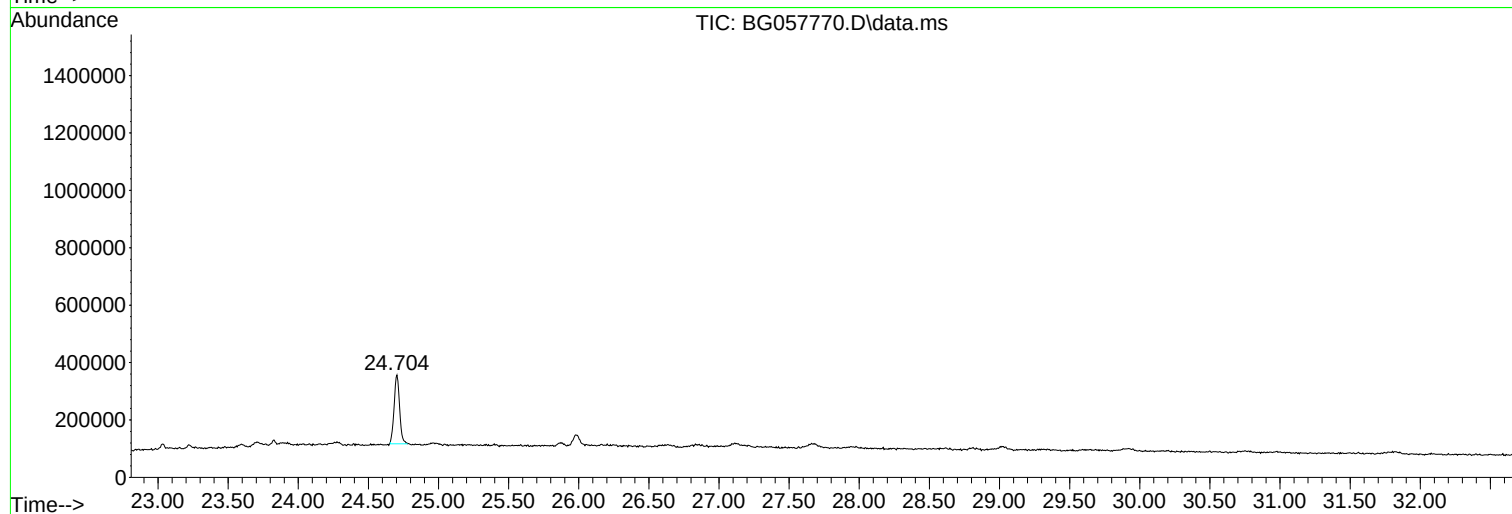
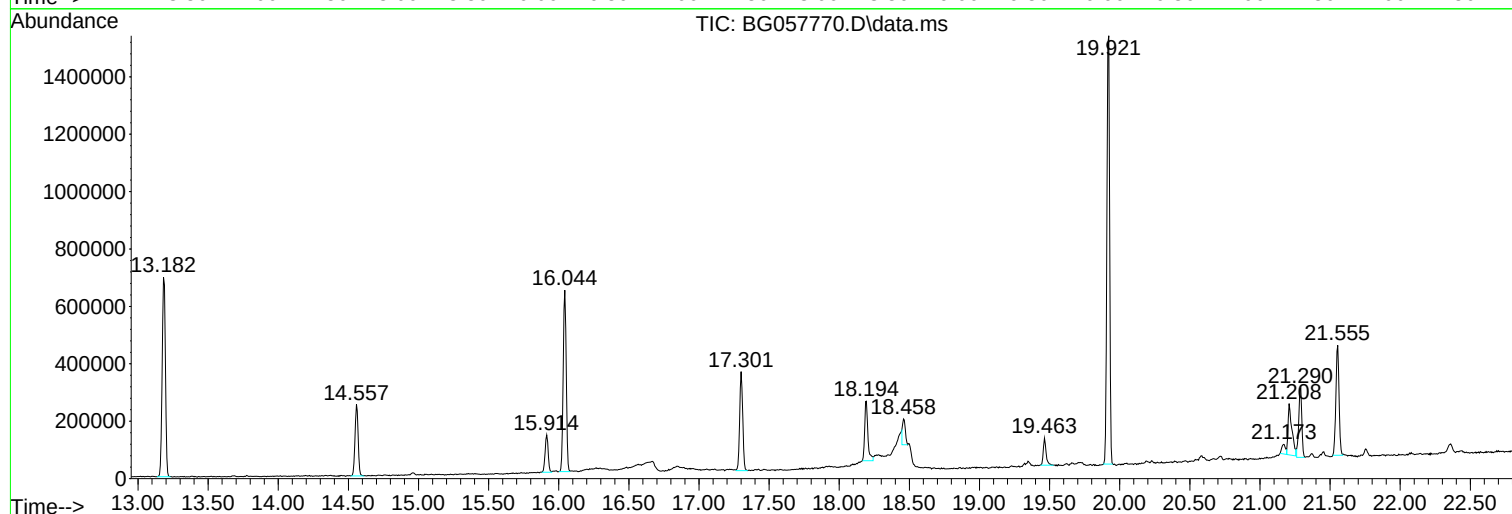
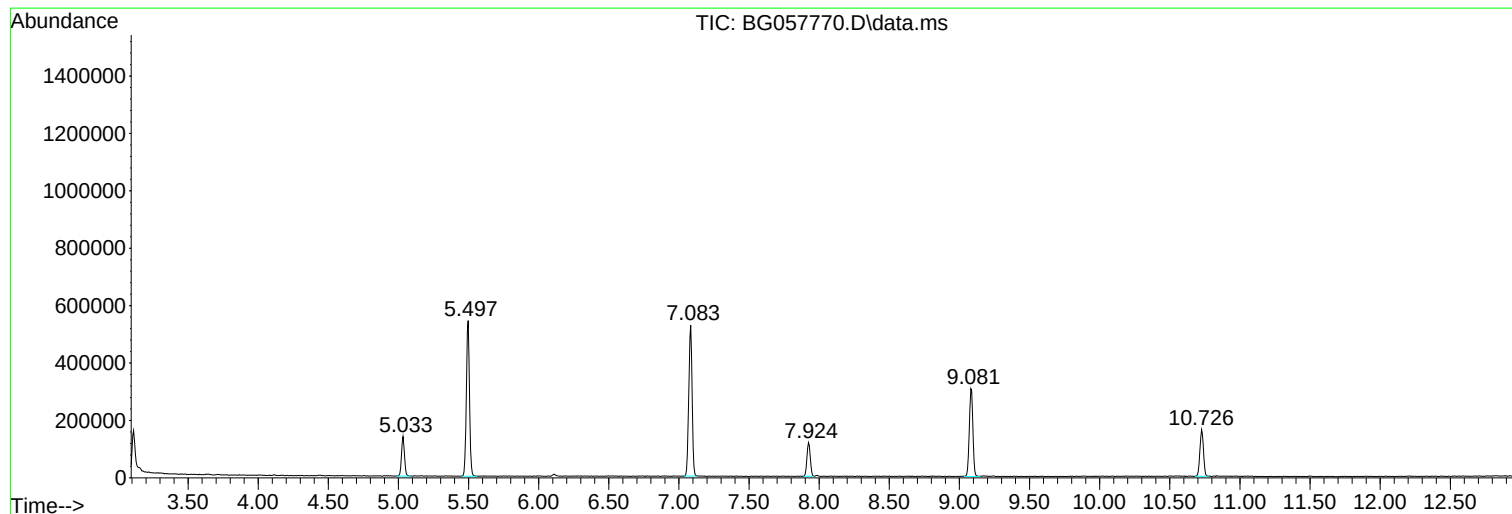
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Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG062023\  
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Misc :  
ALS Vial : 5 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
SB-02-12.0-14.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG061923.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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SB-02-12.0-14.0

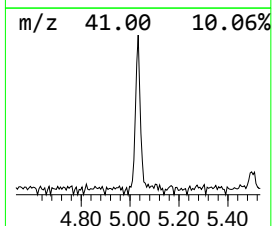
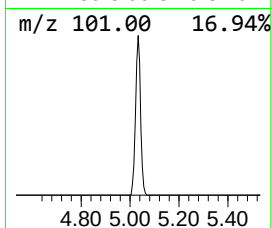
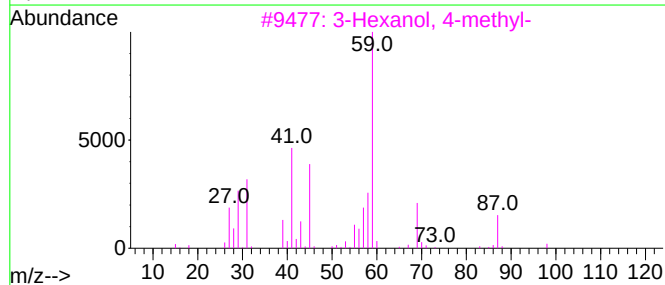
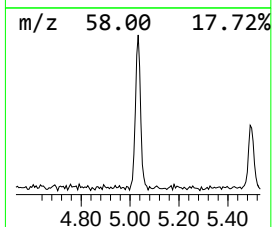
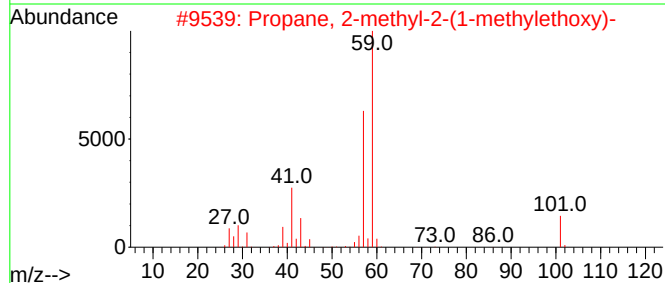
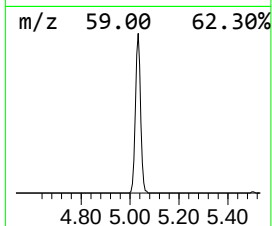
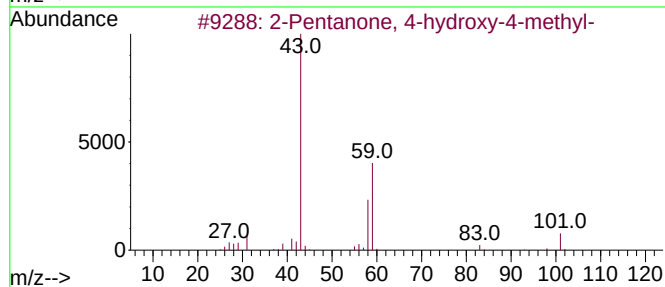
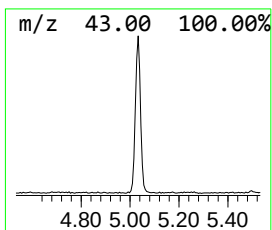
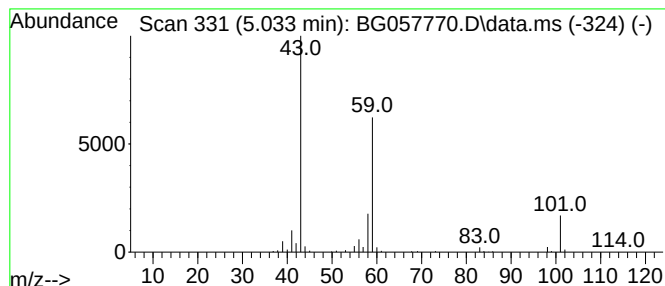
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG061923.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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 1

| R.T.  | EstConc  | Area   | Relative to ISTD       | R.T.  |
|-------|----------|--------|------------------------|-------|
| 5.033 | 20.63 ng | 202054 | 1,4-Dichlorobenzene-d4 | 7.924 |

| Hit# | of                                  | 5   | Tentative ID | MW          | MolForm | CAS# | Qual |
|------|-------------------------------------|-----|--------------|-------------|---------|------|------|
| 1    | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2      | 000123-42-2 | 64      |      |      |
| 2    | Propane, 2-methyl-2-(1-methyleth... | 116 | C7H16O       | 017348-59-3 | 53      |      |      |
| 3    | 3-Hexanol, 4-methyl-                | 116 | C7H16O       | 000615-29-2 | 33      |      |      |
| 4    | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2     | 001116-98-9 | 32      |      |      |
| 5    | 2-Hexanol, 2-methyl-                | 116 | C7H16O       | 000625-23-0 | 28      |      |      |



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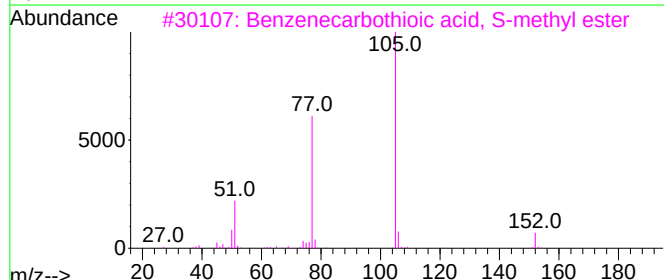
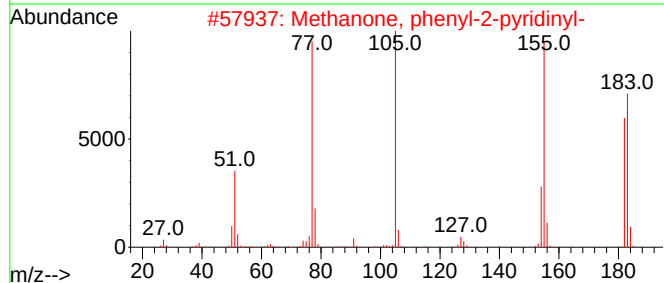
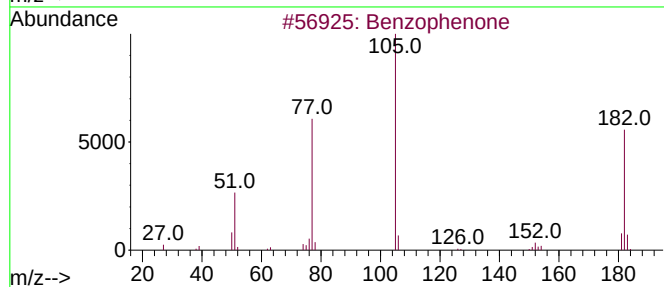
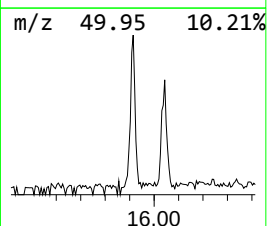
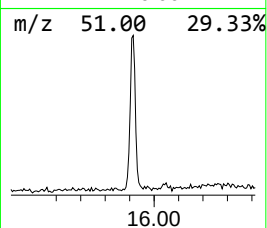
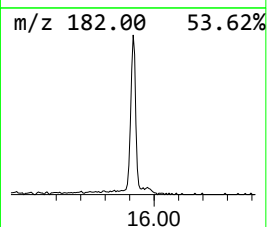
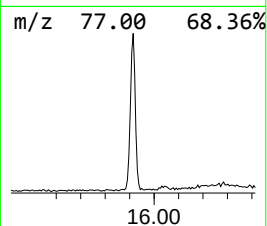
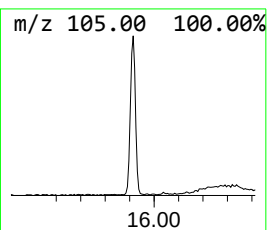
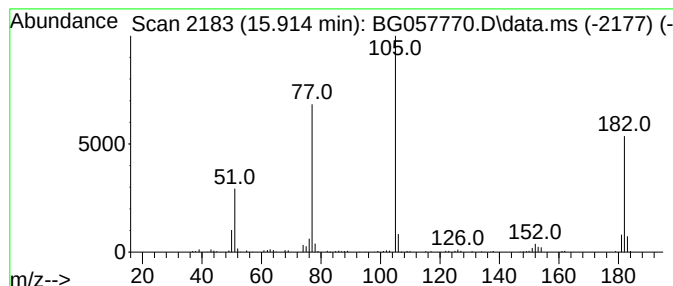
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG061923.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 2 Benzophenone Concentration Rank 5

| R.T.   | EstConc  | Area   | Relative to ISTD | R.T.   |
|--------|----------|--------|------------------|--------|
| 15.914 | 10.07 ng | 191935 | Acenaphthene-d10 | 14.557 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|------------|--------------|------|
| 1    |    |   | Benzophenone                        | 182 | C13H10O    | 000119-61-9  | 96   |
| 2    |    |   | Methanone, phenyl-2-pyridinyl-      | 183 | C12H9NO    | 000091-02-1  | 78   |
| 3    |    |   | Benzenecarbothioic acid, S-methy... | 152 | C8H8OS     | 005925-68-8  | 58   |
| 4    |    |   | N-Methylbenzamide, N-pentafluoro... | 281 | C11H8F5NO2 | 1000446-98-1 | 50   |
| 5    |    |   | N-(1-Cyanovinyl)benzamide           | 172 | C10H8N2O   | 1000186-19-1 | 50   |



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BNA\_G  
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SB-02-12.0-14.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG061923.M  
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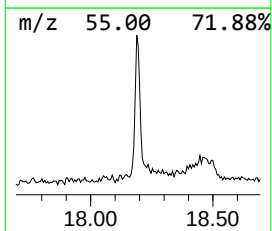
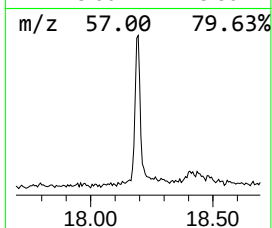
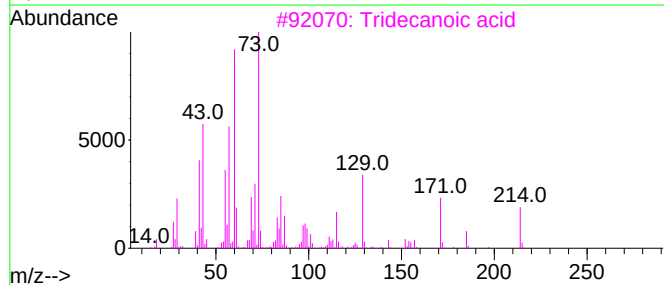
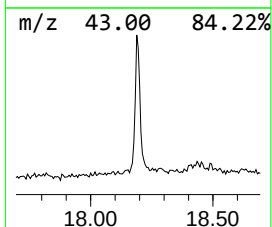
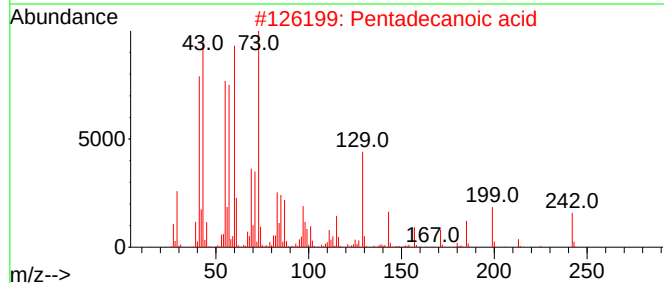
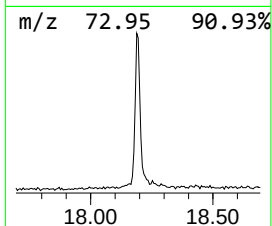
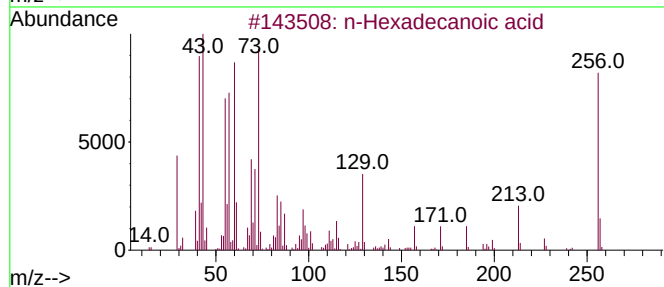
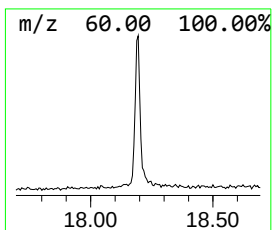
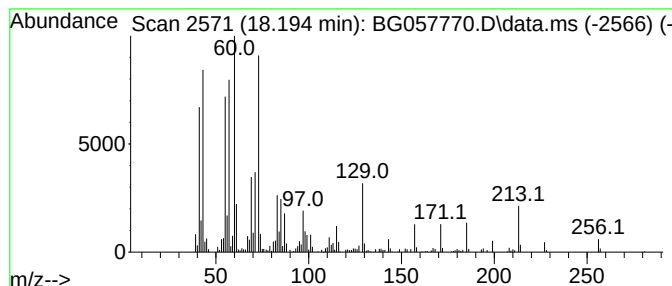
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

| R.T.   | EstConc  | Area   | Relative to ISTD | R.T.   |
|--------|----------|--------|------------------|--------|
| 18.194 | 12.57 ng | 325745 | Phenanthrene-d10 | 17.301 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 97   |
| 2    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 87   |
| 3    |    |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 80   |
| 4    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 72   |
| 5    |    |   | Undecanoic acid     | 186 | C11H22O2 | 000112-37-8 | 58   |



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Instrument :  
BNA\_G  
ClientSampleId :  
SB-02-12.0-14.0

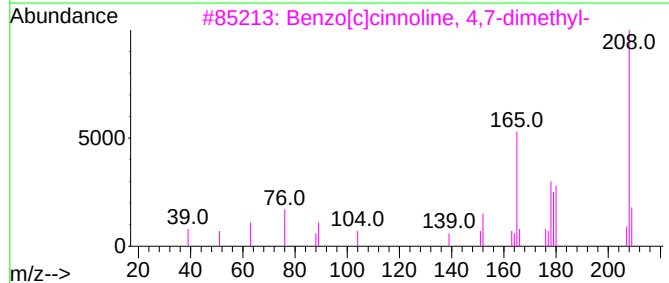
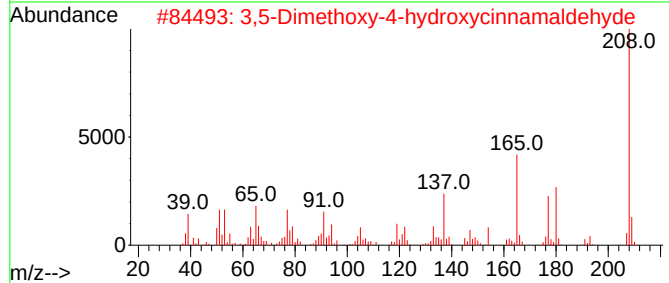
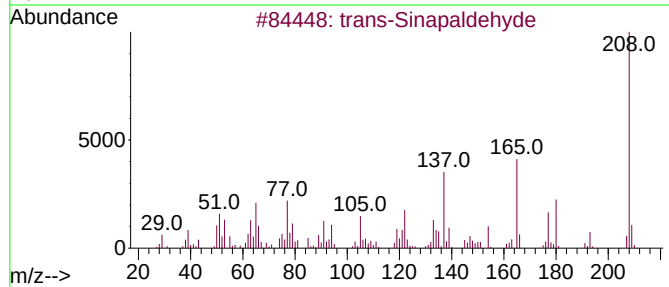
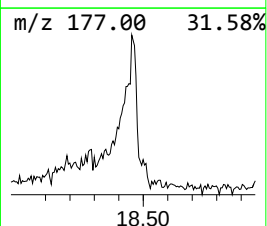
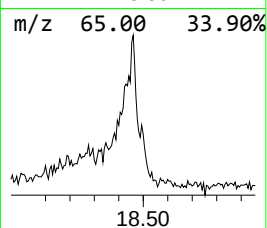
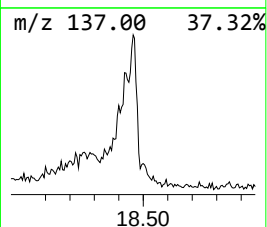
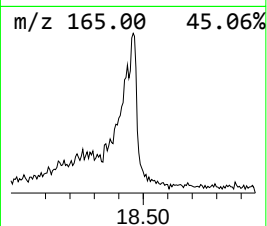
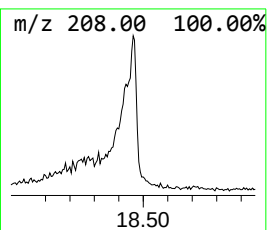
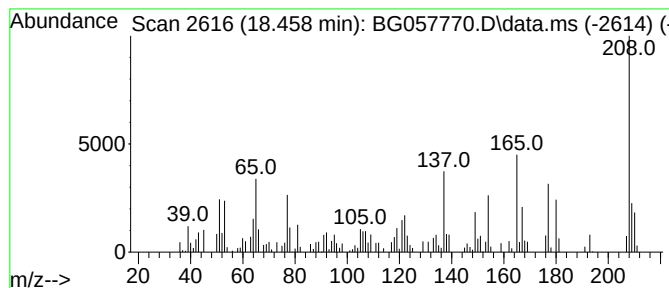
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG061923.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 4 trans-Sinapaldehyde Concentration Rank 6

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 18.458 | 4.57 ng | 118490 | Phenanthrene-d10 | 17.301 |

| Hit# | of | 5 | Tentative ID                          | MW  | MolForm  | CAS#         | Qual |
|------|----|---|---------------------------------------|-----|----------|--------------|------|
| 1    |    |   | trans-Sinapaldehyde                   | 208 | C11H12O4 | 004206-58-0  | 70   |
| 2    |    |   | 3,5-Dimethoxy-4-hydroxycinnamaldehyde | 208 | C11H12O4 | 087345-53-7  | 68   |
| 3    |    |   | Benzo[c]cinnoline, 4,7-dimethyl-      | 208 | C14H12N2 | 020684-54-2  | 49   |
| 4    |    |   | Pyrene, 1,2,3,6,7,8-hexahydro-        | 208 | C16H16   | 001732-13-4  | 49   |
| 5    |    |   | Coumarin, 7,8-dihydro-7-hydroxy-      | 208 | C10H8O5  | 1000263-13-6 | 43   |



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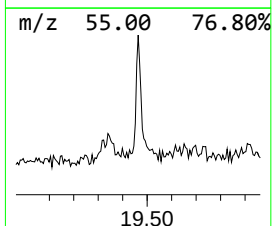
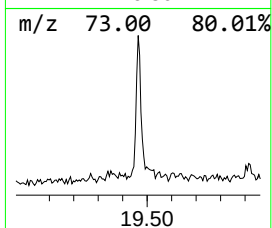
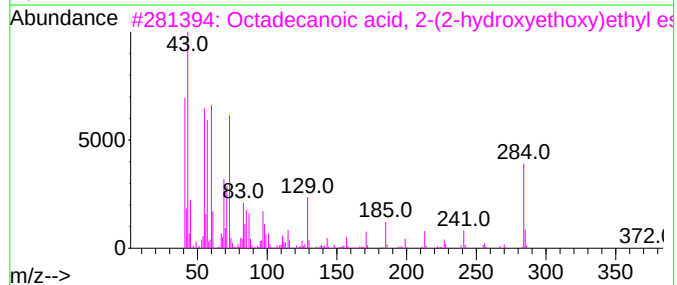
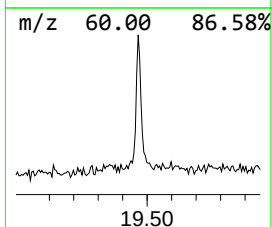
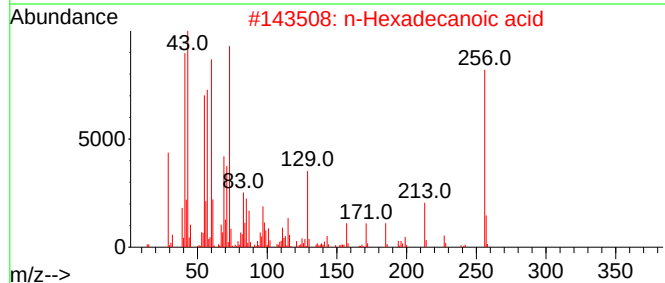
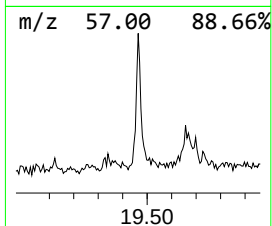
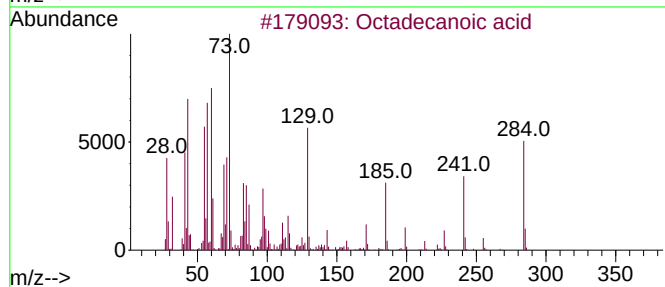
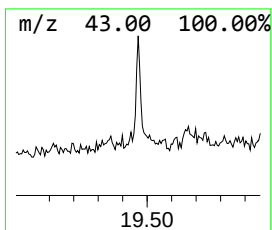
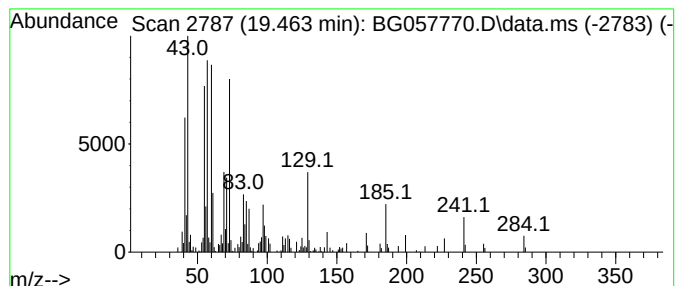
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG061923.M  
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Peak Number 5 Octadecanoic acid Concentration Rank 7

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 19.463 | 4.23 ng | 128856 | Chrysene-d12     | 21.555 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | Octadecanoic acid                   | 284 | C18H36O2 | 000057-11-4 | 97   |
| 2    |    |   | n-Hexadecanoic acid                 | 256 | C16H32O2 | 000057-10-3 | 93   |
| 3    |    |   | Octadecanoic acid, 2-(2-hydroxye... | 372 | C22H44O4 | 000106-11-6 | 86   |
| 4    |    |   | Tetradecanoic acid                  | 228 | C14H28O2 | 000544-63-8 | 83   |
| 5    |    |   | Pentadecanoic acid                  | 242 | C15H30O2 | 001002-84-2 | 72   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG062023\  
Data File : BG057770.D  
Acq On : 20 Jun 2023 10:45  
Operator : CG/JU  
Sample : 03289-05  
Misc :  
ALS Vial : 5 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
SB-02-12.0-14.0

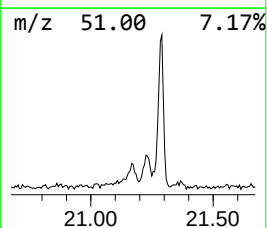
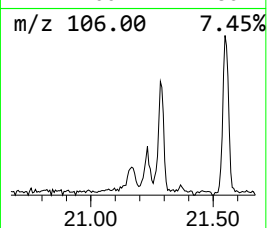
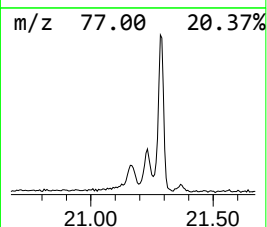
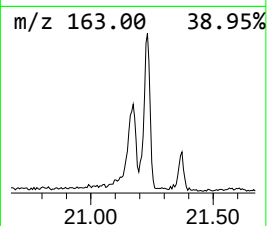
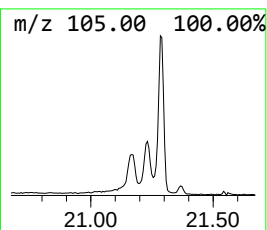
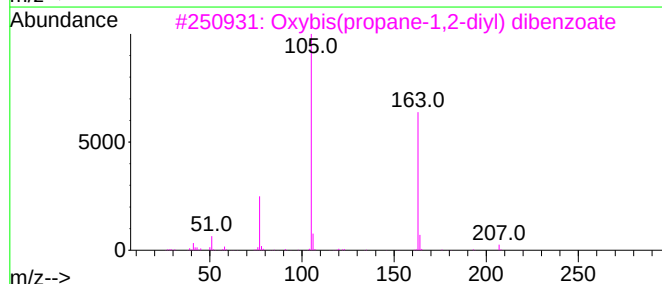
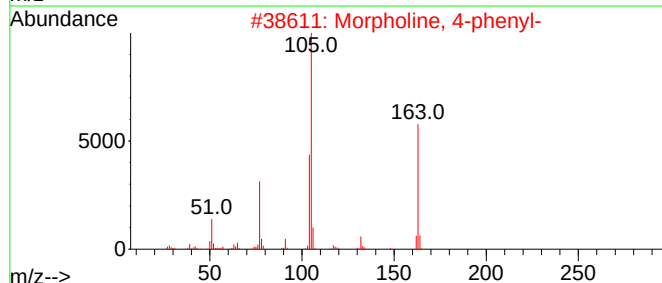
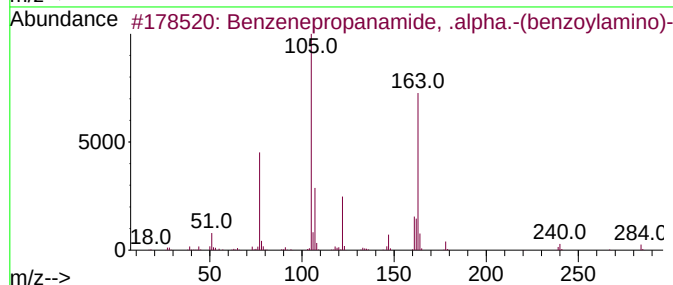
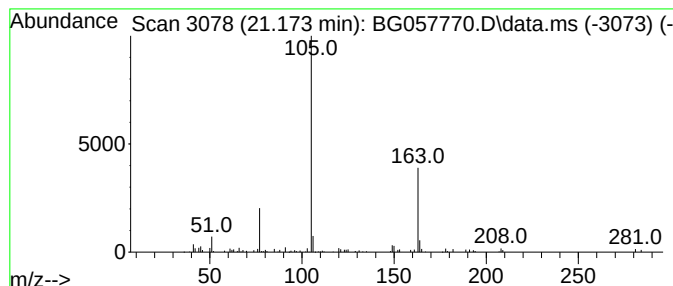
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 6 Benzenepropanamide, .alpha.... Concentration Rank 8

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 21.173 | 2.15 ng | 65315 | Chrysene-d12     | 21.555 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|------------|-------------|------|
| 1    |    |   | Benzenepropanamide, .alpha.-(ben... | 284 | C16H16N2O3 | 058690-81-6 | 59   |
| 2    |    |   | Morpholine, 4-phenyl-               | 163 | C10H13NO   | 000092-53-5 | 59   |
| 3    |    |   | Oxybis(propane-1,2-diyl) dibenzoate | 342 | C20H22O5   | 000094-03-1 | 56   |
| 4    |    |   | Oxirane, (cis)-2-acetoxy-2,3-dip... | 254 | C16H14O3   | 135455-96-8 | 35   |
| 5    |    |   | Ethanone, 2-(acetyloxy)-1-phenyl-   | 178 | C10H10O3   | 002243-35-8 | 27   |





Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG062023\  
Data File : BG057770.D  
Acq On : 20 Jun 2023 10:45  
Operator : CG/JU  
Sample : 03289-05  
Misc :  
ALS Vial : 5 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
SB-02-12.0-14.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG061923.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

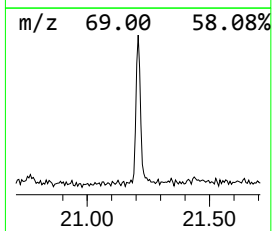
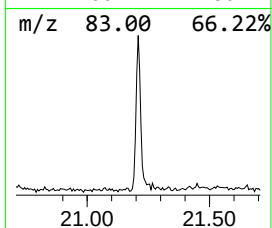
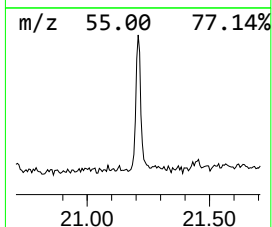
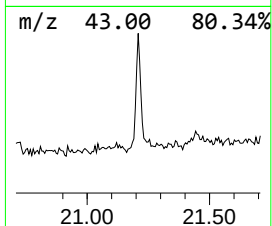
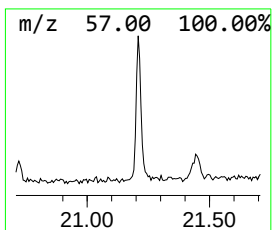
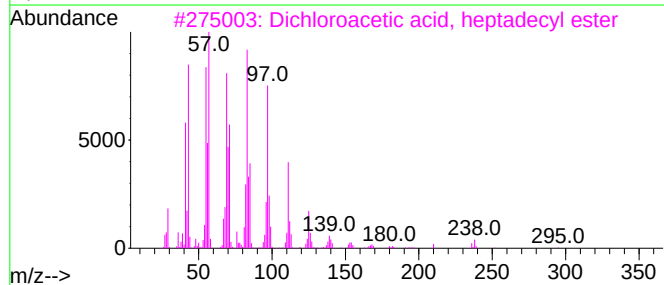
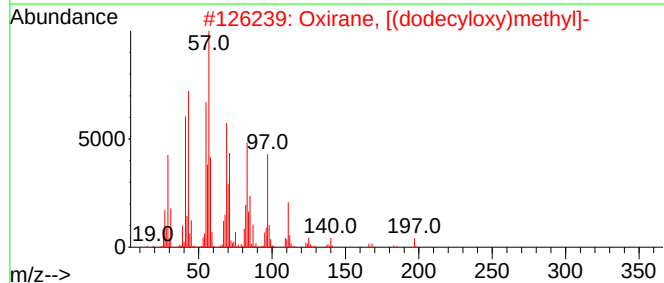
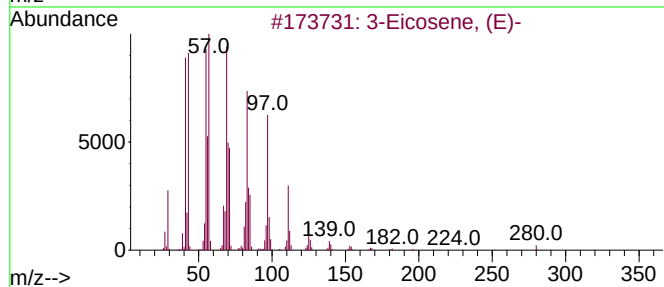
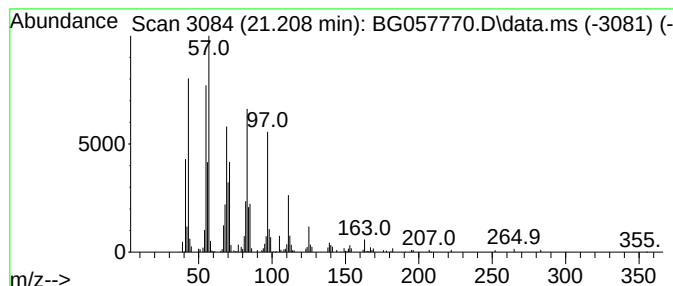
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 7 3-Eicosene, (E)- Concentration Rank 4

| R.T.   | EstConc  | Area   | Relative to ISTD | R.T.   |
|--------|----------|--------|------------------|--------|
| 21.208 | 11.13 ng | 338724 | Chrysene-d12     | 21.555 |

| Hit# | of 5                                | Tentative ID | MW  | MolForm     | CAS#         | Qual |
|------|-------------------------------------|--------------|-----|-------------|--------------|------|
| 1    | 3-Eicosene, (E)-                    |              | 280 | C20H40      | 074685-33-9  | 91   |
| 2    | Oxirane, [(dodecyloxy)methyl]-      |              | 242 | C15H30O2    | 002461-18-9  | 91   |
| 3    | Dichloroacetic acid, heptadecyl ... |              | 366 | C19H36Cl2O2 | 1000282-98-2 | 91   |
| 4    | Heptafluorobutyric acid, hexadec... |              | 438 | C20H33F7O2  | 006385-15-5  | 91   |
| 5    | n-Tetracosanol-1                    |              | 354 | C24H50O     | 000506-51-4  | 87   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG062023\  
Data File : BG057770.D  
Acq On : 20 Jun 2023 10:45  
Operator : CG/JU  
Sample : 03289-05  
Misc :  
ALS Vial : 5 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
SB-02-12.0-14.0

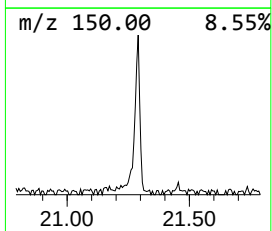
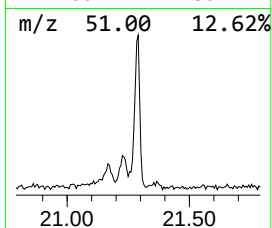
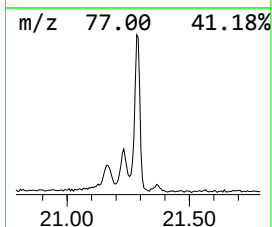
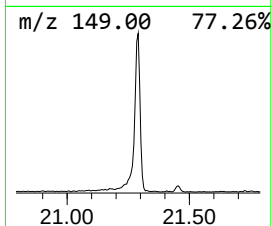
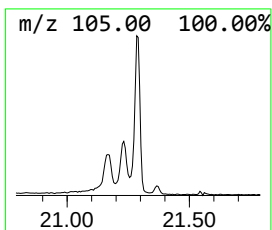
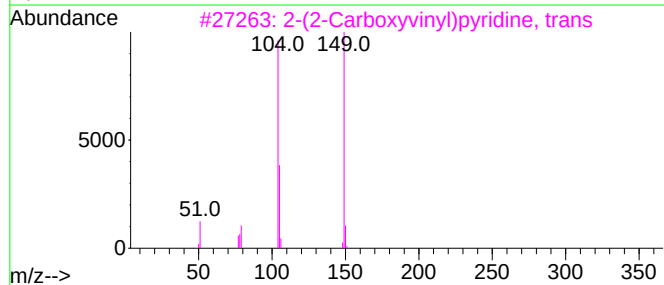
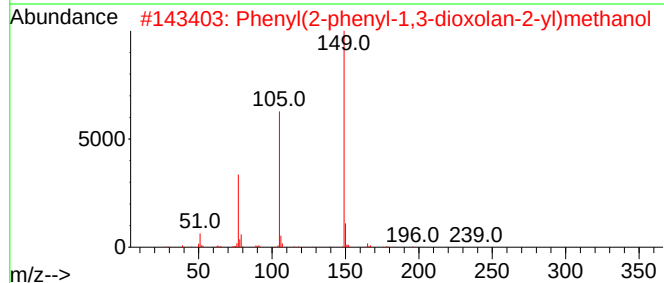
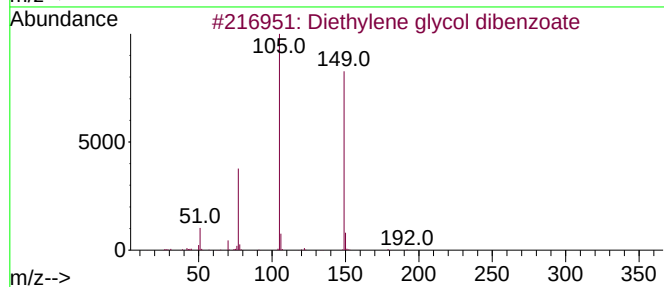
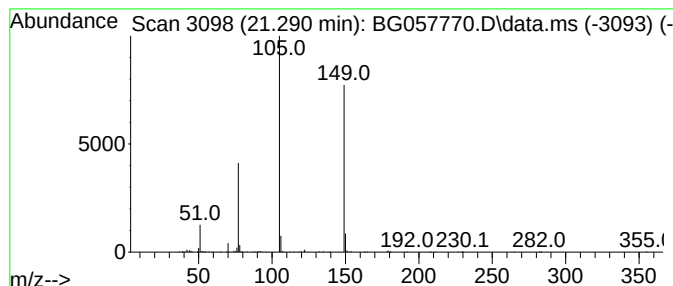
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG061923.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 8 Diethylene glycol dibenzoate Concentration Rank 3

| R.T.   | EstConc  | Area   | Relative to ISTD | R.T.   |
|--------|----------|--------|------------------|--------|
| 21.290 | 11.90 ng | 362286 | Chrysene-d12     | 21.555 |

| Hit# | of | 5 | Tentative ID                               | MW  | MolForm  | CAS#         | Qual |
|------|----|---|--------------------------------------------|-----|----------|--------------|------|
| 1    |    |   | Diethylene glycol dibenzoate               | 314 | C18H18O5 | 000120-55-8  | 90   |
| 2    |    |   | Phenyl(2-phenyl-1,3-dioxolan-2-yl)methanol | 256 | C16H16O3 | 005694-69-9  | 78   |
| 3    |    |   | 2-(2-Carboxyvinyl)pyridine, trans          | 149 | C8H7NO2  | 007340-22-9  | 53   |
| 4    |    |   | 2-Methyl-4-hydroxybenzoxazole              | 149 | C8H7NO2  | 051110-60-2  | 43   |
| 5    |    |   | Phthalic acid, 2-methylbutyl pen...        | 306 | C18H26O4 | 1000322-81-2 | 38   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG062023\  
Data File : BG057770.D  
Acq On : 20 Jun 2023 10:45  
Operator : CG/JU  
Sample : 03289-05  
Misc :  
ALS Vial : 5 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
SB-02-12.0-14.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG061923.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-... | 5.033  | 20.6    | ng    | 202054   | 1                     | 7.924  | 195893 | 20.0 |
| Benzophenone       | 15.914 | 10.1    | ng    | 191935   | 3                     | 14.557 | 381224 | 20.0 |
| n-Hexadecanoic ... | 18.194 | 12.6    | ng    | 325745   | 4                     | 17.301 | 518282 | 20.0 |
| trans-Sinapalde... | 18.458 | 4.6     | ng    | 118490   | 4                     | 17.301 | 518282 | 20.0 |
| Octadecanoic acid  | 19.463 | 4.2     | ng    | 128856   | 5                     | 21.555 | 608929 | 20.0 |
| Benzenepropanam... | 21.173 | 2.1     | ng    | 65315    | 5                     | 21.555 | 608929 | 20.0 |
| 3-Eicosene, (E)-   | 21.208 | 11.1    | ng    | 338724   | 5                     | 21.555 | 608929 | 20.0 |
| Diethylene glyc... | 21.290 | 11.9    | ng    | 362286   | 5                     | 21.555 | 608929 | 20.0 |