

Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG062123\  
 Data File : BG057797.D  
 Acq On : 21 Jun 2023 23:35  
 Operator : CG/JU  
 Sample : 03289-23  
 Misc :  
 ALS Vial : 14 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 SB-08-4.0-6.0

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: BG057797.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         | 5.027       | 324           | 330         | 337          | rBV      | 88581          | 127199        | 7.78%           | 1.458%        |
| 2         | 5.491       | 402           | 409         | 418          | rBV      | 370299         | 566119        | 34.65%          | 6.491%        |
| 3         | 7.077       | 672           | 679         | 690          | rBV      | 382891         | 626340        | 38.33%          | 7.182%        |
| 4         | 7.923       | 816           | 823         | 829          | rVB      | 99891          | 166367        | 10.18%          | 1.908%        |
| 5         | 9.081       | 1012          | 1020        | 1033         | rBV      | 218838         | 373197        | 22.84%          | 4.279%        |
| 6         | 10.726      | 1290          | 1300        | 1309         | rVB      | 146196         | 261538        | 16.01%          | 2.999%        |
| 7         | 13.176      | 1711          | 1717        | 1726         | rVB      | 554766         | 866116        | 53.01%          | 9.931%        |
| 8         | 14.557      | 1945          | 1952        | 1958         | rVB      | 271858         | 402447        | 24.63%          | 4.614%        |
| 9         | 15.908      | 2176          | 2182        | 2189         | rVB      | 69892          | 98487         | 6.03%           | 1.129%        |
| 10        | 16.037      | 2198          | 2204        | 2211         | rBV      | 549925         | 841816        | 51.52%          | 9.652%        |
| 11        | 17.301      | 2412          | 2419        | 2425         | rVB      | 412282         | 585279        | 35.82%          | 6.711%        |
| 12        | 18.188      | 2565          | 2570        | 2581         | rBV      | 99585          | 162478        | 9.94%           | 1.863%        |
| 13        | 19.463      | 2783          | 2787        | 2794         | rBV2     | 31521          | 48836         | 2.99%           | 0.560%        |
| 14        | 19.915      | 2858          | 2864        | 2870         | rBV      | 1243826        | 1633985       | 100.00%         | 18.735%       |
| 15        | 21.167      | 3072          | 3077        | 3080         | rBV2     | 24660          | 43207         | 2.64%           | 0.495%        |
| 16        | 21.208      | 3080          | 3084        | 3092         | rVV3     | 101052         | 200163        | 12.25%          | 2.295%        |
| 17        | 21.284      | 3093          | 3097        | 3108         | rVB      | 116901         | 175026        | 10.71%          | 2.007%        |
| 18        | 21.548      | 3136          | 3142        | 3150         | rBV      | 411057         | 657426        | 40.23%          | 7.538%        |
| 19        | 21.754      | 3173          | 3177        | 3183         | rVB      | 24722          | 33741         | 2.06%           | 0.387%        |
| 20        | 22.348      | 3274          | 3278        | 3284         | rBV5     | 23838          | 40083         | 2.45%           | 0.460%        |
| 21        | 23.029      | 3390          | 3394        | 3401         | rVB4     | 16894          | 25258         | 1.55%           | 0.290%        |
| 22        | 23.217      | 3421          | 3426        | 3431         | rVB2     | 21941          | 41084         | 2.51%           | 0.471%        |
| 23        | 24.704      | 3669          | 3679        | 3695         | rVB      | 258435         | 745174        | 45.60%          | 8.544%        |

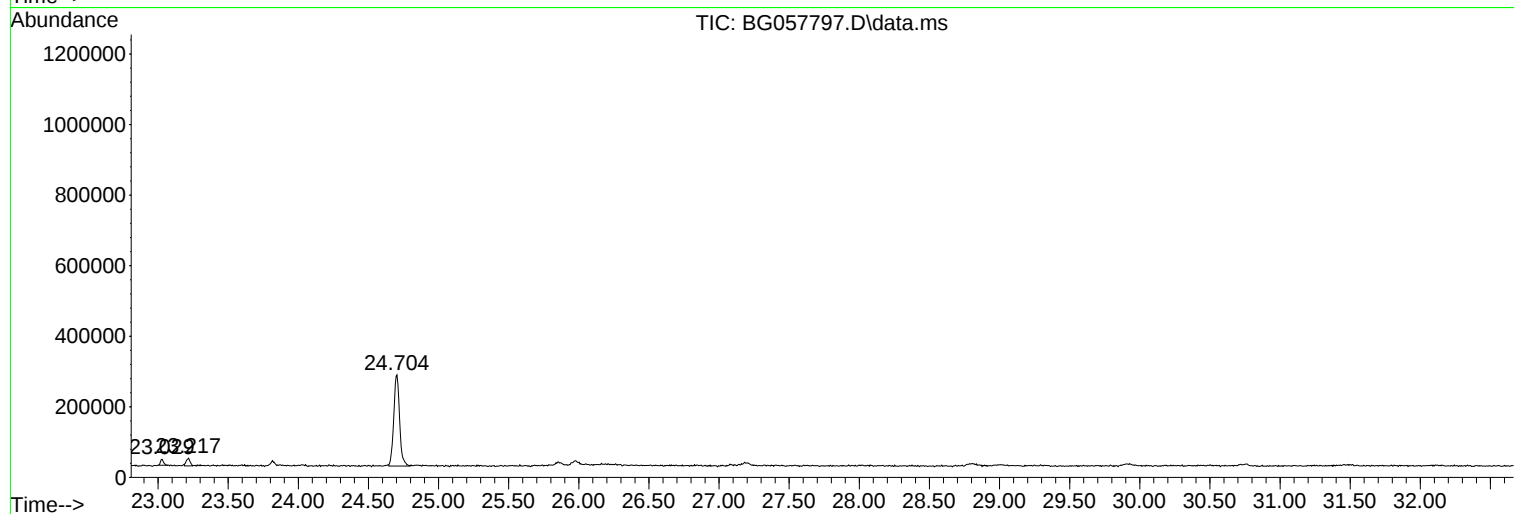
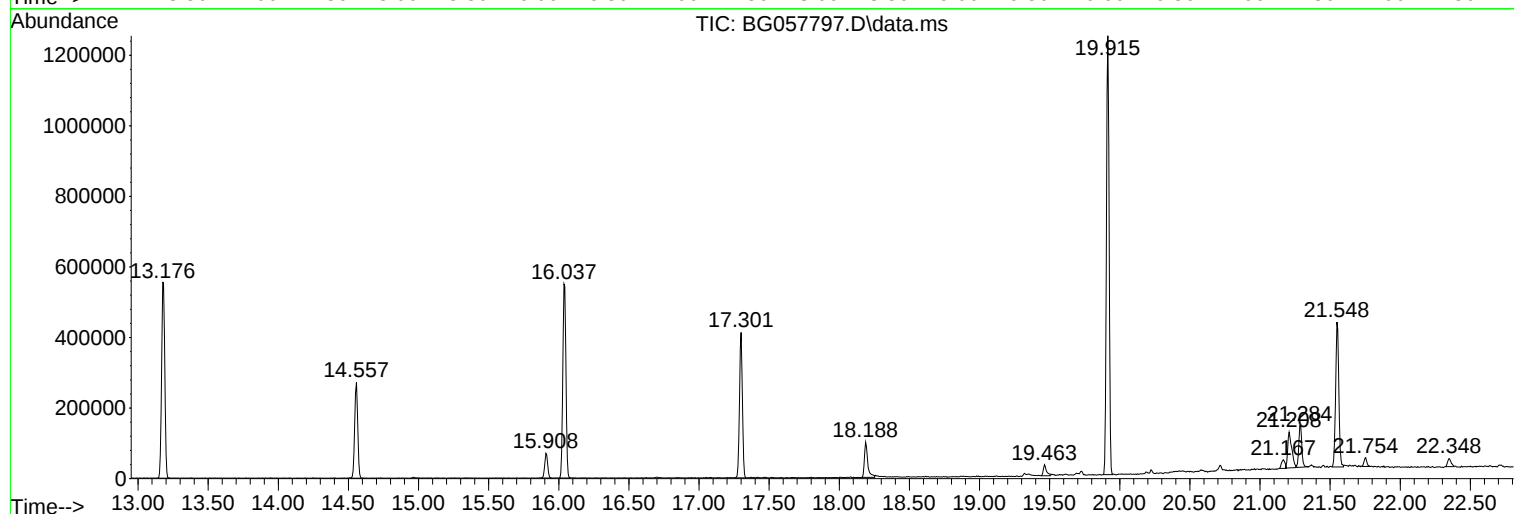
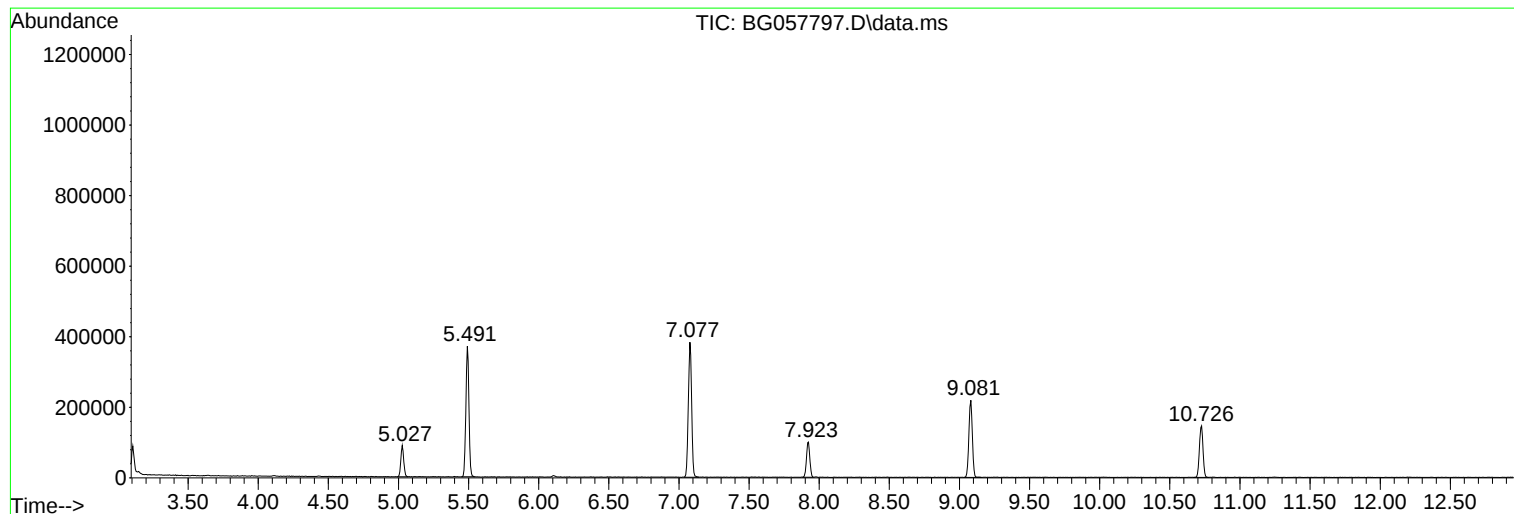
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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG061923.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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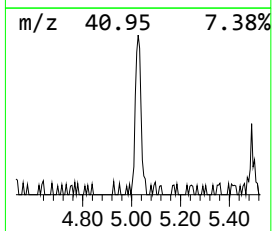
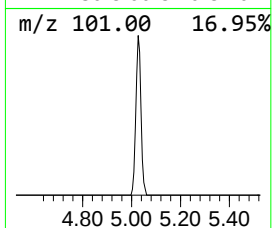
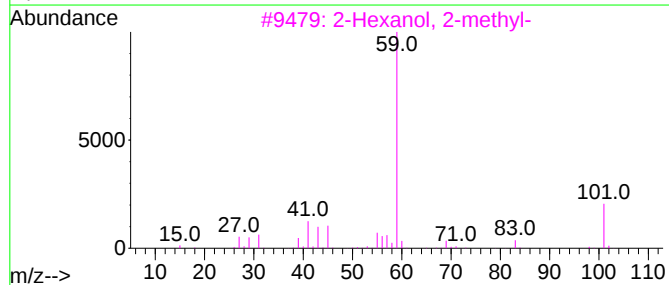
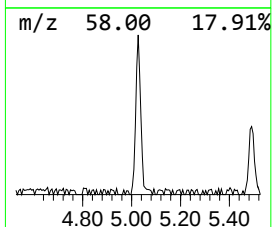
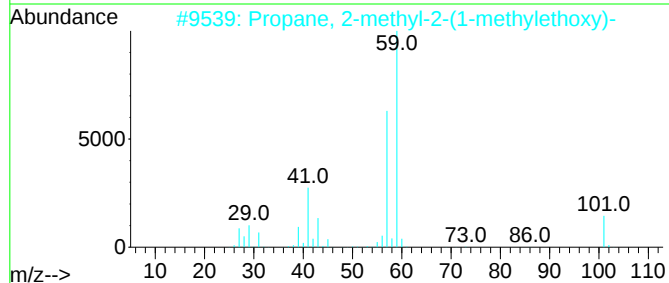
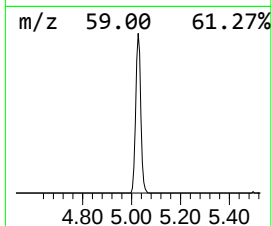
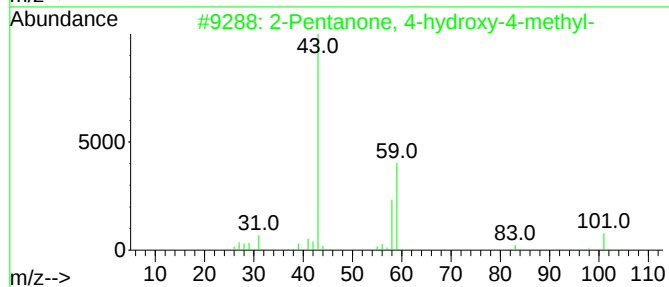
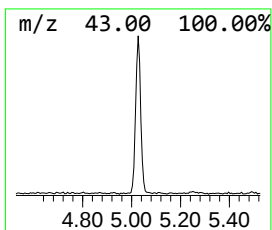
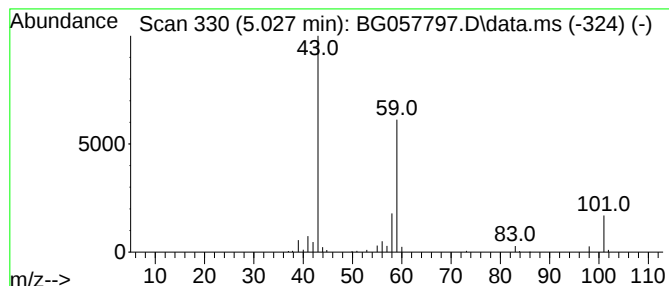
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

| R.T.  | EstConc  | Area   | Relative to ISTD       | R.T.  |
|-------|----------|--------|------------------------|-------|
| 5.027 | 15.29 ng | 127199 | 1,4-Dichlorobenzene-d4 | 7.923 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2  | 000123-42-2 | 56   |
| 2    |    |   | Propane, 2-methyl-2-(1-methyleth... | 116 | C7H16O   | 017348-59-3 | 42   |
| 3    |    |   | 2-Hexanol, 2-methyl-                | 116 | C7H16O   | 000625-23-0 | 38   |
| 4    |    |   | 2-Pentanol, 2,4-dimethyl-           | 116 | C7H16O   | 000625-06-9 | 28   |
| 5    |    |   | 1,8-Nonanediol, 8-methyl-           | 174 | C10H22O2 | 054725-73-4 | 25   |



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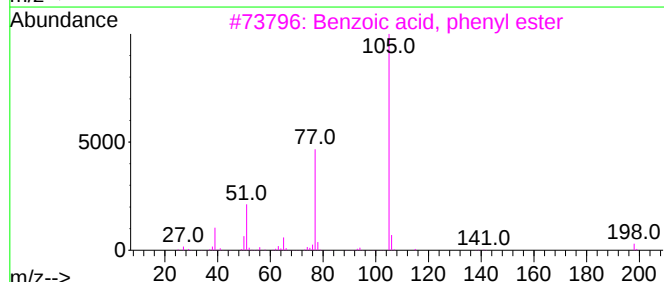
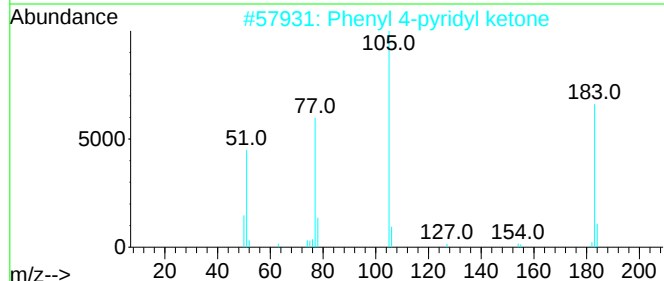
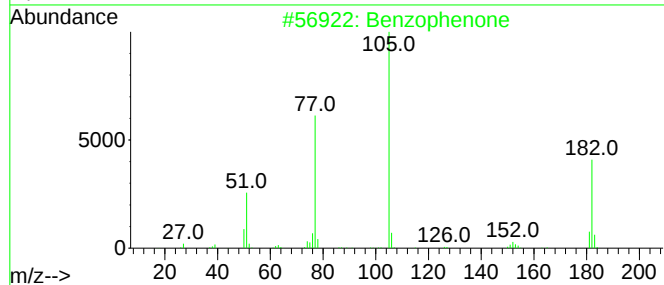
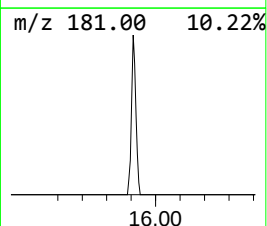
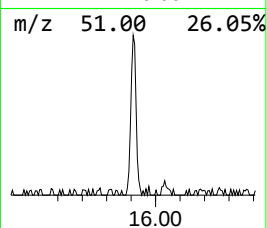
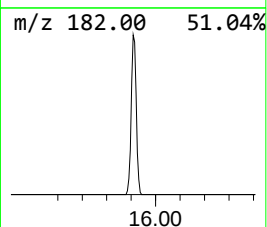
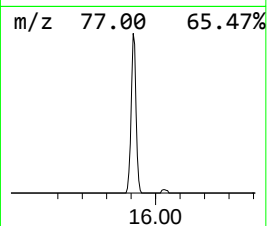
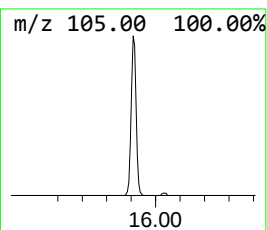
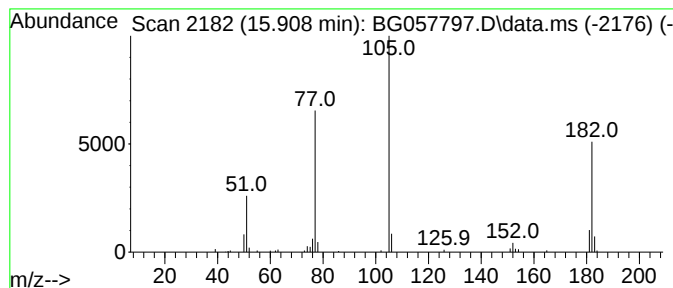
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG061923.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.   |
|--------|---------|-------|------------------|--------|
| 15.908 | 4.89 ng | 98487 | Acenaphthene-d10 | 14.557 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|----------|--------------|------|
| 1    |    |   | Benzophenone                        | 182 | C13H10O  | 000119-61-9  | 96   |
| 2    |    |   | Phenyl 4-pyridyl ketone             | 183 | C12H9NO  | 014548-46-0  | 53   |
| 3    |    |   | Benzoic acid, phenyl ester          | 198 | C13H10O2 | 000093-99-2  | 47   |
| 4    |    |   | N-(1-Cyanovinyl)benzamide           | 172 | C10H8N2O | 1000186-19-1 | 47   |
| 5    |    |   | Benzenecarbothioic acid, S-methy... | 152 | C8H8OS   | 005925-68-8  | 47   |



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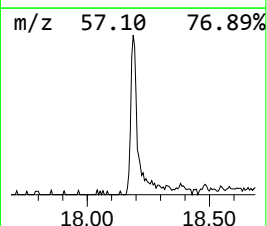
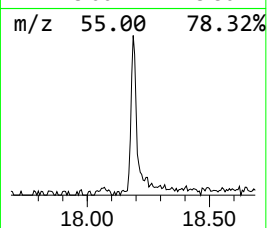
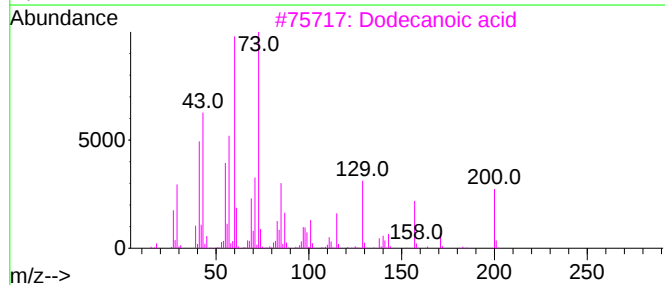
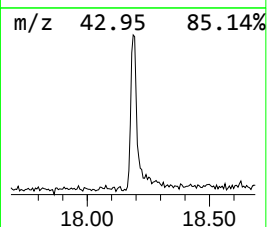
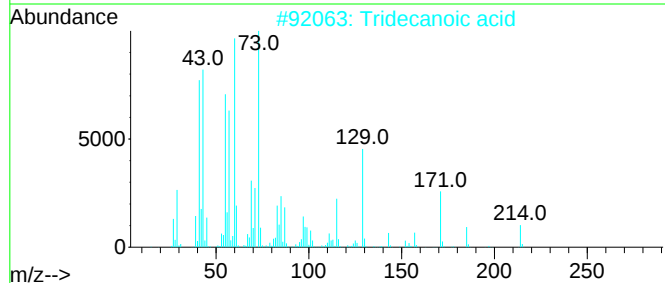
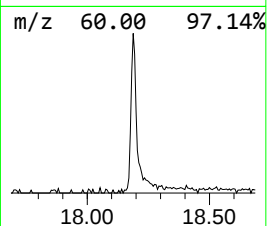
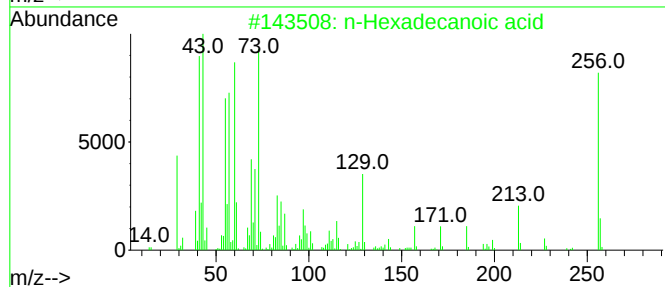
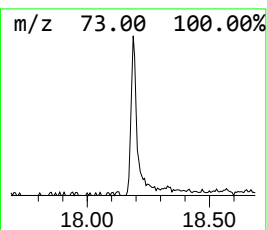
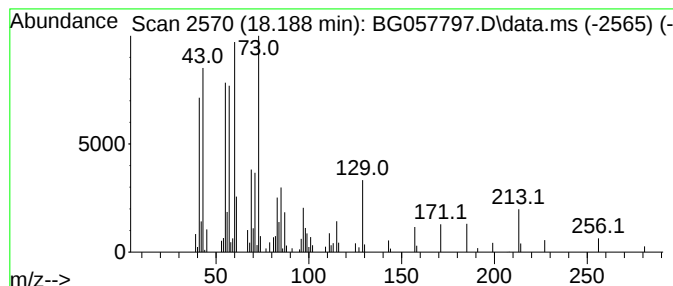
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 18.188 | 5.55 ng | 162478 | Phenanthrene-d10 | 17.301 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 98   |
| 2    |    |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 90   |
| 3    |    |   | Dodecanoic acid     | 200 | C12H24O2 | 000143-07-7 | 64   |
| 4    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 64   |
| 5    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 62   |



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

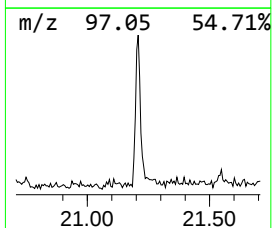
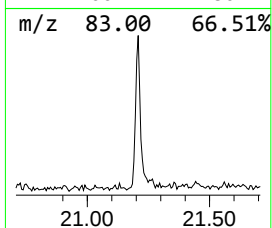
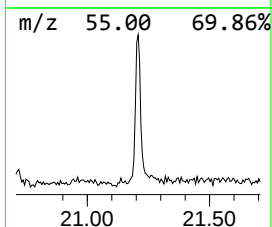
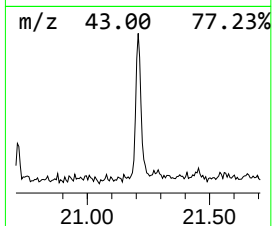
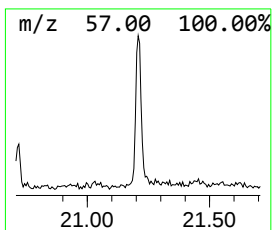
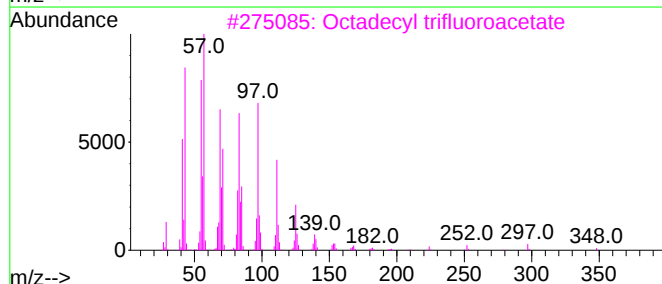
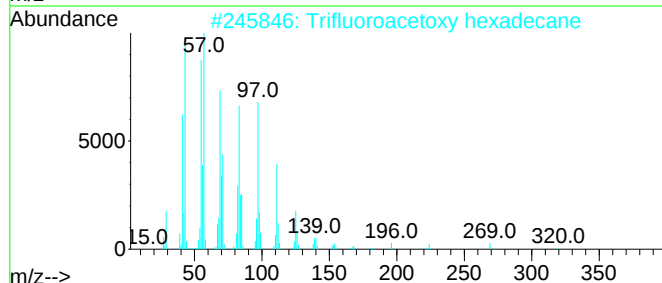
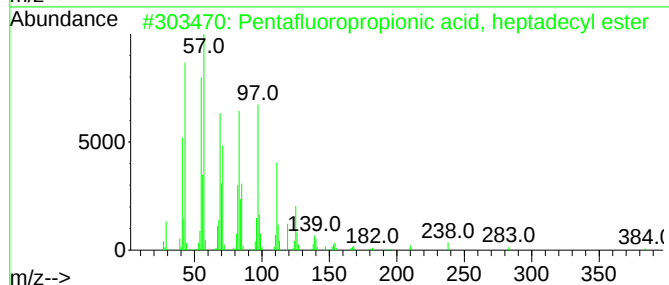
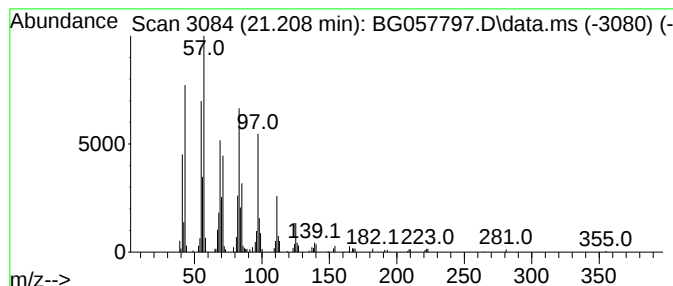
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Peak Number 4 Pentafluoropropionic acid, ... Concentration Rank 2

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 21.208 | 6.09 ng | 200163 | Chrysene-d12     | 21.548 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|------------|-------------|------|
| 1    |    |   | Pentafluoropropionic acid, hepta... | 402 | C20H35F5O2 | 959218-78-1 | 91   |
| 2    |    |   | Trifluoroacetoxy hexadecane         | 338 | C18H33F3O2 | 006222-03-3 | 91   |
| 3    |    |   | Octadecyl trifluoroacetate          | 366 | C20H37F3O2 | 079392-43-1 | 91   |
| 4    |    |   | Heptafluorobutyric acid, pentade... | 424 | C19H31F7O2 | 959261-23-5 | 91   |
| 5    |    |   | Heptadecyl heptafluorobutyrate      | 452 | C21H35F7O2 | 959085-66-6 | 91   |



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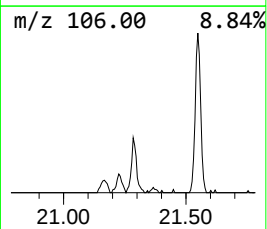
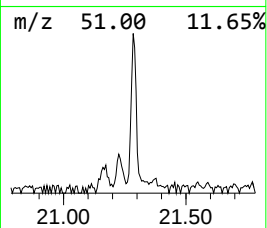
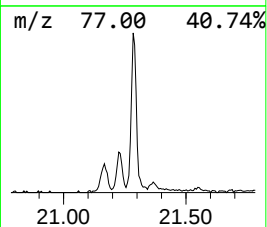
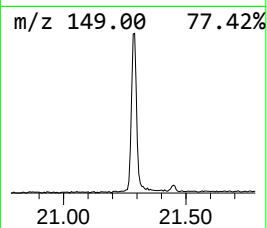
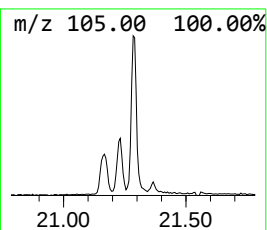
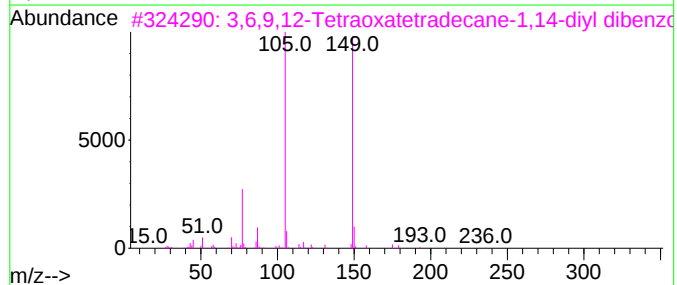
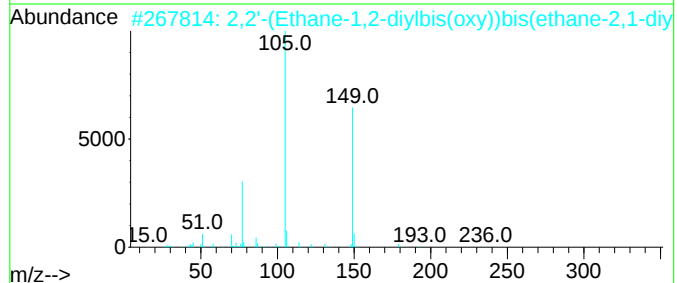
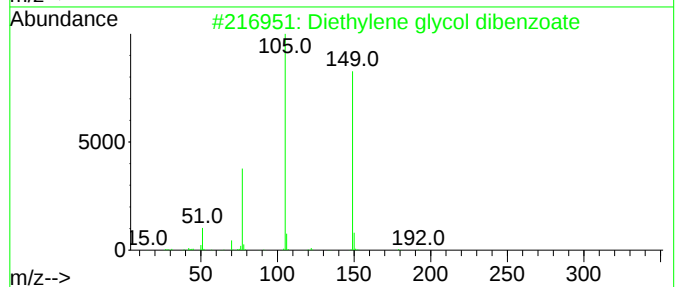
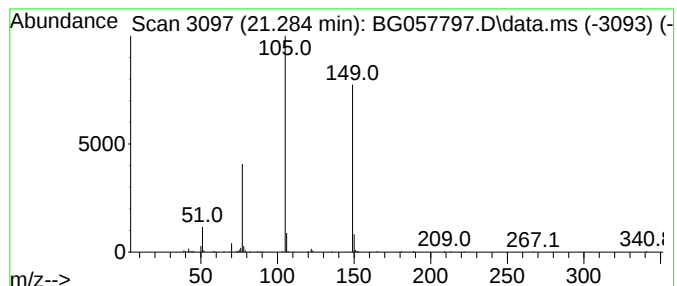
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG061923.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 5 Diethylene glycol dibenzoate Concentration Rank 4

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 21.284 | 5.32 ng | 175026 | Chrysene-d12     | 21.548 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|----------|--------------|------|
| 1    |    |   | Diethylene glycol dibenzoate        | 314 | C18H18O5 | 000120-55-8  | 90   |
| 2    |    |   | 2,2'-(Ethane-1,2-diylbis(oxy))bi... | 358 | C20H22O6 | 1000366-99-4 | 83   |
| 3    |    |   | 3,6,9,12-Tetraoxatetradecane-1,1... | 446 | C24H30O8 | 1000366-97-0 | 83   |
| 4    |    |   | 2-(2-Carboxyvinyl)pyridine, trans   | 149 | C8H7NO2  | 007340-22-9  | 52   |
| 5    |    |   | 2-Methyl-4-hydroxybenzoxazole       | 149 | C8H7NO2  | 051110-60-2  | 43   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG062123\  
Data File : BG057797.D  
Acq On : 21 Jun 2023 23:35  
Operator : CG/JU  
Sample : 03289-23  
Misc :  
ALS Vial : 14 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
SB-08-4.0-6.0

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

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| 2-Pentanone, 4-... | 5.027  | 15.3    | ng    | 127199   | 1                     | 7.923  | 166367 | 20.0 |
| Benzophenone       | 15.908 | 4.9     | ng    | 98487    | 3                     | 14.557 | 402447 | 20.0 |
| n-Hexadecanoic ... | 18.188 | 5.5     | ng    | 162478   | 4                     | 17.301 | 585279 | 20.0 |
| Pentafluoroprop... | 21.208 | 6.1     | ng    | 200163   | 5                     | 21.548 | 657426 | 20.0 |
| Diethylene glyc... | 21.284 | 5.3     | ng    | 175026   | 5                     | 21.548 | 657426 | 20.0 |