

Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG062321\  
 Data File : BG049069.D  
 Acq On : 23 Jun 2021 20:13  
 Operator : CG/JU  
 Sample : M2795-07  
 Misc :  
 ALS Vial : 13 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 B4-0-2

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA\_G\METHODS\8270-BG061121.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG049069.D\data.ms

| peak<br># | R.T.<br>min | first<br>scan | max<br>scan | last<br>scan | PK<br>TY | peak<br>height | corr.<br>area | corr.<br>% max. | % of<br>total |
|-----------|-------------|---------------|-------------|--------------|----------|----------------|---------------|-----------------|---------------|
| 1         | 3.159       | 14            | 20          | 30           | rBV2     | 48105          | 101366        | 12.38%          | 1.915%        |
| 2         | 3.235       | 30            | 33          | 37           | rVB3     | 10563          | 12813         | 1.56%           | 0.242%        |
| 3         | 4.581       | 257           | 262         | 269          | rBV      | 46244          | 75786         | 9.26%           | 1.432%        |
| 4         | 5.186       | 360           | 365         | 374          | rVB      | 106764         | 167144        | 20.41%          | 3.158%        |
| 5         | 5.656       | 439           | 445         | 455          | rVB      | 114920         | 192287        | 23.48%          | 3.633%        |
| 6         | 7.254       | 710           | 717         | 731          | rBV2     | 148371         | 269272        | 32.89%          | 5.088%        |
| 7         | 8.106       | 855           | 862         | 868          | rBV      | 107080         | 186394        | 22.77%          | 3.522%        |
| 8         | 9.269       | 1052          | 1060        | 1068         | rBV2     | 94813          | 180995        | 22.11%          | 3.420%        |
| 9         | 10.691      | 1296          | 1302        | 1310         | rBV3     | 21877          | 43627         | 5.33%           | 0.824%        |
| 10        | 10.926      | 1333          | 1342        | 1351         | rBV      | 139988         | 248737        | 30.38%          | 4.700%        |
| 11        | 13.370      | 1751          | 1758        | 1765         | rBV      | 248830         | 387600        | 47.34%          | 7.324%        |
| 12        | 14.745      | 1985          | 1992        | 2001         | rBV      | 222425         | 359331        | 43.89%          | 6.790%        |
| 13        | 15.474      | 2110          | 2116        | 2123         | rBV2     | 22220          | 32126         | 3.92%           | 0.607%        |
| 14        | 16.232      | 2239          | 2245        | 2253         | rBV2     | 90716          | 137542        | 16.80%          | 2.599%        |
| 15        | 17.495      | 2452          | 2460        | 2465         | rBV      | 355667         | 539688        | 65.91%          | 10.198%       |
| 16        | 17.536      | 2465          | 2467        | 2472         | rVB2     | 14497          | 18423         | 2.25%           | 0.348%        |
| 17        | 18.376      | 2605          | 2610        | 2614         | rBV3     | 11990          | 18104         | 2.21%           | 0.342%        |
| 18        | 19.322      | 2767          | 2771        | 2774         | rBV5     | 12512          | 13699         | 1.67%           | 0.259%        |
| 19        | 19.540      | 2803          | 2808        | 2815         | rBV2     | 25315          | 36991         | 4.52%           | 0.699%        |
| 20        | 19.904      | 2867          | 2870        | 2876         | rVB2     | 27397          | 40978         | 5.00%           | 0.774%        |
| 21        | 20.098      | 2896          | 2903        | 2910         | rBV      | 632605         | 818770        | 100.00%         | 15.471%       |
| 22        | 20.779      | 3016          | 3019        | 3024         | rVB8     | 9446           | 14736         | 1.80%           | 0.278%        |
| 23        | 21.408      | 3122          | 3126        | 3131         | rBV7     | 27191          | 46982         | 5.74%           | 0.888%        |
| 24        | 21.778      | 3183          | 3189        | 3196         | rBV2     | 360663         | 630777        | 77.04%          | 11.919%       |
| 25        | 22.971      | 3387          | 3392        | 3394         | rBV6     | 6738           | 12011         | 1.47%           | 0.227%        |
| 26        | 24.040      | 3569          | 3574        | 3578         | rBV7     | 9658           | 18710         | 2.29%           | 0.354%        |
| 27        | 25.098      | 3744          | 3754        | 3772         | rVB2     | 218950         | 679108        | 82.94%          | 12.832%       |
| 28        | 26.332      | 3961          | 3964        | 3966         | rBV4     | 7281           | 8204          | 1.00%           | 0.155%        |

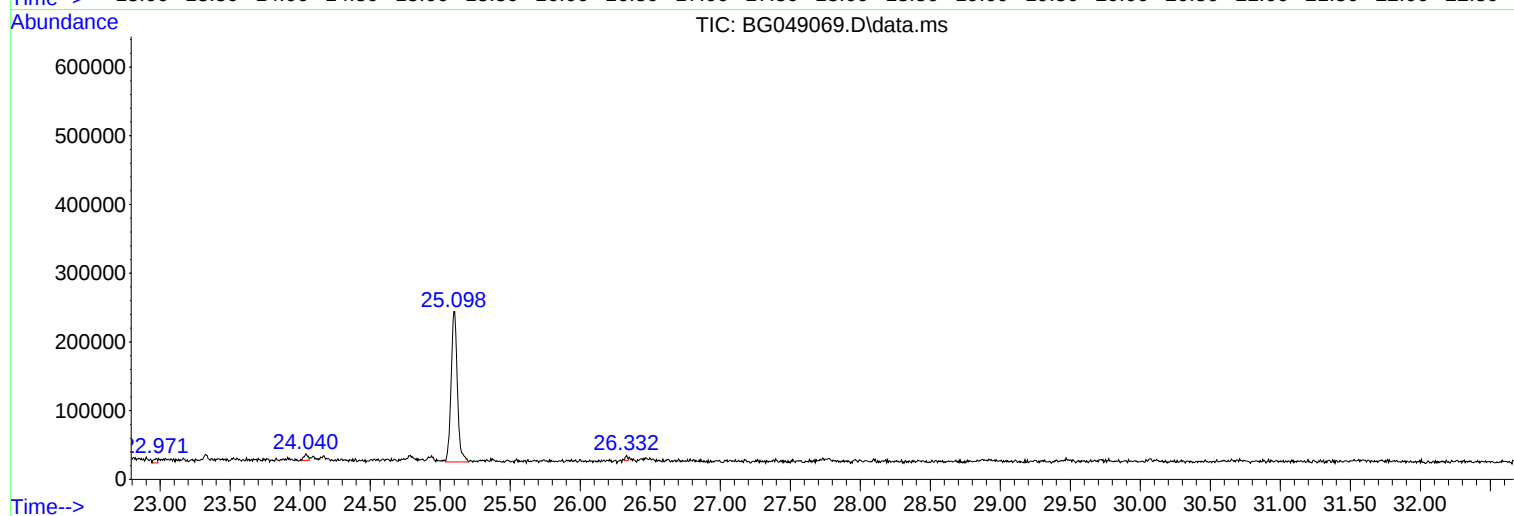
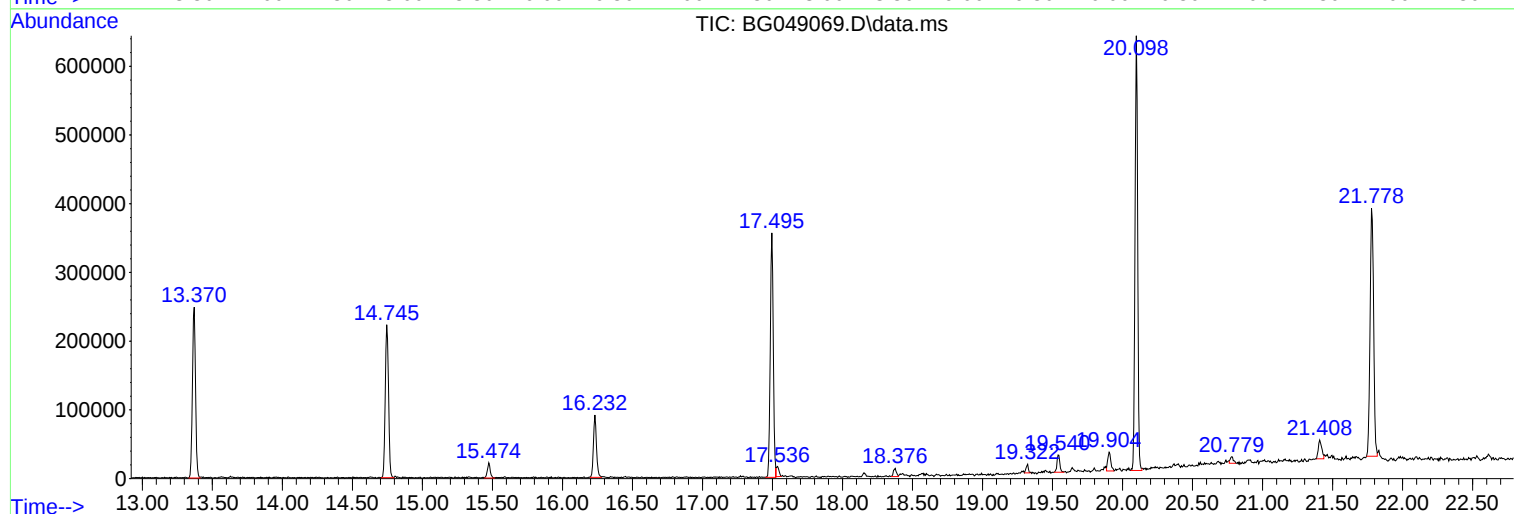
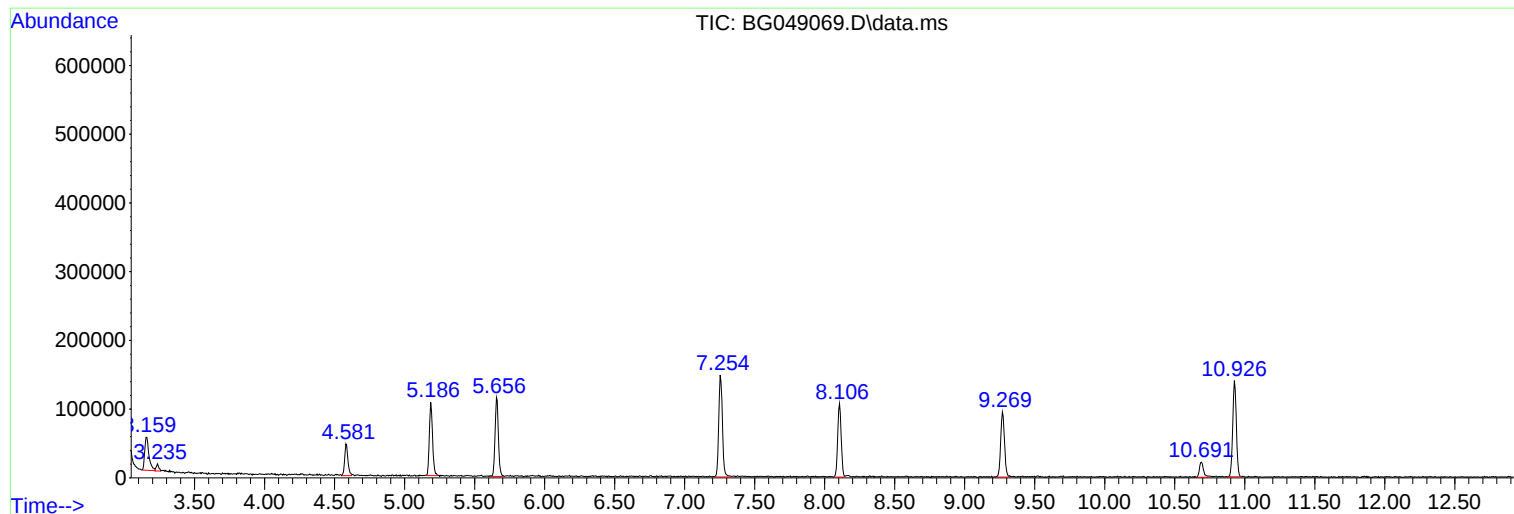
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BNA\_G  
ClientSampleId :  
B4-0-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_G\METHODS\8270-BG061121.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L  
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG062321\  
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Instrument :  
BNA\_G  
ClientSampleId :  
B4-0-2

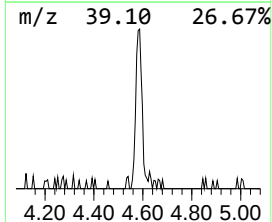
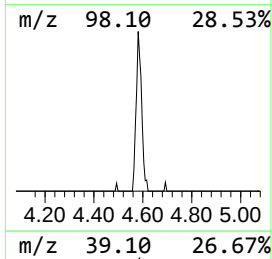
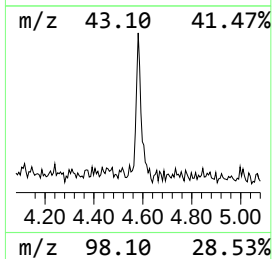
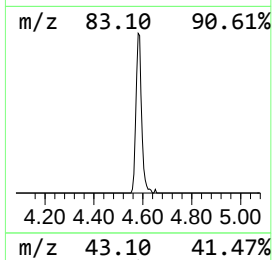
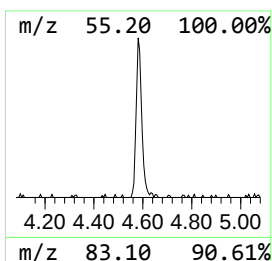
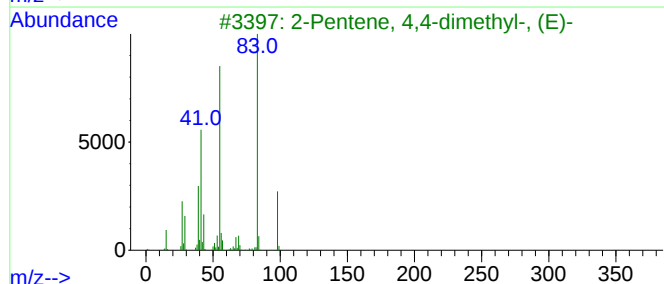
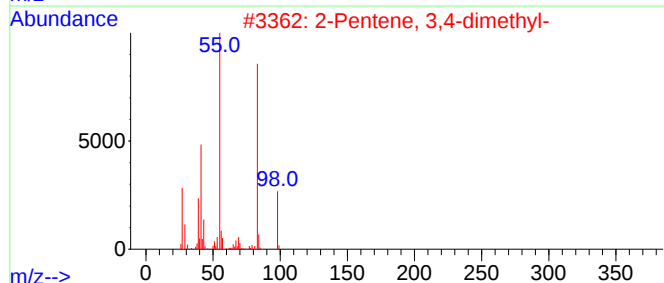
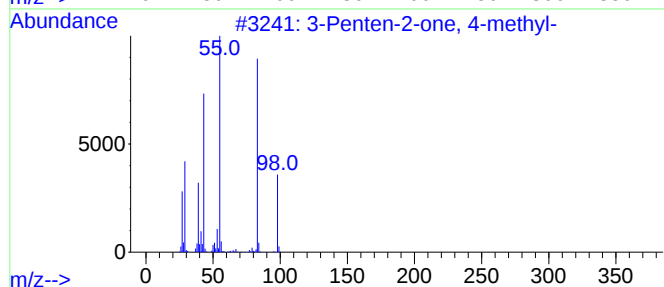
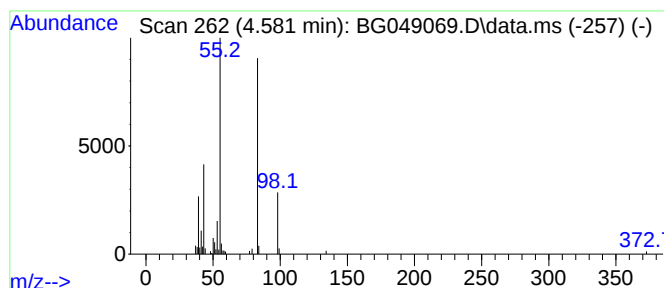
Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_G\METHODS\8270-BG061121.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 3

| R.T.  | EstConc | Area  | Relative to ISTD       | R.T.  |
|-------|---------|-------|------------------------|-------|
| 4.581 | 8.13 ng | 75786 | 1,4-Dichlorobenzene-d4 | 8.106 |

| Hit# | of 5 | Tentative ID                   | MW | MolForm | CAS#        | Qual |
|------|------|--------------------------------|----|---------|-------------|------|
| 1    |      | 3-Penten-2-one, 4-methyl-      | 98 | C6H10O  | 000141-79-7 | 86   |
| 2    |      | 2-Pentene, 3,4-dimethyl-       | 98 | C7H14   | 024910-63-2 | 72   |
| 3    |      | 2-Pentene, 4,4-dimethyl-, (E)- | 98 | C7H14   | 000690-08-4 | 72   |
| 4    |      | 3-Hexen-2-one                  | 98 | C6H10O  | 000763-93-9 | 72   |
| 5    |      | 2-Pentene, 2,4-dimethyl-       | 98 | C7H14   | 000625-65-0 | 72   |



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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

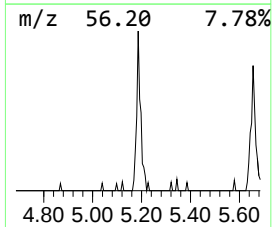
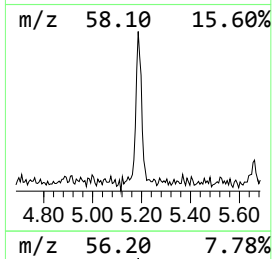
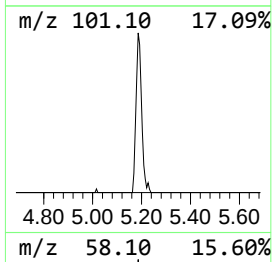
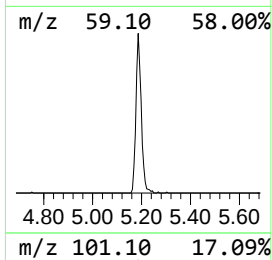
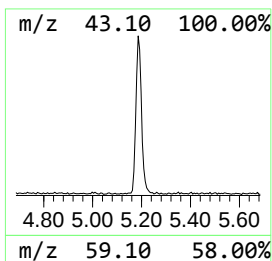
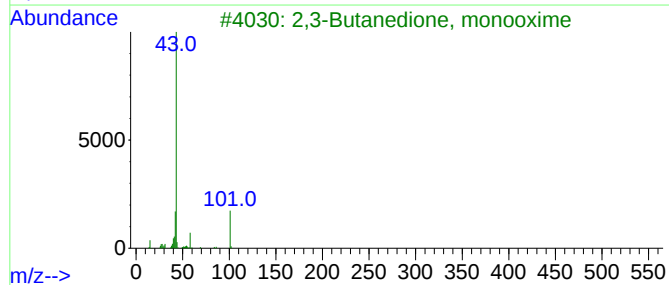
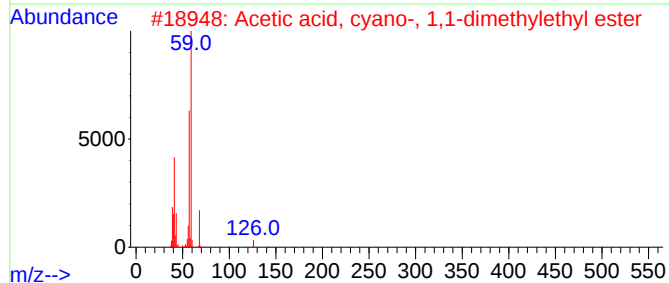
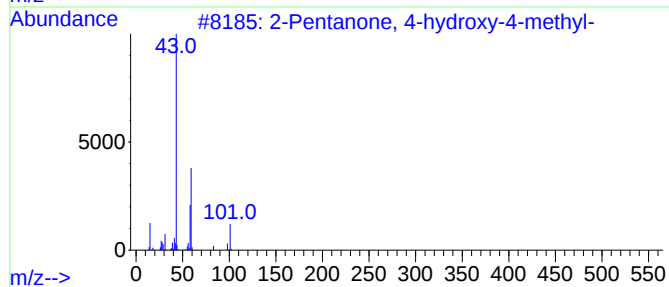
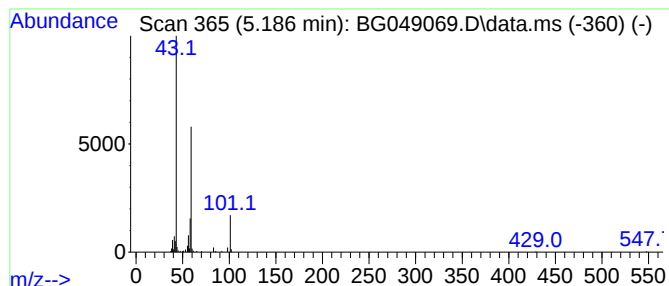
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TIC Integration Parameters: LSCINT.P

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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

| R.T.  | EstConc  | Area   | Relative to ISTD       | R.T.  |
|-------|----------|--------|------------------------|-------|
| 5.186 | 17.93 ng | 167144 | 1,4-Dichlorobenzene-d4 | 8.106 |

| Hit# | of                                  | 5   | Tentative ID | MW          | MolForm | CAS# | Qual |
|------|-------------------------------------|-----|--------------|-------------|---------|------|------|
| 1    | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2      | 000123-42-2 | 50      |      |      |
| 2    | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2     | 001116-98-9 | 23      |      |      |
| 3    | 2,3-Butanedione, monooxime          | 101 | C4H7NO2      | 000057-71-6 | 16      |      |      |
| 4    | Acetone                             | 58  | C3H6O        | 000067-64-1 | 10      |      |      |
| 5    | Guanidine                           | 59  | CH5N3        | 000113-00-8 | 9       |      |      |



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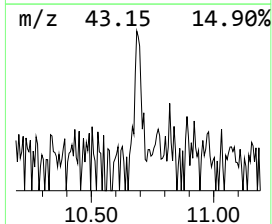
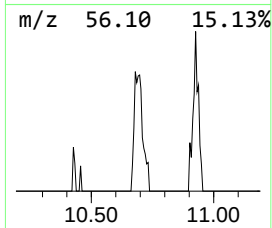
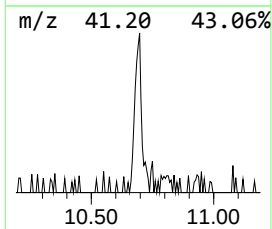
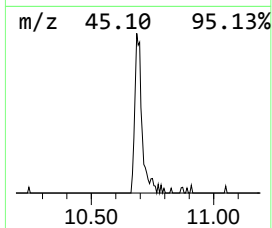
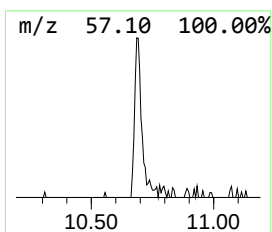
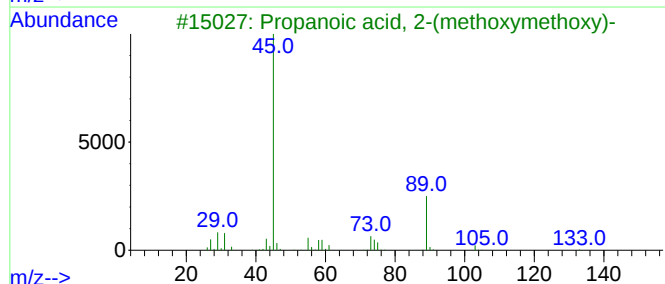
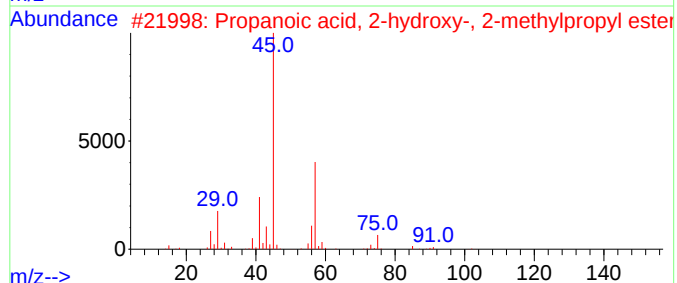
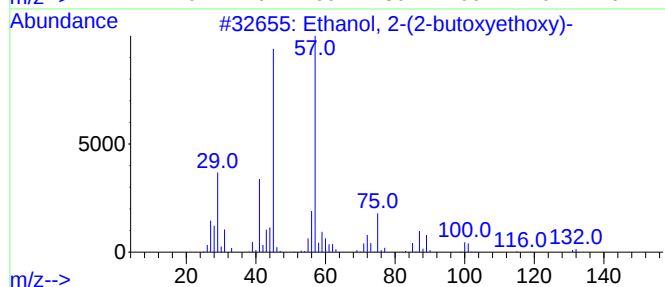
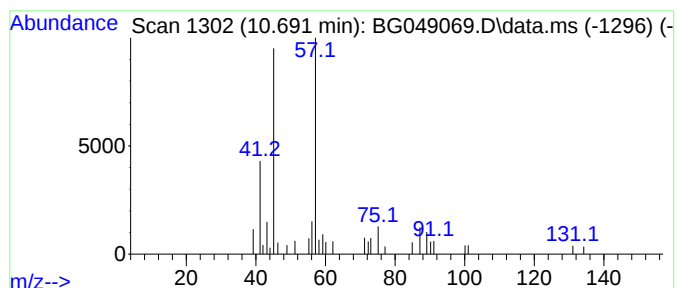
Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_G\METHODS\8270-BG061121.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 10.691 | 3.51 ng | 43627 | Naphthalene-d8   | 10.926 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|---------|-------------|------|
| 1    |    |   | Ethanol, 2-(2-butoxyethoxy)-        | 162 | C8H18O3 | 000112-34-5 | 72   |
| 2    |    |   | Propanoic acid, 2-hydroxy-, 2-me... | 146 | C7H14O3 | 000585-24-0 | 53   |
| 3    |    |   | Propanoic acid, 2-(methoxymethoxy)- | 134 | C5H10O4 | 081327-29-9 | 50   |
| 4    |    |   | Ethylene glycol diglycidyl ether    | 174 | C8H14O4 | 002224-15-9 | 50   |
| 5    |    |   | 12-Crown-4                          | 176 | C8H16O4 | 000294-93-9 | 45   |



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| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| 3-Penten-2-one,... | 4.581  | 8.1     | ng    | 75786    | 1                     | 8.106  | 186394 | 20.0 |
| 2-Pentanone, 4-... | 5.186  | 17.9    | ng    | 167144   | 1                     | 8.106  | 186394 | 20.0 |
| Ethanol, 2-(2-b... | 10.691 | 3.5     | ng    | 43627    | 2                     | 10.926 | 248737 | 20.0 |