

Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG052223\  
 Data File : BG057488.D  
 Acq On : 22 May 2023 11:06  
 Operator : CG/JU  
 Sample : PB152920BL  
 Misc :  
 ALS Vial : 3 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 PB152920BL

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-BG042723.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057488.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         | 4.762       | 203           | 208         | 215          | rBB      | 19636          | 27960         | 1.43%           | 0.389%        |
| 2         | 5.390       | 308           | 315         | 324          | rBV      | 82620          | 125191        | 6.42%           | 1.743%        |
| 3         | 5.878       | 391           | 398         | 410          | rBV      | 349500         | 551915        | 28.32%          | 7.684%        |
| 4         | 7.505       | 668           | 675         | 693          | rBV      | 356529         | 626383        | 32.14%          | 8.721%        |
| 5         | 8.363       | 813           | 821         | 828          | rBV      | 62220          | 103226        | 5.30%           | 1.437%        |
| 6         | 9.544       | 1013          | 1022        | 1031         | rBV      | 219436         | 393035        | 20.17%          | 5.472%        |
| 7         | 11.200      | 1297          | 1304        | 1314         | rVB      | 81821          | 148316        | 7.61%           | 2.065%        |
| 8         | 13.603      | 1706          | 1713        | 1723         | rBV      | 716694         | 1085901       | 55.72%          | 15.119%       |
| 9         | 14.977      | 1941          | 1947        | 1957         | rVB      | 154594         | 240620        | 12.35%          | 3.350%        |
| 10        | 16.464      | 2193          | 2200        | 2216         | rBV      | 581550         | 922568        | 47.34%          | 12.845%       |
| 11        | 17.715      | 2407          | 2413        | 2421         | rBV      | 222902         | 347612        | 17.84%          | 4.840%        |
| 12        | 20.288      | 2845          | 2851        | 2860         | rBV      | 1546043        | 1949010       | 100.00%         | 27.136%       |
| 13        | 22.027      | 3140          | 3147        | 3155         | rVB2     | 189350         | 337295        | 17.31%          | 4.696%        |
| 14        | 25.534      | 3734          | 3744        | 3755         | rVB      | 107967         | 323470        | 16.60%          | 4.504%        |

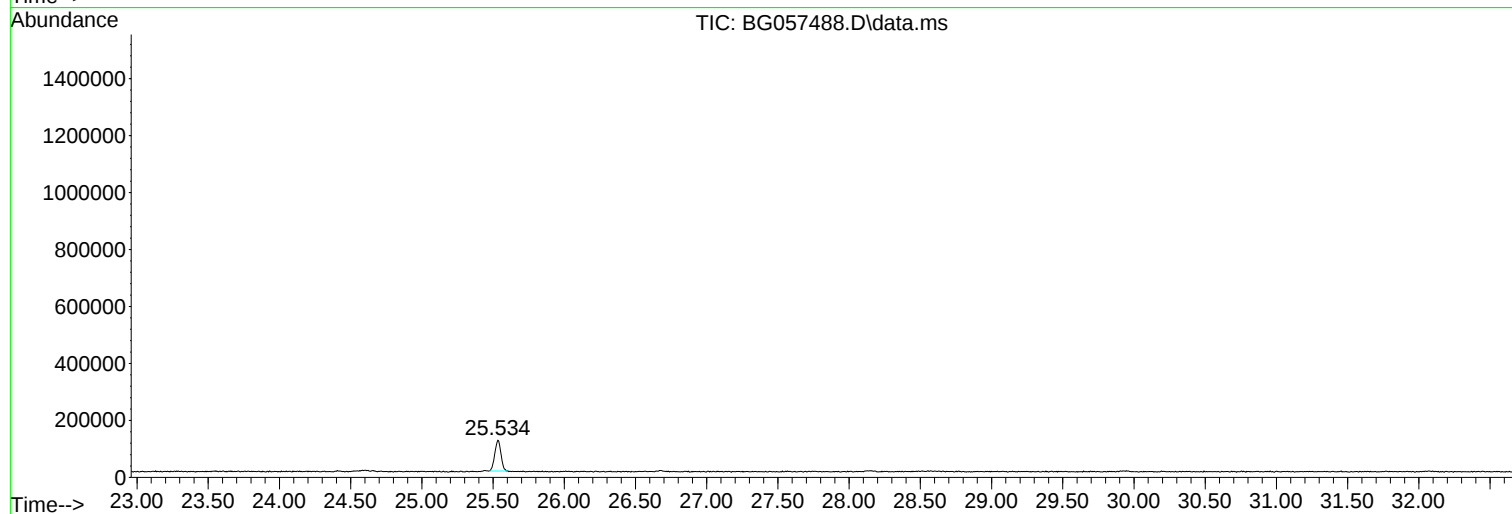
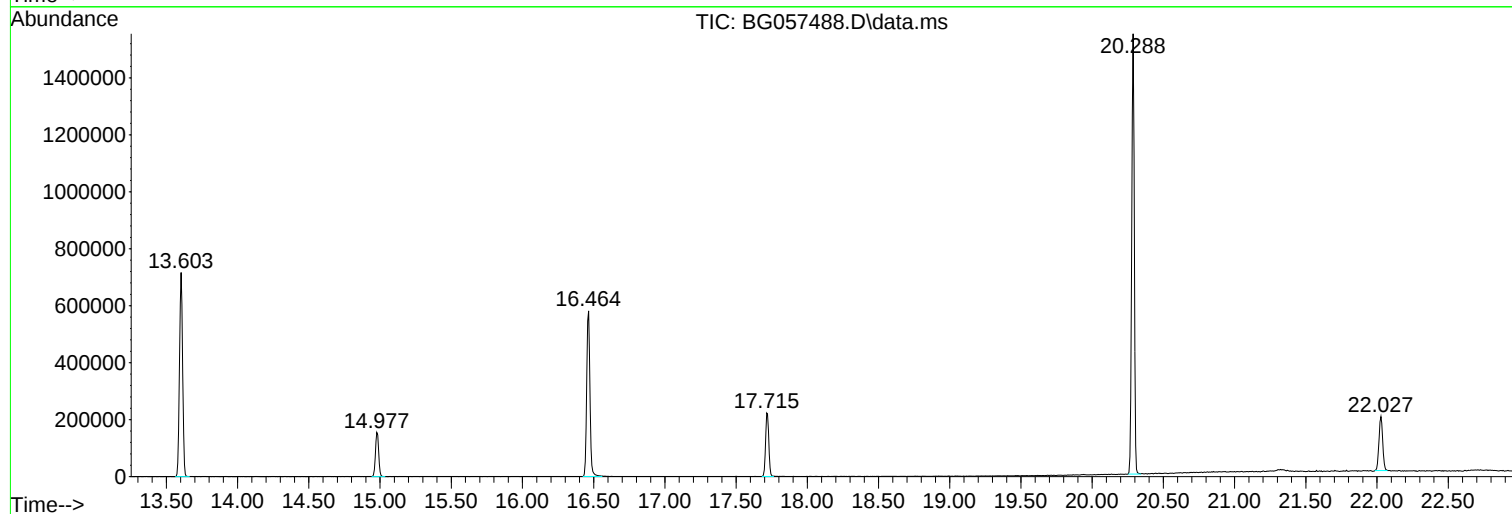
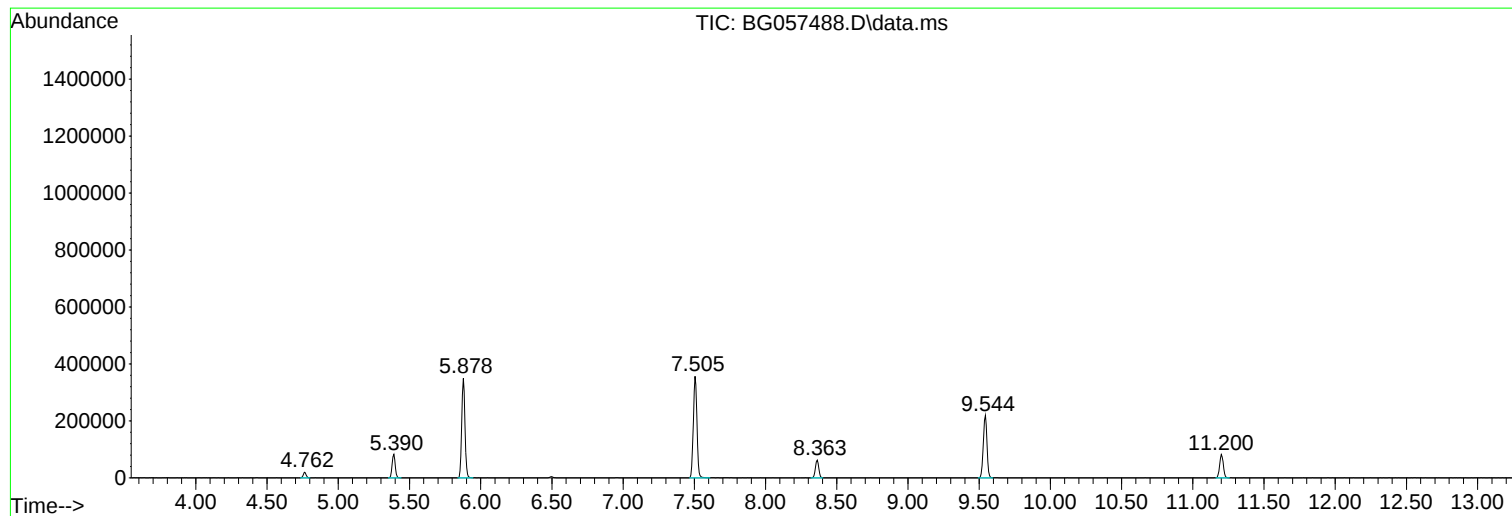
Sum of corrected areas: 7182502

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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG042723.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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Operator : CG/JU  
Sample : PB152920BL  
Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
PB152920BL

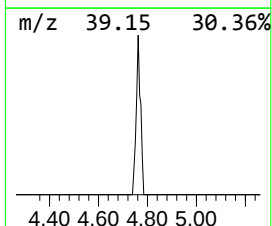
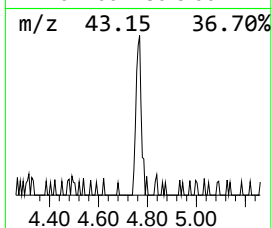
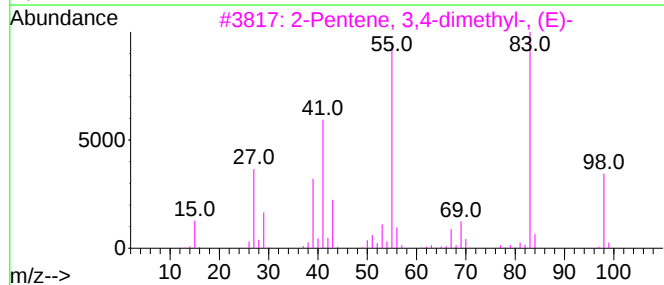
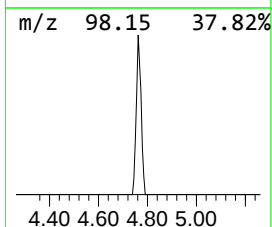
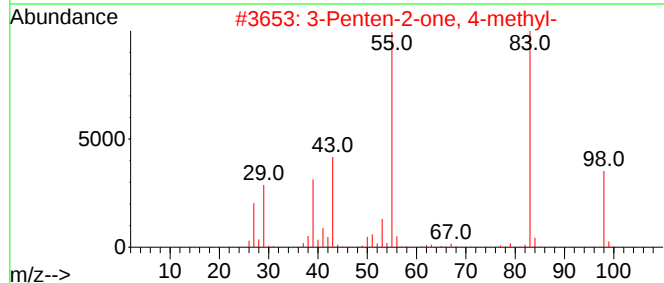
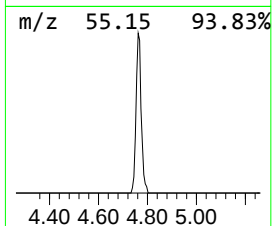
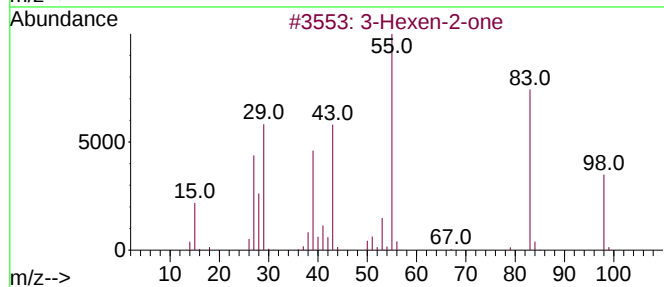
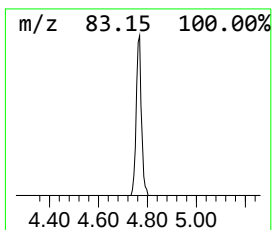
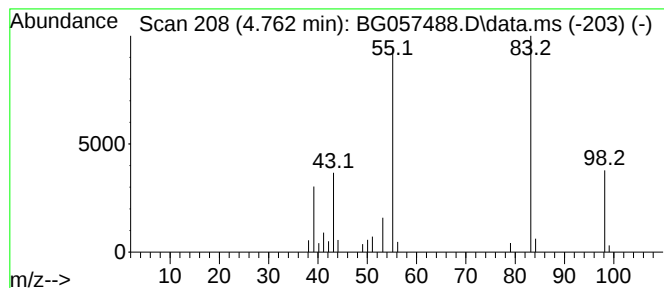
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG042723.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

| R.T.  | EstConc | Area  | Relative to ISTD       | R.T.  |
|-------|---------|-------|------------------------|-------|
| 4.762 | 5.42 ng | 27960 | 1,4-Dichlorobenzene-d4 | 8.363 |

| Hit# | of | 5 | Tentative ID                   | MW | MolForm | CAS#        | Qual |
|------|----|---|--------------------------------|----|---------|-------------|------|
| 1    |    |   | 3-Hexen-2-one                  | 98 | C6H10O  | 000763-93-9 | 90   |
| 2    |    |   | 3-Penten-2-one, 4-methyl-      | 98 | C6H10O  | 000141-79-7 | 90   |
| 3    |    |   | 2-Pentene, 3,4-dimethyl-, (E)- | 98 | C7H14   | 004914-92-5 | 86   |
| 4    |    |   | 2-Pentene, 3,4-dimethyl-, (Z)- | 98 | C7H14   | 004914-91-4 | 86   |
| 5    |    |   | 2-Pentene, 4,4-dimethyl-, (Z)- | 98 | C7H14   | 000762-63-0 | 86   |



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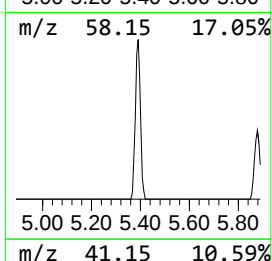
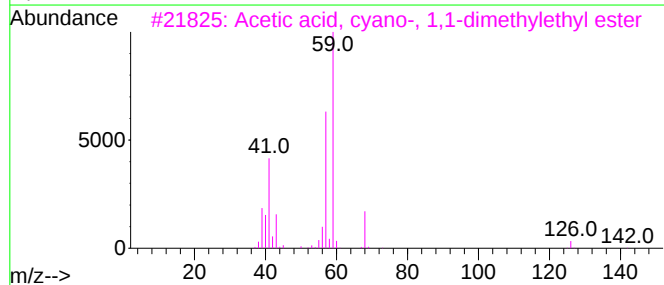
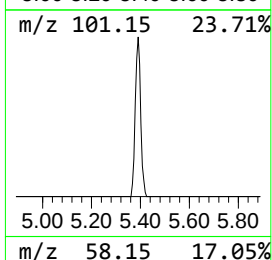
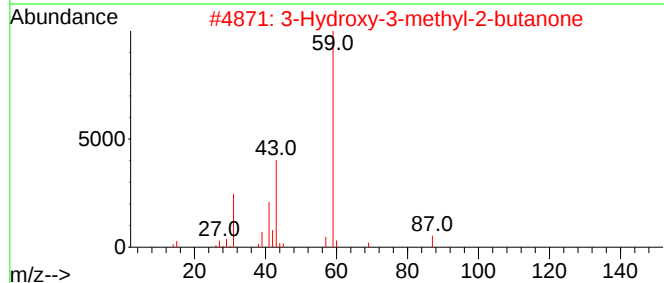
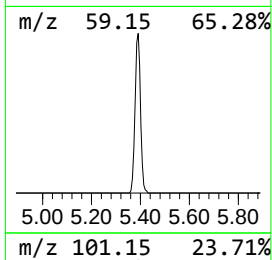
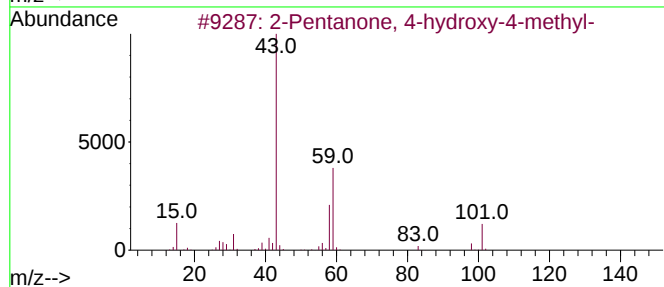
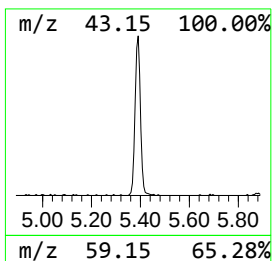
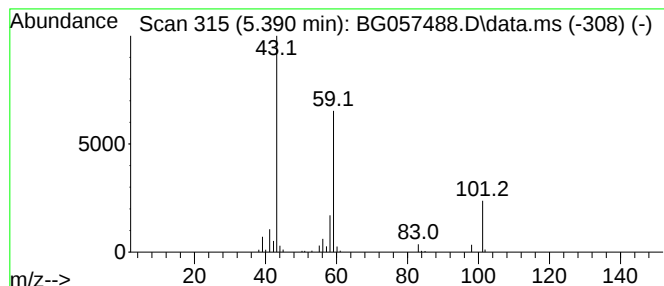
Instrument :  
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ClientSampleId :  
PB152920BL

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TIC Integration Parameters: LSCINT.P

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

| R.T.      | EstConc                             | Area   | Relative to ISTD       | R.T.        |      |
|-----------|-------------------------------------|--------|------------------------|-------------|------|
| 5.390     | 24.26 ng                            | 125191 | 1,4-Dichlorobenzene-d4 | 8.363       |      |
| Hit# of 5 | Tentative ID                        | MW     | MolForm                | CAS#        | Qual |
| 1         | 2-Pentanone, 4-hydroxy-4-methyl-    | 116    | C6H12O2                | 000123-42-2 | 56   |
| 2         | 3-Hydroxy-3-methyl-2-butanone       | 102    | C5H10O2                | 000115-22-0 | 25   |
| 3         | Acetic acid, cyano-, 1,1-dimethy... | 141    | C7H11NO2               | 001116-98-9 | 17   |
| 4         | 1-Propen-2-ol, acetate              | 100    | C5H8O2                 | 000108-22-5 | 10   |
| 5         | Morpholine, 4-methyl-               | 101    | C5H11NO                | 000109-02-4 | 9    |



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

| TIC Top Hit name   | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|--------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                    |       |         |       |          | #                     | RT    | Resp   | Conc |
| 3-Hexen-2-one      | 4.762 | 5.4     | ng    | 27960    | 1                     | 8.363 | 103226 | 20.0 |
| 2-Pentanone, 4-... | 5.390 | 24.3    | ng    | 125191   | 1                     | 8.363 | 103226 | 20.0 |