

Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG010821\  
 Data File : BG047899.D  
 Acq On : 8 Jan 2021 23:25  
 Operator : CG/JU  
 Sample : M1044-16  
 Misc :  
 ALS Vial : 14 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 TP-8

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-BG121720.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG047899.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         | 3.510       | 22            | 29          | 35           | rBV      | 80485          | 101362        | 2.87%           | 0.687%        |
| 2         | 4.708       | 227           | 233         | 240          | rBV      | 121820         | 179411        | 5.08%           | 1.216%        |
| 3         | 5.178       | 307           | 313         | 316          | rBV      | 74903          | 114272        | 3.24%           | 0.774%        |
| 4         | 5.214       | 316           | 319         | 326          | rVB2     | 35141          | 53286         | 1.51%           | 0.361%        |
| 5         | 5.748       | 402           | 410         | 421          | rBV      | 934577         | 1637136       | 46.39%          | 11.095%       |
| 6         | 7.399       | 683           | 691         | 708          | rBV      | 728132         | 1695850       | 48.06%          | 11.493%       |
| 7         | 8.163       | 814           | 821         | 829          | rBV      | 187633         | 304324        | 8.62%           | 2.062%        |
| 8         | 9.332       | 1012          | 1020        | 1029         | rBV      | 628600         | 1113232       | 31.55%          | 7.544%        |
| 9         | 10.989      | 1296          | 1302        | 1309         | rBV      | 175585         | 325487        | 9.22%           | 2.206%        |
| 10        | 13.422      | 1707          | 1716        | 1726         | rBV      | 1100243        | 1699664       | 48.16%          | 11.518%       |
| 11        | 14.232      | 1848          | 1854        | 1859         | rBV2     | 28677          | 43874         | 1.24%           | 0.297%        |
| 12        | 14.791      | 1942          | 1949        | 1956         | rVB      | 250976         | 381489        | 10.81%          | 2.585%        |
| 13        | 16.283      | 2195          | 2203        | 2212         | rBV      | 1129952        | 1734591       | 49.15%          | 11.755%       |
| 14        | 17.534      | 2408          | 2416        | 2422         | rBV      | 346407         | 539444        | 15.29%          | 3.656%        |
| 15        | 20.126      | 2850          | 2857        | 2863         | rBV      | 2803315        | 3528904       | 100.00%         | 23.915%       |
| 16        | 21.424      | 3074          | 3078        | 3086         | rBV8     | 20094          | 43433         | 1.23%           | 0.294%        |
| 17        | 21.806      | 3136          | 3143        | 3152         | rBV      | 387098         | 651037        | 18.45%          | 4.412%        |
| 18        | 25.137      | 3699          | 3710        | 3719         | rVB2     | 204579         | 609211        | 17.26%          | 4.129%        |

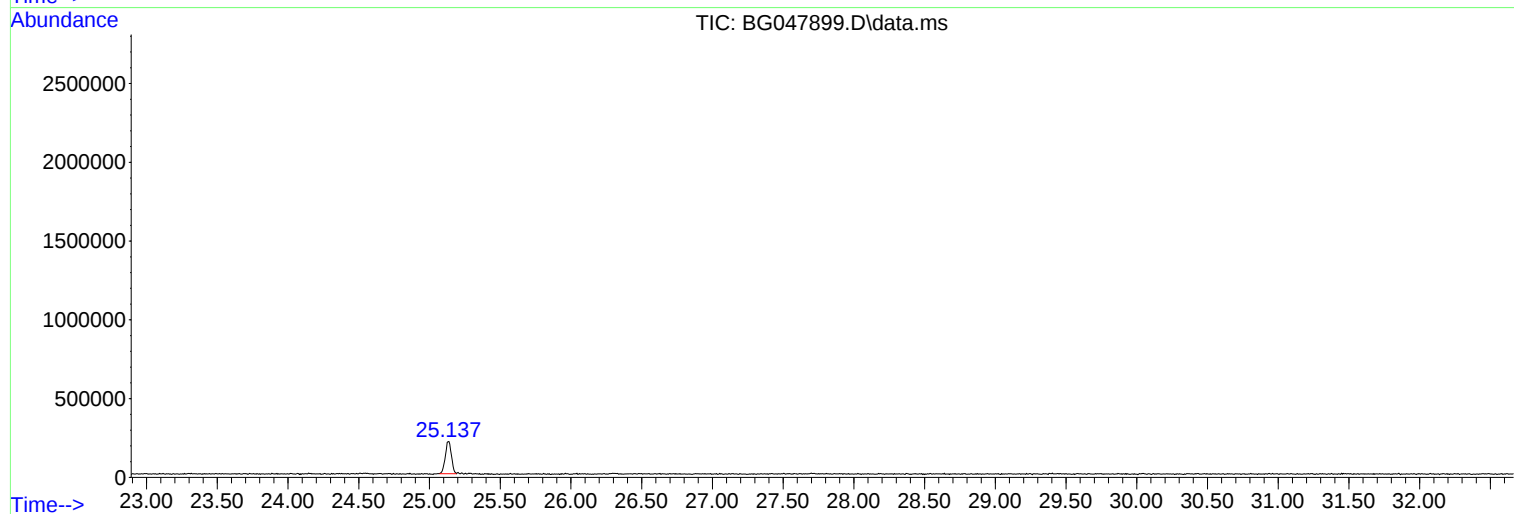
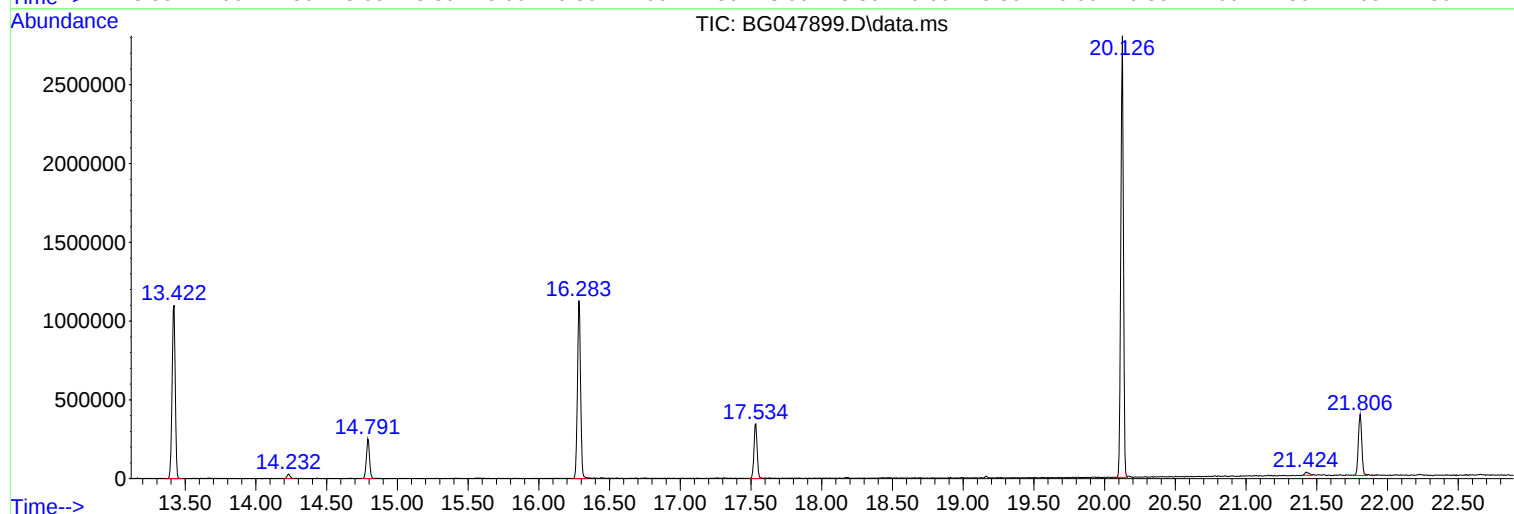
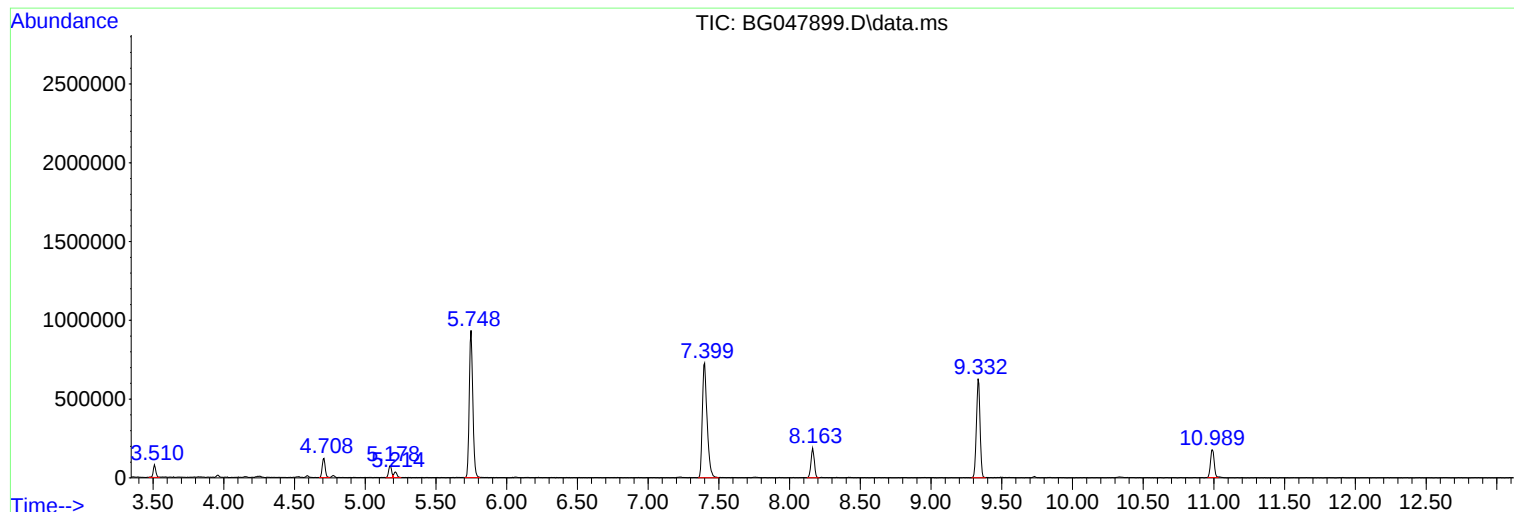
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BNA\_G  
ClientSampleId :  
TP-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_G\METHODS\8270-BG121720.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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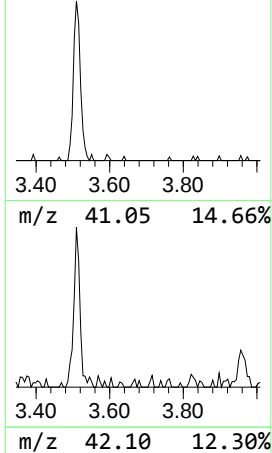
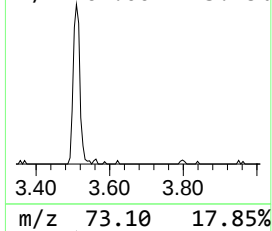
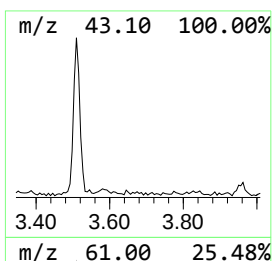
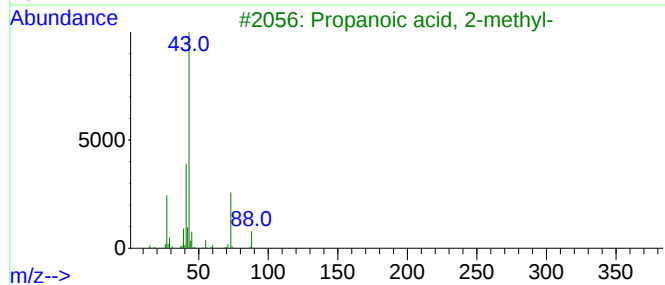
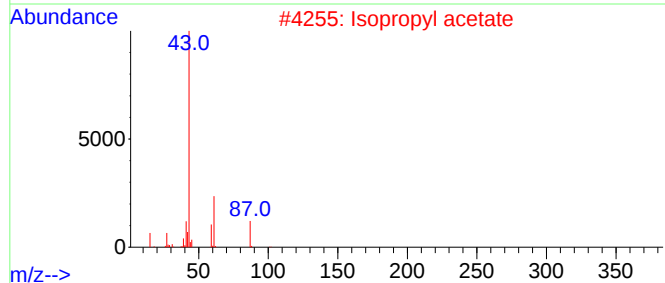
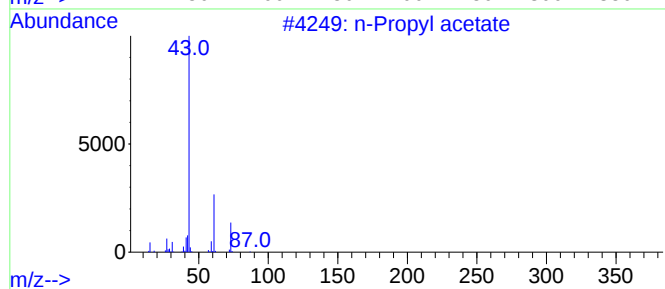
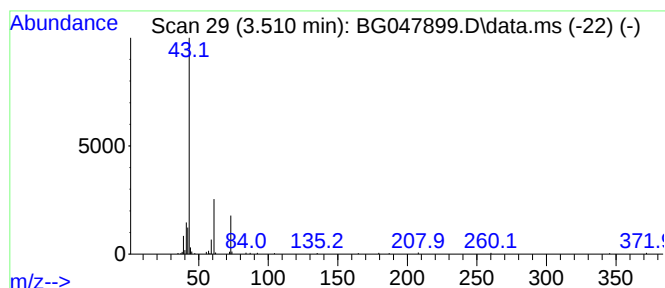
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Peak Number 1 n-Propyl acetate Concentration Rank 3

| R.T.  | EstConc | Area   | Relative to ISTD       | R.T.  |
|-------|---------|--------|------------------------|-------|
| 3.510 | 6.66 ng | 101362 | 1,4-Dichlorobenzene-d4 | 8.163 |

| Hit# | of | 5 | Tentative ID                   | MW  | MolForm   | CAS#        | Qual |
|------|----|---|--------------------------------|-----|-----------|-------------|------|
| 1    |    |   | n-Propyl acetate               | 102 | C5H10O2   | 000109-60-4 | 64   |
| 2    |    |   | Isopropyl acetate              | 102 | C5H10O2   | 000108-21-4 | 33   |
| 3    |    |   | Propanoic acid, 2-methyl-      | 88  | C4H8O2    | 000079-31-2 | 23   |
| 4    |    |   | Acetic acid, pentyl ester      | 130 | C7H14O2   | 000628-63-7 | 23   |
| 5    |    |   | 1-Pentanol, 5-chloro-, acetate | 164 | C7H13ClO2 | 020395-28-2 | 9    |



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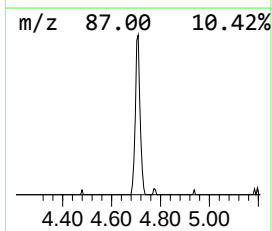
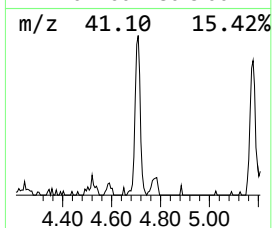
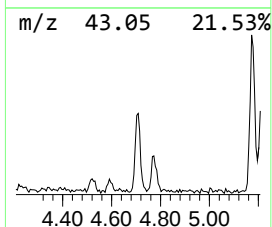
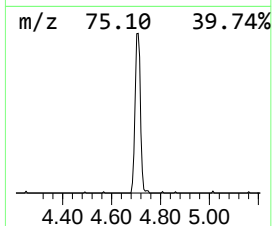
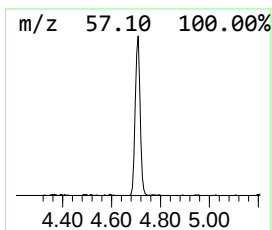
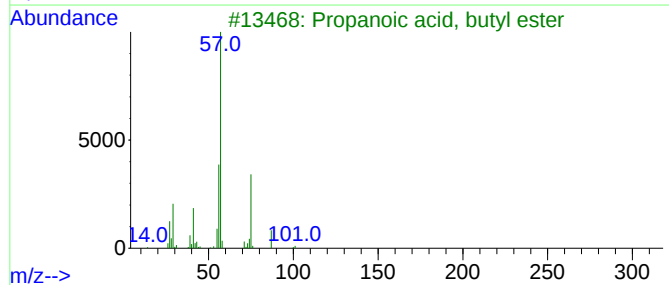
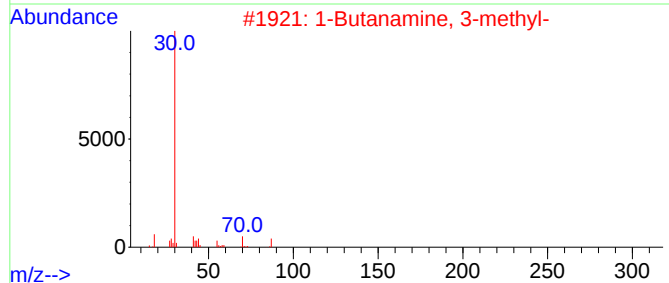
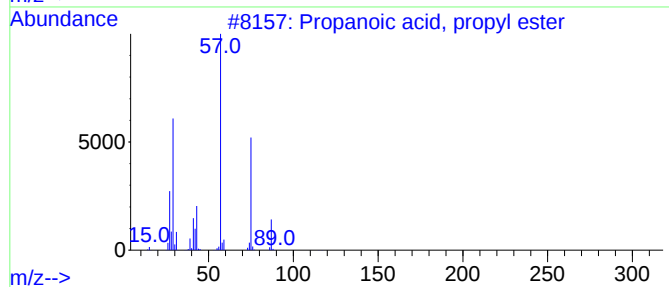
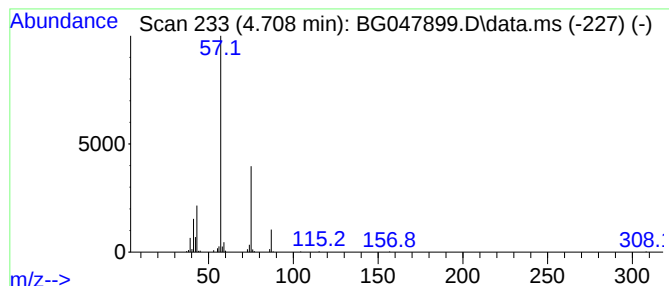
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Peak Number 2 Propanoic acid, propyl ester Concentration Rank 1

| R.T.  | EstConc  | Area   | Relative to ISTD       | R.T.  |
|-------|----------|--------|------------------------|-------|
| 4.708 | 11.79 ng | 179411 | 1,4-Dichlorobenzene-d4 | 8.163 |

| Hit# | of 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|------|-------------------------------------|-----|----------|-------------|------|
| 1    |      | Propanoic acid, propyl ester        | 116 | C6H12O2  | 000106-36-5 | 83   |
| 2    |      | 1-Butanamine, 3-methyl-             | 87  | C5H13N   | 000107-85-7 | 9    |
| 3    |      | Propanoic acid, butyl ester         | 130 | C7H14O2  | 000590-01-2 | 9    |
| 4    |      | Propanoic acid, 1-methylethyl ester | 116 | C6H12O2  | 000637-78-5 | 9    |
| 5    |      | di-tert-Butyl dicarbonate           | 218 | C10H18O5 | 024424-99-5 | 9    |



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ALS Vial : 14 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
TP-8

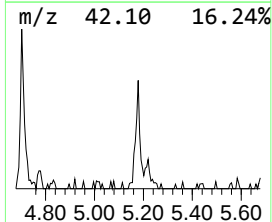
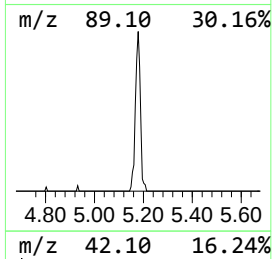
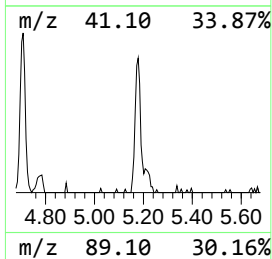
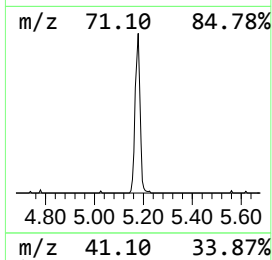
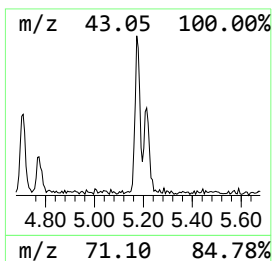
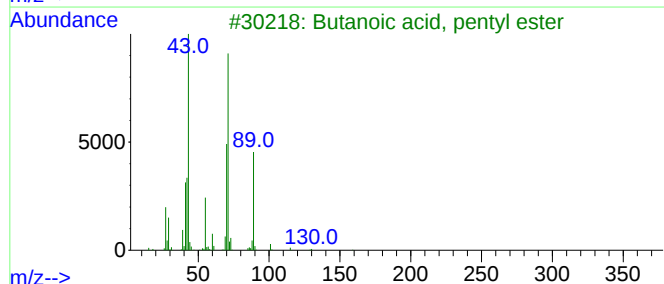
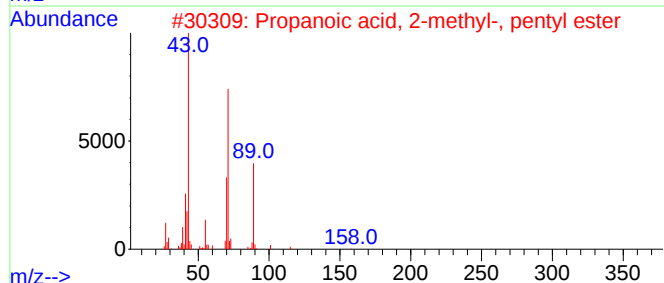
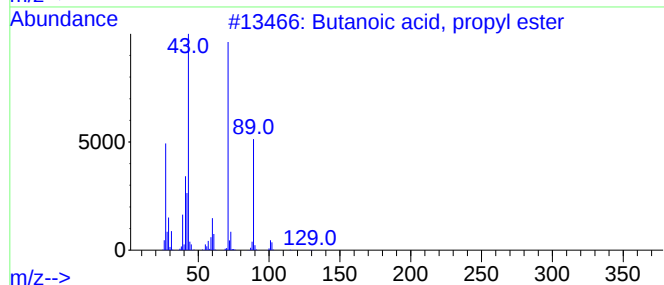
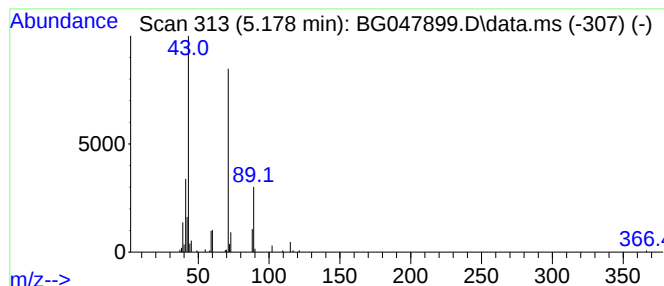
Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_G\METHODS\8270-BG121720.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 3 Butanoic acid, propyl ester Concentration Rank 2

| R.T.  | EstConc | Area   | Relative to ISTD       | R.T.  |
|-------|---------|--------|------------------------|-------|
| 5.178 | 7.51 ng | 114272 | 1,4-Dichlorobenzene-d4 | 8.163 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|----------|--------------|------|
| 1    |    |   | Butanoic acid, propyl ester         | 130 | C7H14O2  | 000105-66-8  | 72   |
| 2    |    |   | Propanoic acid, 2-methyl-, penty... | 158 | C9H18O2  | 002445-72-9  | 72   |
| 3    |    |   | Butanoic acid, pentyl ester         | 158 | C9H18O2  | 000540-18-1  | 64   |
| 4    |    |   | Sulfurous acid, isobutyl 2-penty... | 208 | C9H20O3S | 1000309-15-2 | 59   |
| 5    |    |   | Butanoic acid, 1-methylethyl ester  | 130 | C7H14O2  | 000638-11-9  | 59   |



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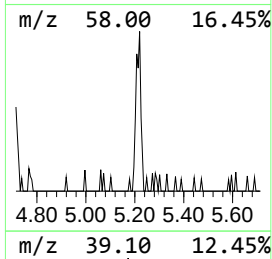
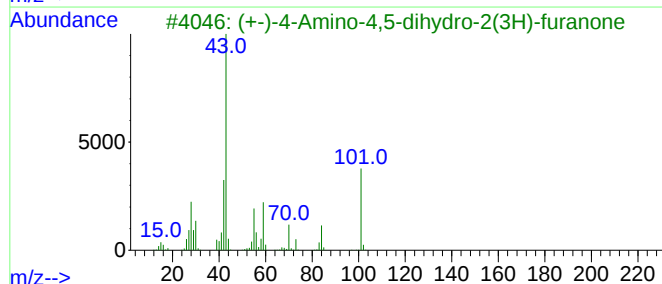
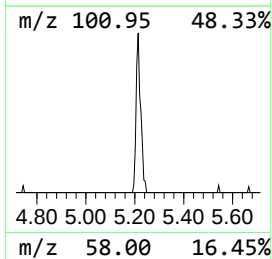
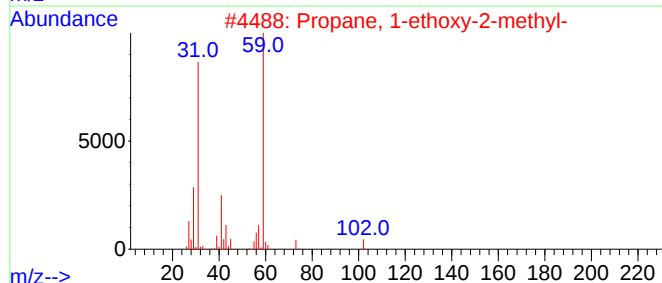
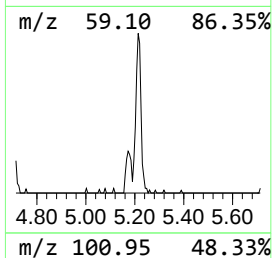
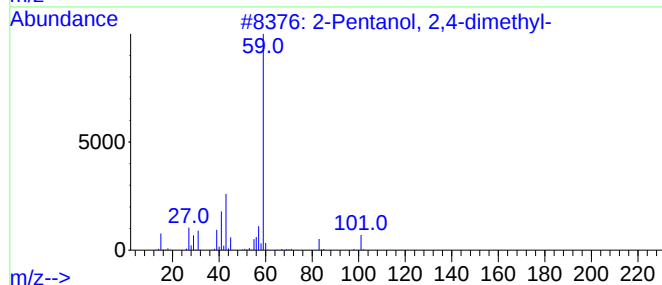
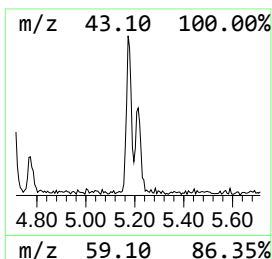
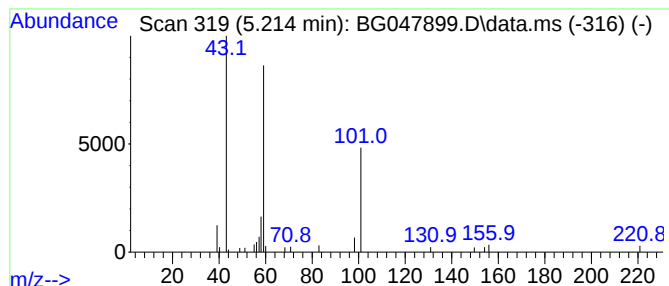
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Peak Number 4 unknown5.214 Concentration Rank 4

| R.T.  | EstConc | Area  | Relative to ISTD       | R.T.  |
|-------|---------|-------|------------------------|-------|
| 5.214 | 3.50 ng | 53286 | 1,4-Dichlorobenzene-d4 | 8.163 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|----------|--------------|------|
| 1    |    |   | 2-Pentanol, 2,4-dimethyl-           | 116 | C7H16O   | 000625-06-9  | 23   |
| 2    |    |   | Propane, 1-ethoxy-2-methyl-         | 102 | C6H14O   | 000627-02-1  | 17   |
| 3    |    |   | (+)-4-Amino-4,5-dihydro-2(3H)-f...  | 101 | C4H7NO2  | 016504-58-8  | 9    |
| 4    |    |   | 3-Heptanol, 4-methyl-               | 130 | C8H18O   | 014979-39-6  | 9    |
| 5    |    |   | Succinic acid, heptyl 2-methoxye... | 274 | C14H26O5 | 1000325-80-7 | 9    |



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| TIC Top Hit name   | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|--------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                    |       |         |       |          | #                     | RT    | Resp   | Conc |
| n-Propyl acetate   | 3.510 | 6.7     | ng    | 101362   | 1                     | 8.163 | 304324 | 20.0 |
| Propanoic acid,... | 4.708 | 11.8    | ng    | 179411   | 1                     | 8.163 | 304324 | 20.0 |
| Butanoic acid, ... | 5.178 | 7.5     | ng    | 114272   | 1                     | 8.163 | 304324 | 20.0 |
| unknown5.214       | 5.214 | 3.5     | ng    | 53286    | 1                     | 8.163 | 304324 | 20.0 |