

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG062518\  
 Data File : BG035377.D  
 Acq On : 25 Jun 2018 14:19  
 Operator : JU/SJ  
 Sample : J3627-27  
 Misc :  
 ALS Vial : 8 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 26KV-CC-14

Integration Parameters: rteint.p  
 Integrator: RTE  
 Smoothing : ON  
 Sampling : 1  
 Start Thrs: 0.2  
 Stop Thrs : 0  
 Filtering: 5  
 Min Area: 3 % of largest Peak  
 Max Peaks: 100  
 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-BG060718.M  
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

| 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         | 4.568       | 213           | 218         | 228          | rVB      | 66072          | 103662        | 3.41%           | 0.703%        |
| 2         | 5.167       | 313           | 320         | 332          | rVB      | 125896         | 205800        | 6.77%           | 1.396%        |
| 3         | 5.625       | 392           | 398         | 409          | rBV      | 508691         | 847806        | 27.88%          | 5.749%        |
| 4         | 7.211       | 660           | 668         | 680          | rBV      | 627915         | 1094254       | 35.98%          | 7.421%        |
| 5         | 7.587       | 724           | 732         | 740          | rBV      | 566033         | 968909        | 31.86%          | 6.571%        |
| 6         | 8.051       | 804           | 811         | 819          | rVB2     | 151348         | 262024        | 8.62%           | 1.777%        |
| 7         | 8.374       | 858           | 866         | 874          | rBV      | 450154         | 794934        | 26.14%          | 5.391%        |
| 8         | 9.214       | 1000          | 1009        | 1022         | rBV2     | 356974         | 671546        | 22.08%          | 4.554%        |
| 9         | 10.853      | 1279          | 1288        | 1298         | rBV      | 186229         | 345545        | 11.36%          | 2.343%        |
| 10        | 13.297      | 1697          | 1704        | 1712         | rBV      | 1120321        | 1712102       | 56.30%          | 11.611%       |
| 11        | 14.119      | 1838          | 1844        | 1851         | rBV      | 63195          | 96071         | 3.16%           | 0.652%        |
| 12        | 14.672      | 1932          | 1938        | 1948         | rVB2     | 329696         | 547064        | 17.99%          | 3.710%        |
| 13        | 15.512      | 2076          | 2081        | 2087         | rVB3     | 21279          | 30589         | 1.01%           | 0.207%        |
| 14        | 16.158      | 2181          | 2191        | 2201         | rBV      | 659717         | 991326        | 32.60%          | 6.723%        |
| 15        | 16.375      | 2223          | 2228        | 2236         | rVB      | 26414          | 44594         | 1.47%           | 0.302%        |
| 16        | 17.415      | 2398          | 2405        | 2416         | rBV2     | 504699         | 793558        | 26.10%          | 5.382%        |
| 17        | 20.023      | 2842          | 2849        | 2858         | rBV      | 2390436        | 3040917       | 100.00%         | 20.622%       |
| 18        | 20.323      | 2897          | 2900        | 2906         | rVB2     | 35815          | 44979         | 1.48%           | 0.305%        |
| 19        | 20.816      | 2980          | 2984        | 2988         | rBV2     | 43102          | 52972         | 1.74%           | 0.359%        |
| 20        | 21.321      | 3064          | 3070        | 3080         | rBV2     | 70318          | 126795        | 4.17%           | 0.860%        |
| 21        | 21.680      | 3125          | 3131        | 3139         | rBV2     | 544638         | 902579        | 29.68%          | 6.121%        |
| 22        | 21.874      | 3160          | 3164        | 3169         | rVB2     | 37225          | 50441         | 1.66%           | 0.342%        |
| 23        | 22.485      | 3262          | 3268        | 3272         | rBV2     | 31027          | 49638         | 1.63%           | 0.337%        |
| 24        | 23.178      | 3381          | 3386        | 3391         | rVB5     | 21843          | 37066         | 1.22%           | 0.251%        |
| 25        | 23.982      | 3517          | 3523        | 3530         | rVB8     | 20528          | 42942         | 1.41%           | 0.291%        |
| 26        | 24.905      | 3667          | 3680        | 3690         | rBV3     | 295763         | 887881        | 29.20%          | 6.021%        |

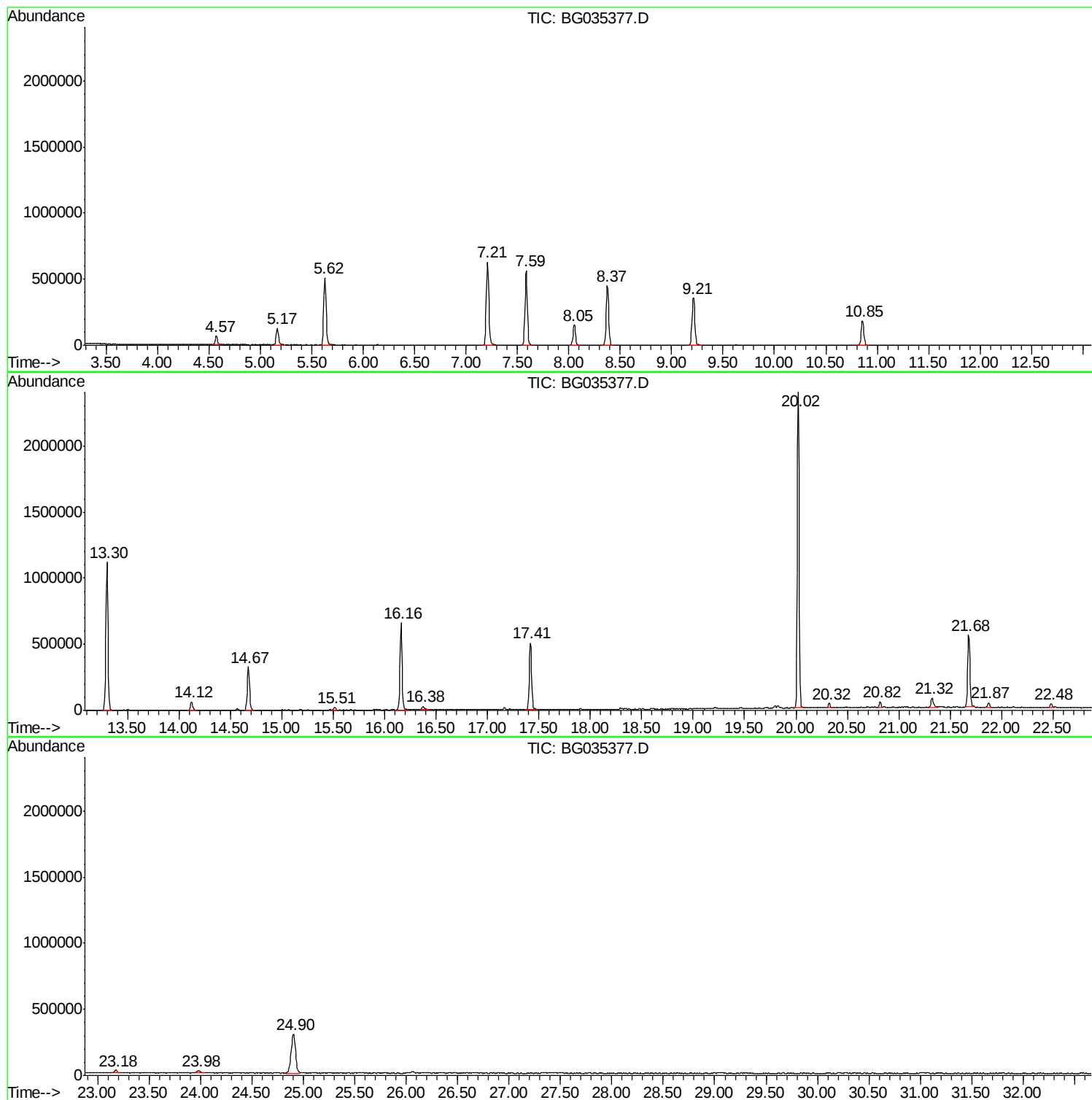
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG060718.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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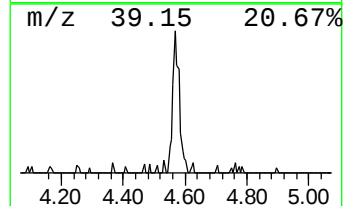
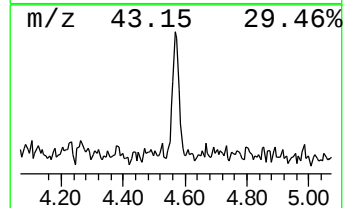
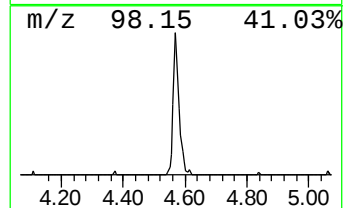
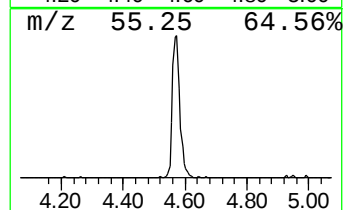
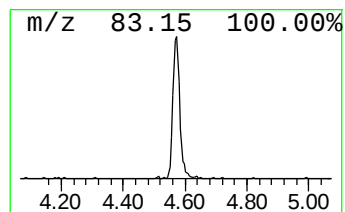
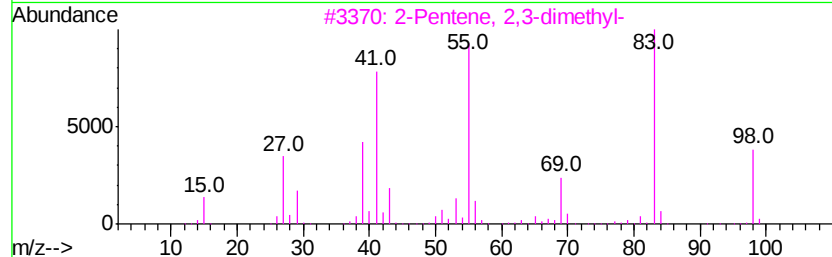
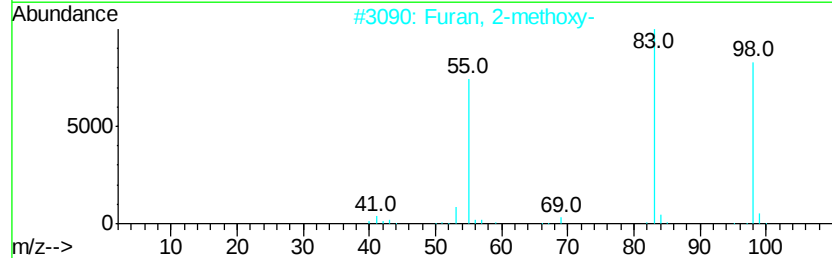
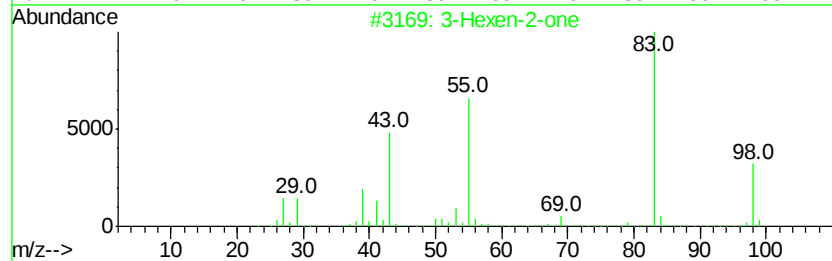
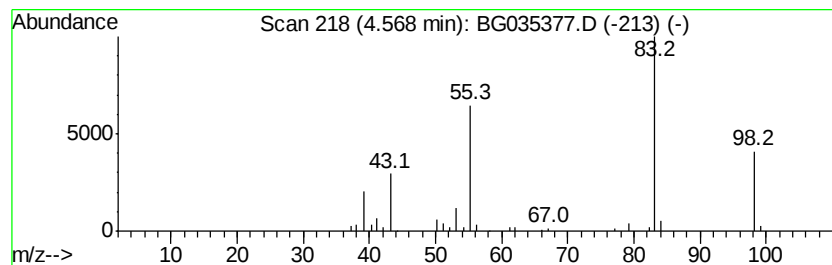
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG060718.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 3-Hexen-2-one Concentration Rank 4

| R.T. | EstConc | Area   | Relative to ISTD       | R.T. |
|------|---------|--------|------------------------|------|
| 4.57 | 7.91 ng | 103662 | 1,4-Dichlorobenzene-d4 | 8.05 |

| Hit# | of | 5 | Tentative ID                   | MW | MolForm | CAS#        | Qual |
|------|----|---|--------------------------------|----|---------|-------------|------|
| 1    |    |   | 3-Hexen-2-one                  | 98 | C6H10O  | 000763-93-9 | 86   |
| 2    |    |   | Furan, 2-methoxy-              | 98 | C5H6O2  | 025414-22-6 | 78   |
| 3    |    |   | 2-Pentene, 2,3-dimethyl-       | 98 | C7H14   | 010574-37-5 | 78   |
| 4    |    |   | 2-Pentene, 3,4-dimethyl-, (E)- | 98 | C7H14   | 004914-92-5 | 78   |
| 5    |    |   | 3-Penten-2-one, 4-methyl-      | 98 | C6H10O  | 000141-79-7 | 78   |



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ClientSampled :  
26KV-CC-14

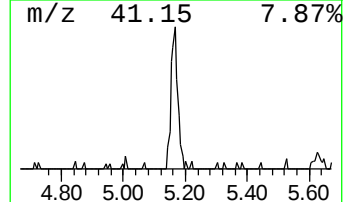
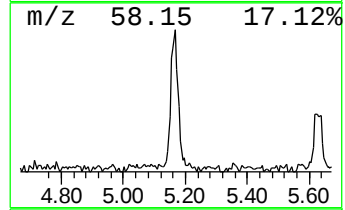
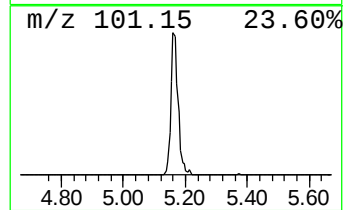
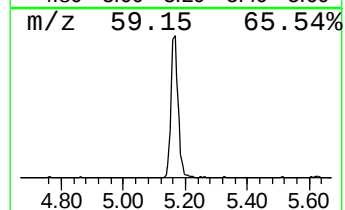
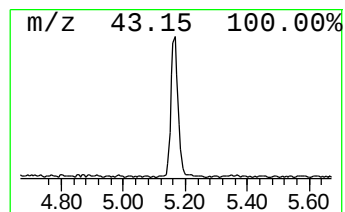
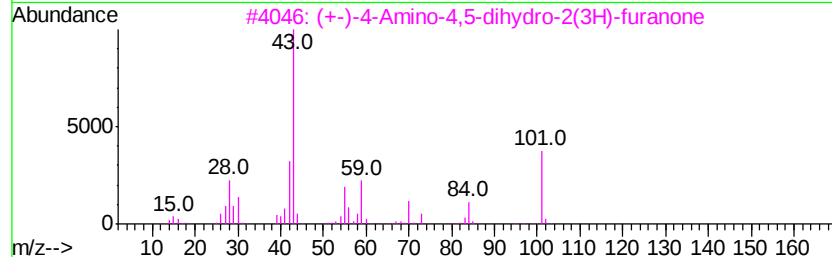
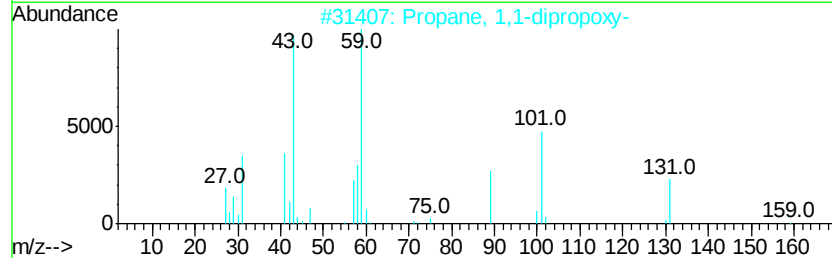
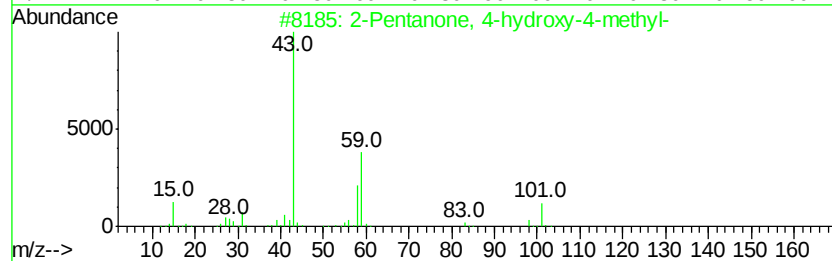
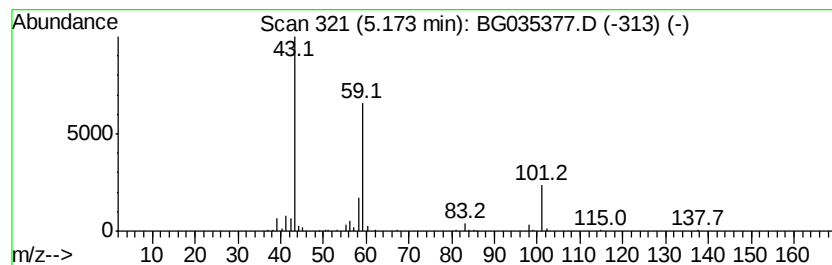
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG060718.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

| R.T. | EstConc  | Area   | Relative to ISTD       | R.T. |
|------|----------|--------|------------------------|------|
| 5.17 | 15.71 ng | 205800 | 1,4-Dichlorobenzene-d4 | 8.05 |

| Hit# | of | Tentative ID                           | MW  | MolForm  | CAS#         | Qual |
|------|----|----------------------------------------|-----|----------|--------------|------|
| 1    | 5  | 2-Pentanone, 4-hydroxy-4-methyl-       | 116 | C6H12O2  | 000123-42-2  | 59   |
| 2    |    | Propane, 1,1-dipropoxy-                | 160 | C9H20O2  | 004744-11-0  | 45   |
| 3    |    | (+)-4-Amino-4,5-dihydro-2(3H)-furanone | 101 | C4H7NO2  | 016504-58-8  | 37   |
| 4    |    | Dimethadione                           | 129 | C5H7NO3  | 000695-53-4  | 33   |
| 5    |    | Succinic acid, heptyl 2-methoxy-       | 274 | C14H26O5 | 1000325-80-7 | 28   |



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Instrument :  
BNA\_G  
ClientSampleId :  
26KV-CC-14

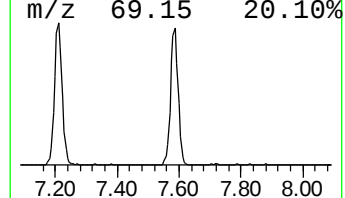
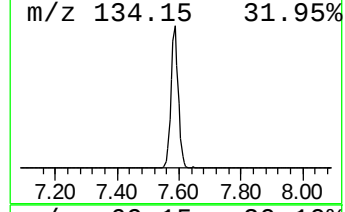
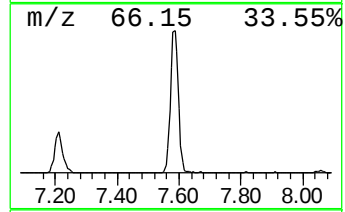
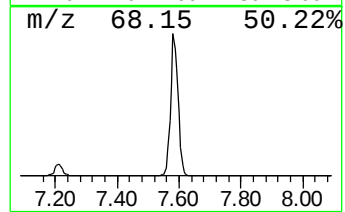
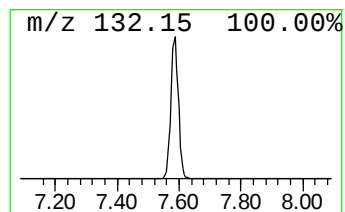
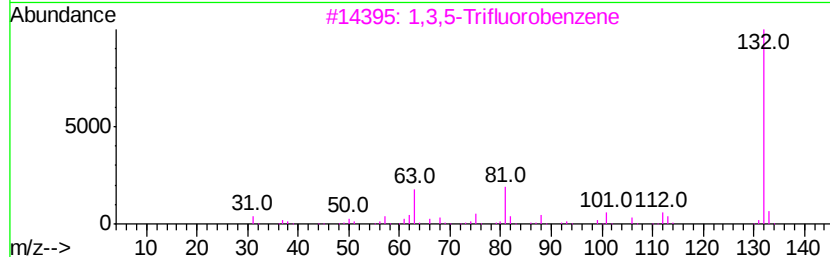
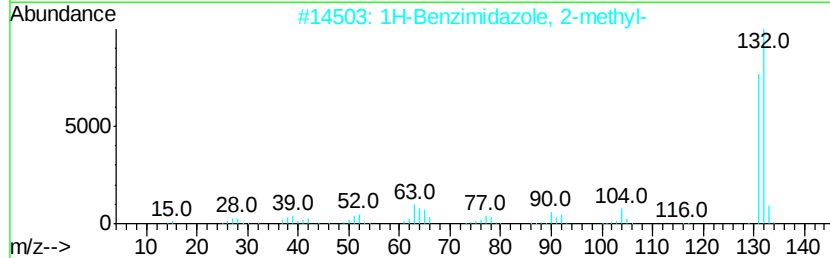
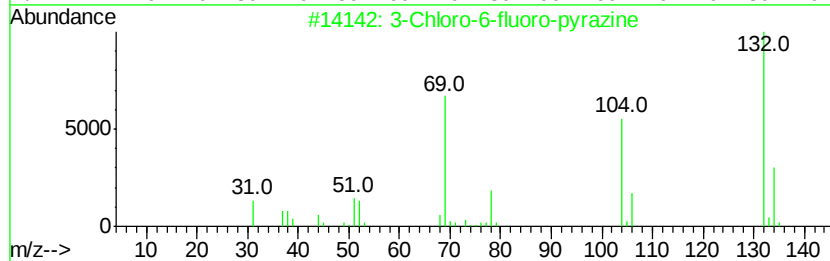
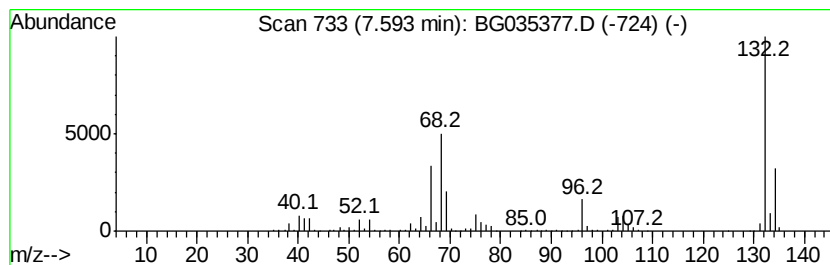
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 3 unknown7.59 Concentration Rank 1

| R.T. | EstConc  | Area   | Relative to ISTD       | R.T. |
|------|----------|--------|------------------------|------|
| 7.59 | 73.96 ng | 968909 | 1,4-Dichlorobenzene-d4 | 8.05 |

| Hit# | of | Tentative ID                | MW  | MolForm   | CAS#         | Qual |
|------|----|-----------------------------|-----|-----------|--------------|------|
| 1    | 5  | 3-Chloro-6-fluoro-pyrazine  | 132 | C4H2ClFN2 | 1000146-10-7 | 27   |
| 2    |    | 1H-Benzimidazole, 2-methyl- | 132 | C8H8N2    | 000615-15-6  | 22   |
| 3    |    | 1,3,5-Trifluorobenzene      | 132 | C6H3F3    | 000372-38-3  | 14   |
| 4    |    | 5-Aminoindole               | 132 | C8H8N2    | 005192-03-0  | 12   |
| 5    |    | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0  | 12   |



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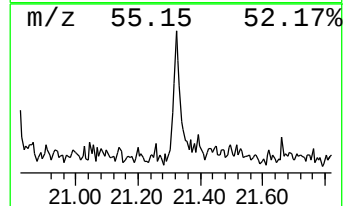
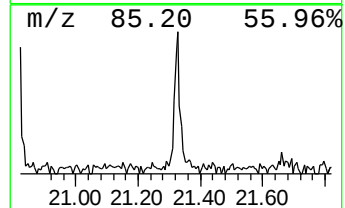
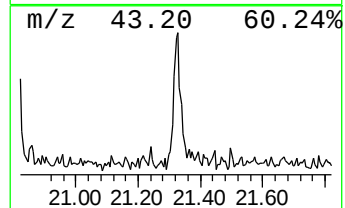
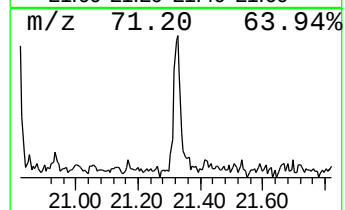
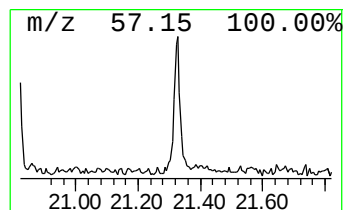
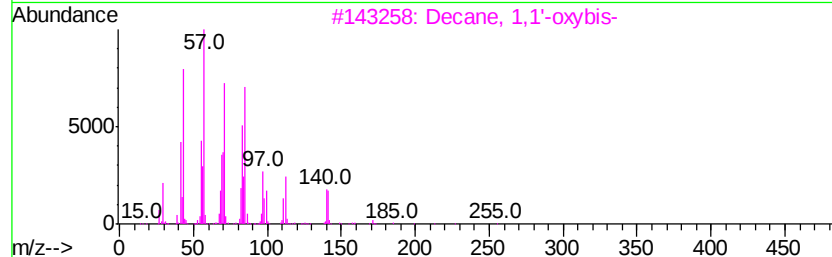
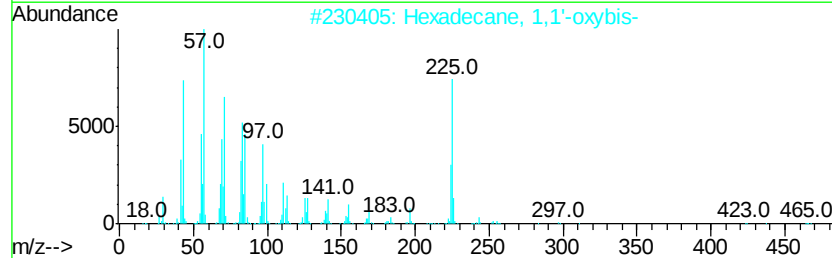
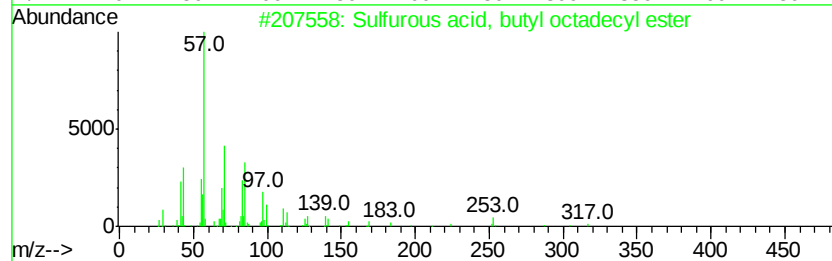
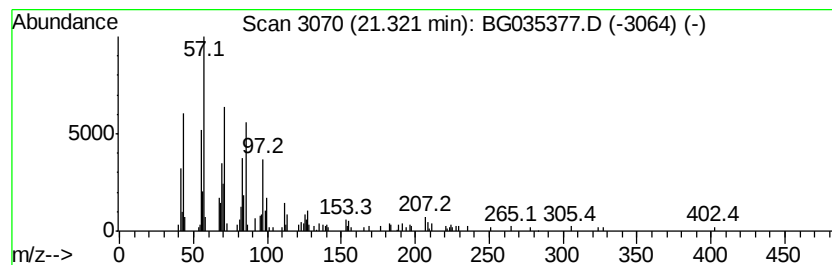
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\*\*\*\*\*  
Peak Number 5 Sulfurous acid, butyl octadecad... Concentration Rank 5

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 21.32 | 2.81 ng | 126795 | Chrysene-d12     | 21.68 |

| Hit# | of | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|-------------------------------------|-----|-----------|--------------|------|
| 1    | 5  | Sulfurous acid, butyl octadecyl ... | 390 | C22H46O3S | 1000309-18-5 | 86   |
| 2    |    | Hexadecane, 1,1'-oxybis-            | 467 | C32H66O   | 004113-12-6  | 72   |
| 3    |    | Decane, 1,1'-oxybis-                | 298 | C20H42O   | 002456-28-2  | 68   |
| 4    |    | Hexadecane                          | 226 | C16H34    | 000544-76-3  | 58   |
| 5    |    | Cyclotetradecane                    | 196 | C14H28    | 000295-17-0  | 53   |



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

| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                      |       |         |       |          | #                     | RT    | Resp   | Conc |
| 3-Hexen-2-one        | 4.57  | 7.9     | ng    | 103662   | 1                     | 8.05  | 262024 | 20.0 |
| 2-Pentanone, 4-hy... | 5.17  | 15.7    | ng    | 205800   | 1                     | 8.05  | 262024 | 20.0 |
| unknown7.59          | 7.59  | 74.0    | ng    | 968909   | 1                     | 8.05  | 262024 | 20.0 |
| Sulfurous acid, b... | 21.32 | 2.8     | ng    | 126795   | 5                     | 21.68 | 902579 | 20.0 |