

Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG062823\  
 Data File : BG057884.D  
 Acq On : 28 Jun 2023 8:57  
 Operator : CG/JU  
 Sample : PB153813BL  
 Misc :  
 ALS Vial : 3 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 PB153813BL

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-BG062723.M  
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057884.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         | 4.428       | 223           | 228         | 233          | rBV      | 64840          | 93223         | 2.36%           | 0.606%        |
| 2         | 5.027       | 323           | 330         | 345          | rBB      | 360972         | 532481        | 13.49%          | 3.464%        |
| 3         | 5.497       | 403           | 410         | 419          | rBV      | 814305         | 1262901       | 32.00%          | 8.215%        |
| 4         | 7.083       | 672           | 680         | 690          | rBV      | 805599         | 1352728       | 34.27%          | 8.799%        |
| 5         | 7.918       | 815           | 822         | 830          | rBV      | 124040         | 212095        | 5.37%           | 1.380%        |
| 6         | 9.081       | 1011          | 1020        | 1030         | rBV      | 455970         | 785020        | 19.89%          | 5.106%        |
| 7         | 10.726      | 1292          | 1300        | 1307         | rBV      | 174943         | 316953        | 8.03%           | 2.062%        |
| 8         | 13.182      | 1710          | 1718        | 1727         | rBV      | 1160766        | 1799731       | 45.60%          | 11.707%       |
| 9         | 14.557      | 1944          | 1952        | 1959         | rBV      | 302546         | 471093        | 11.94%          | 3.064%        |
| 10        | 16.044      | 2198          | 2205        | 2221         | rBV      | 1173893        | 1835385       | 46.50%          | 11.939%       |
| 11        | 17.301      | 2412          | 2419        | 2425         | rBV      | 494237         | 747023        | 18.93%          | 4.859%        |
| 12        | 19.915      | 2858          | 2864        | 2870         | rBV      | 2981048        | 3946757       | 100.00%         | 25.673%       |
| 13        | 21.549      | 3135          | 3142        | 3149         | rBV2     | 570906         | 889700        | 22.54%          | 5.787%        |
| 14        | 24.698      | 3667          | 3678        | 3691         | rBV      | 361937         | 1018347       | 25.80%          | 6.624%        |
| 15        | 25.844      | 3865          | 3873        | 3882         | rVB5     | 18603          | 53430         | 1.35%           | 0.348%        |
| 16        | 27.166      | 4090          | 4098        | 4106         | rVB8     | 16631          | 56316         | 1.43%           | 0.366%        |

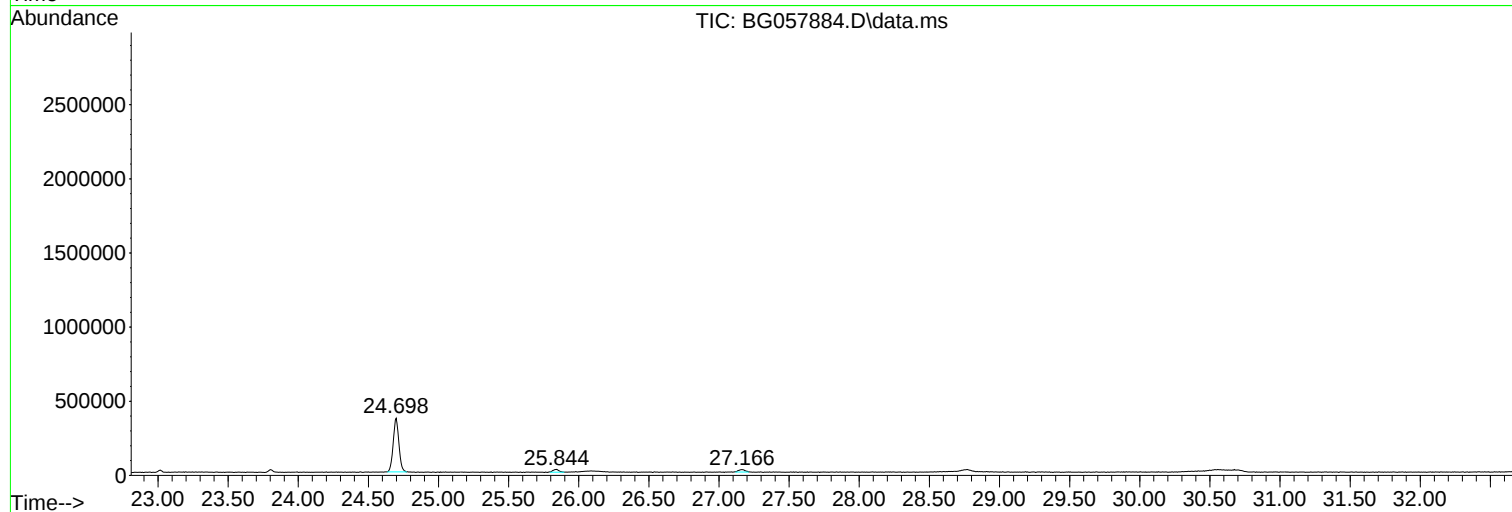
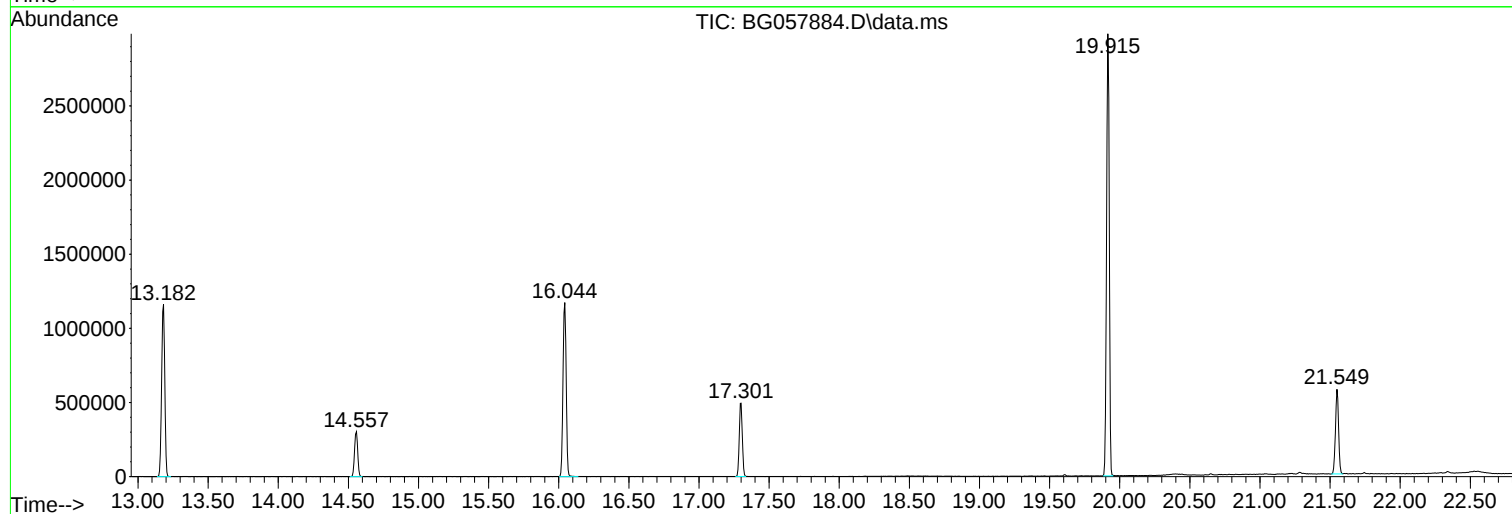
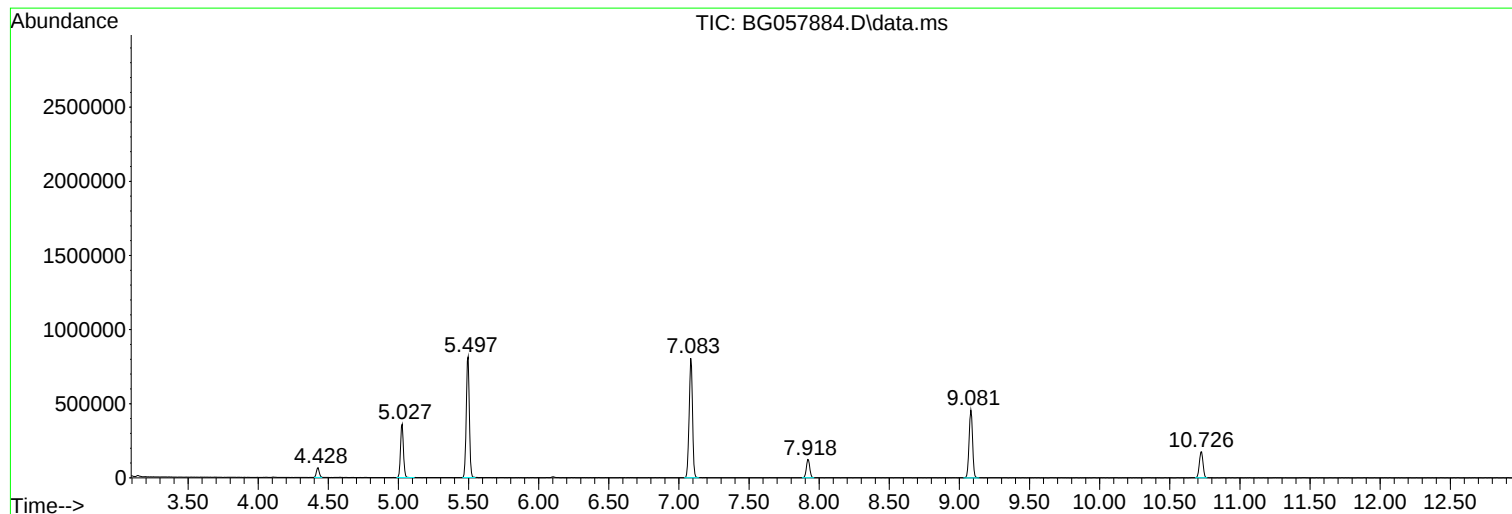
Sum of corrected areas: 15373183

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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG062723.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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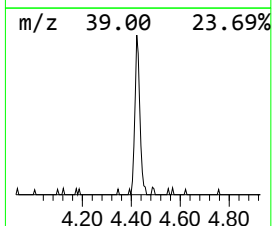
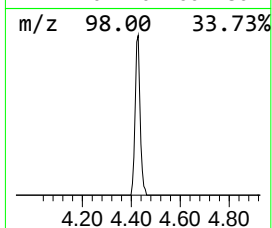
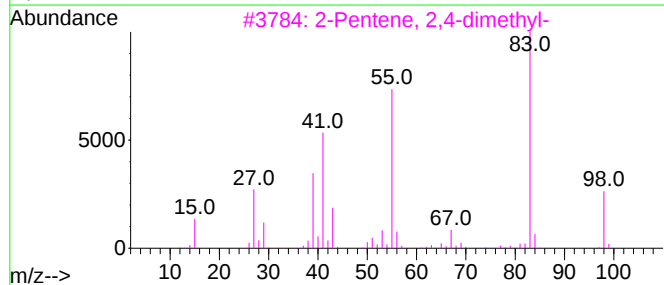
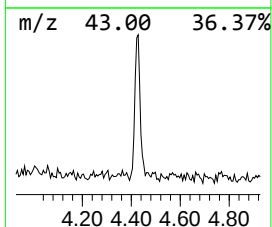
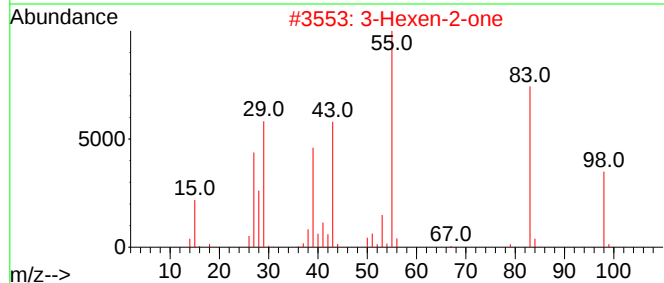
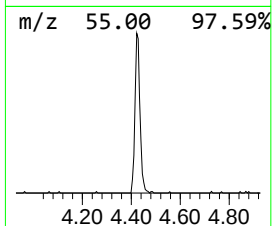
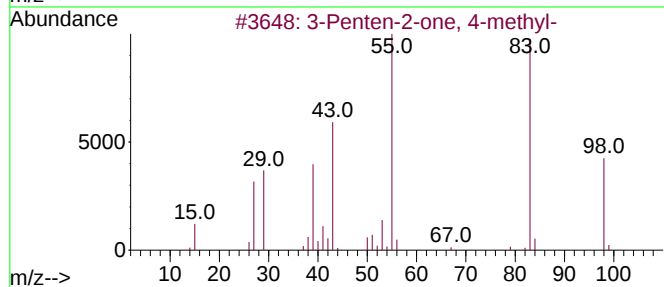
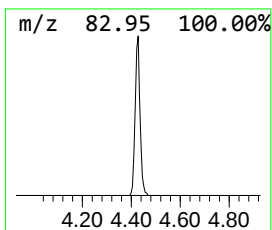
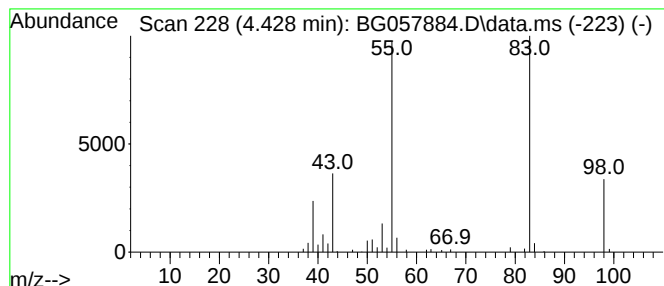
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG062723.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 2

| R.T.  | EstConc | Area  | Relative to ISTD       | R.T.  |
|-------|---------|-------|------------------------|-------|
| 4.428 | 8.79 ng | 93223 | 1,4-Dichlorobenzene-d4 | 7.924 |

| Hit# | of 5 | Tentative ID                   | MW | MolForm | CAS#        | Qual |
|------|------|--------------------------------|----|---------|-------------|------|
| 1    |      | 3-Penten-2-one, 4-methyl-      | 98 | C6H10O  | 000141-79-7 | 91   |
| 2    |      | 3-Hexen-2-one                  | 98 | C6H10O  | 000763-93-9 | 91   |
| 3    |      | 2-Pentene, 2,4-dimethyl-       | 98 | C7H14   | 000625-65-0 | 80   |
| 4    |      | 2-Pentene, 4,4-dimethyl-, (E)- | 98 | C7H14   | 000690-08-4 | 78   |
| 5    |      | 2-Pentene, 3,4-dimethyl-, (E)- | 98 | C7H14   | 004914-92-5 | 72   |



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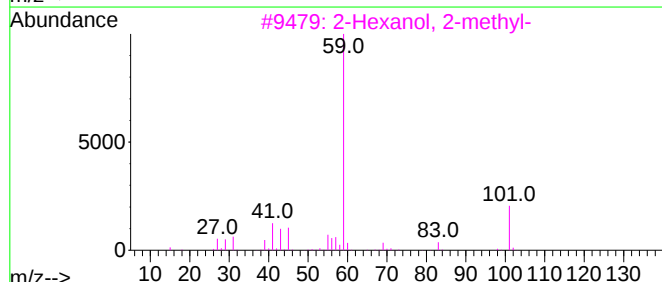
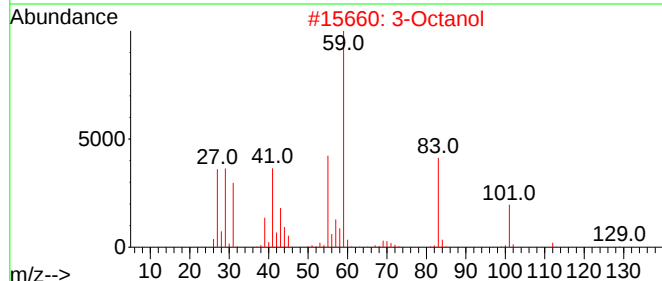
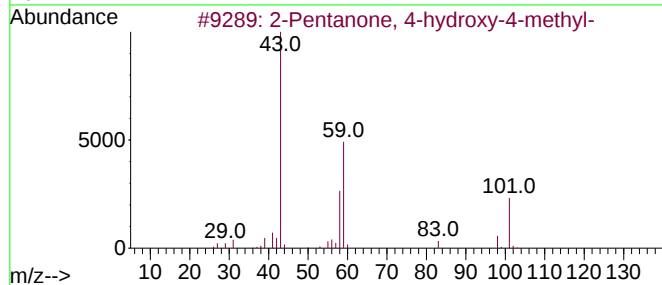
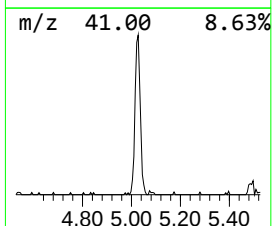
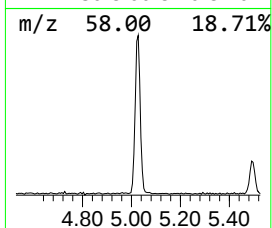
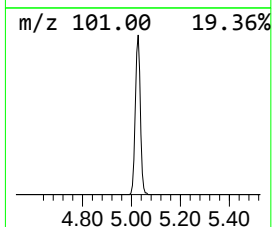
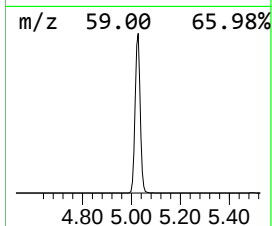
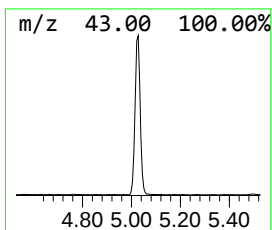
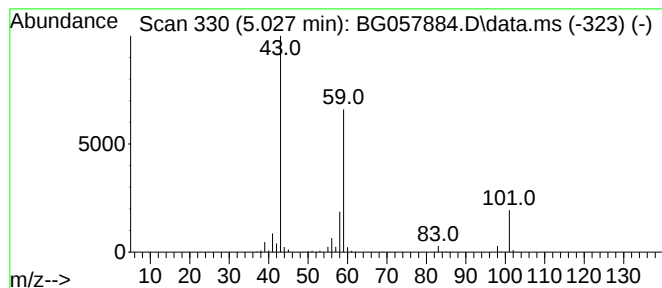
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TIC Integration Parameters: LSCINT.P

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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.  |
|-------|----------|--------|------------------------|-------|
| 5.027 | 50.21 ng | 532481 | 1,4-Dichlorobenzene-d4 | 7.924 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2  | 000123-42-2 | 64   |
| 2    |    |   | 3-Octanol                           | 130 | C8H18O   | 000589-98-0 | 33   |
| 3    |    |   | 2-Hexanol, 2-methyl-                | 116 | C7H16O   | 000625-23-0 | 33   |
| 4    |    |   | 3-Hexanol, 4-methyl-                | 116 | C7H16O   | 000615-29-2 | 28   |
| 5    |    |   | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 23   |



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| TIC Top Hit name   | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|--------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                    |       |         |       |          | #                     | RT    | Resp   | Conc |
| 3-Penten-2-one,... | 4.428 | 8.8     | ng    | 93223    | 1                     | 7.924 | 212095 | 20.0 |
| 2-Pentanone, 4-... | 5.027 | 50.2    | ng    | 532481   | 1                     | 7.924 | 212095 | 20.0 |