

Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG081123\  
 Data File : BG058705.D  
 Acq On : 11 Aug 2023 16:40  
 Operator : MA/JU  
 Sample : 03971-09  
 Misc :  
 ALS Vial : 5 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 B-PP08A

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-BG072823.M  
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG058705.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         | 4.310       | 202           | 208         | 215          | rBV      | 65226          | 98988         | 5.11%           | 1.093%        |
| 2         | 4.909       | 305           | 310         | 319          | rBV      | 79295          | 119964        | 6.19%           | 1.325%        |
| 3         | 5.385       | 384           | 391         | 403          | rBV      | 411545         | 661716        | 34.15%          | 7.306%        |
| 4         | 6.983       | 656           | 663         | 679          | rBV      | 442186         | 783348        | 40.43%          | 8.649%        |
| 5         | 7.812       | 796           | 804         | 811          | rBV      | 143202         | 242587        | 12.52%          | 2.678%        |
| 6         | 8.975       | 995           | 1002        | 1021         | rBV      | 249814         | 493347        | 25.46%          | 5.447%        |
| 7         | 10.614      | 1273          | 1281        | 1296         | rBV      | 181188         | 367975        | 18.99%          | 4.063%        |
| 8         | 13.076      | 1693          | 1700        | 1716         | rBV      | 659888         | 1148626       | 59.28%          | 12.682%       |
| 9         | 14.463      | 1927          | 1936        | 1952         | rBV      | 306114         | 534079        | 27.56%          | 5.897%        |
| 10        | 15.955      | 2184          | 2190        | 2208         | rBV      | 197260         | 389253        | 20.09%          | 4.298%        |
| 11        | 17.207      | 2396          | 2403        | 2416         | rBV      | 413252         | 701474        | 36.20%          | 7.745%        |
| 12        | 19.821      | 2843          | 2848        | 2865         | rBV      | 1353070        | 1937632       | 100.00%         | 21.393%       |
| 13        | 21.102      | 3061          | 3066        | 3074         | rBV3     | 23920          | 60583         | 3.13%           | 0.669%        |
| 14        | 21.449      | 3119          | 3125        | 3141         | rBV      | 383639         | 743853        | 38.39%          | 8.213%        |
| 15        | 23.029      | 3389          | 3394        | 3400         | rVB3     | 13590          | 24820         | 1.28%           | 0.274%        |
| 16        | 24.527      | 3637          | 3649        | 3672         | rBV      | 204785         | 748917        | 38.65%          | 8.269%        |

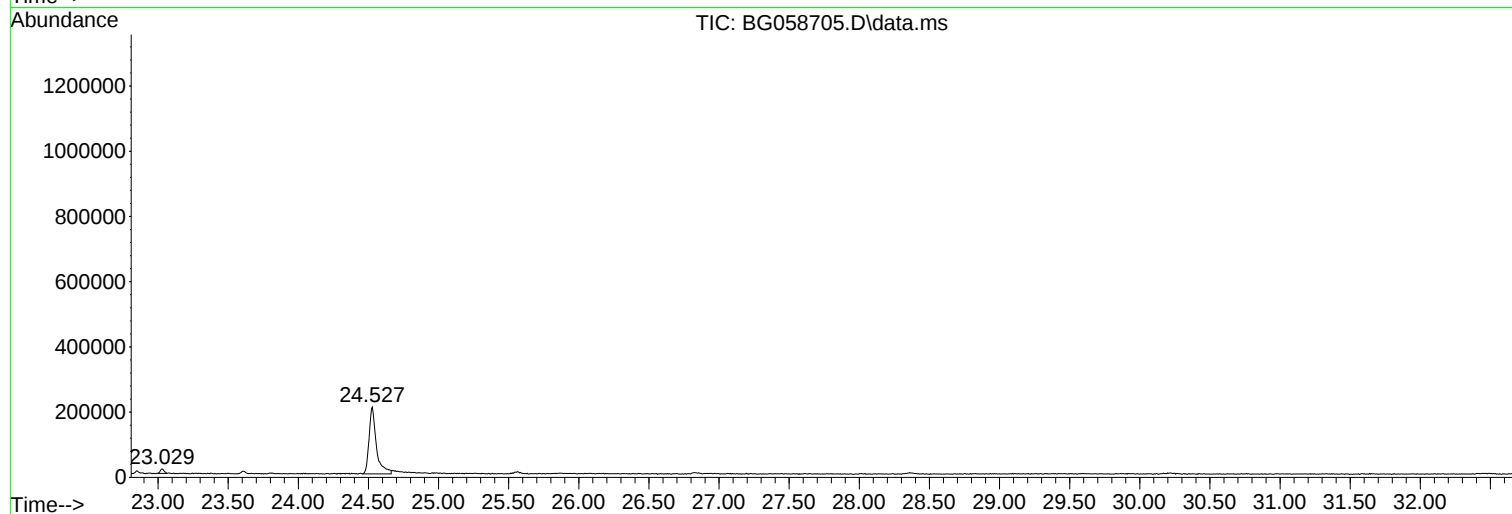
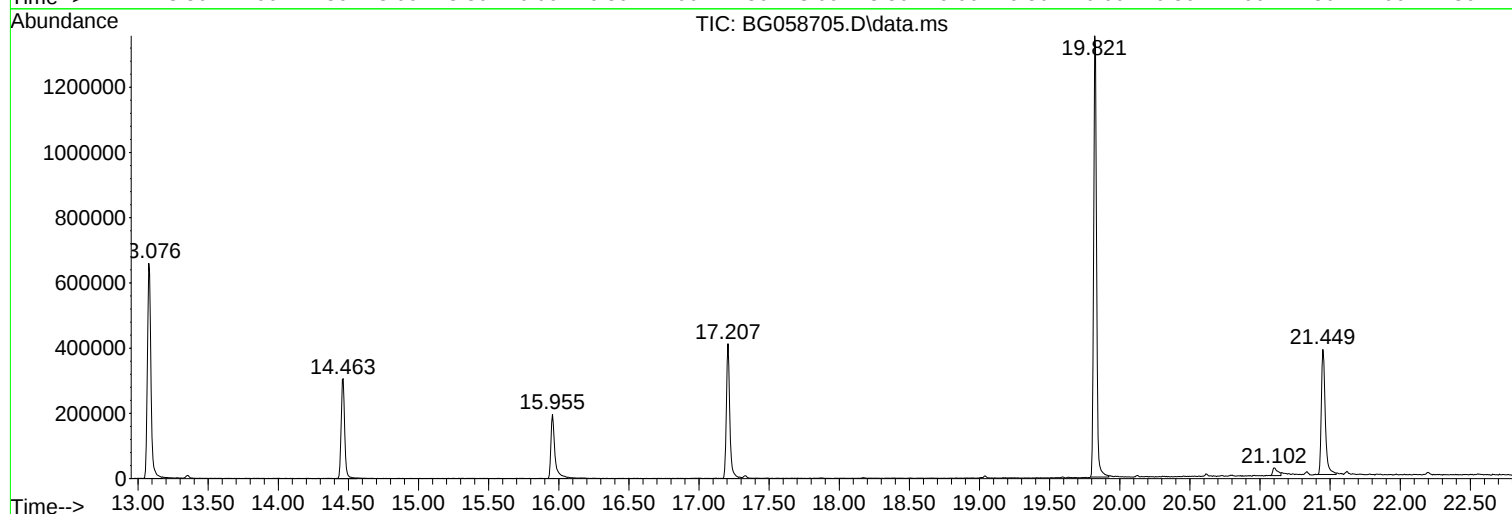
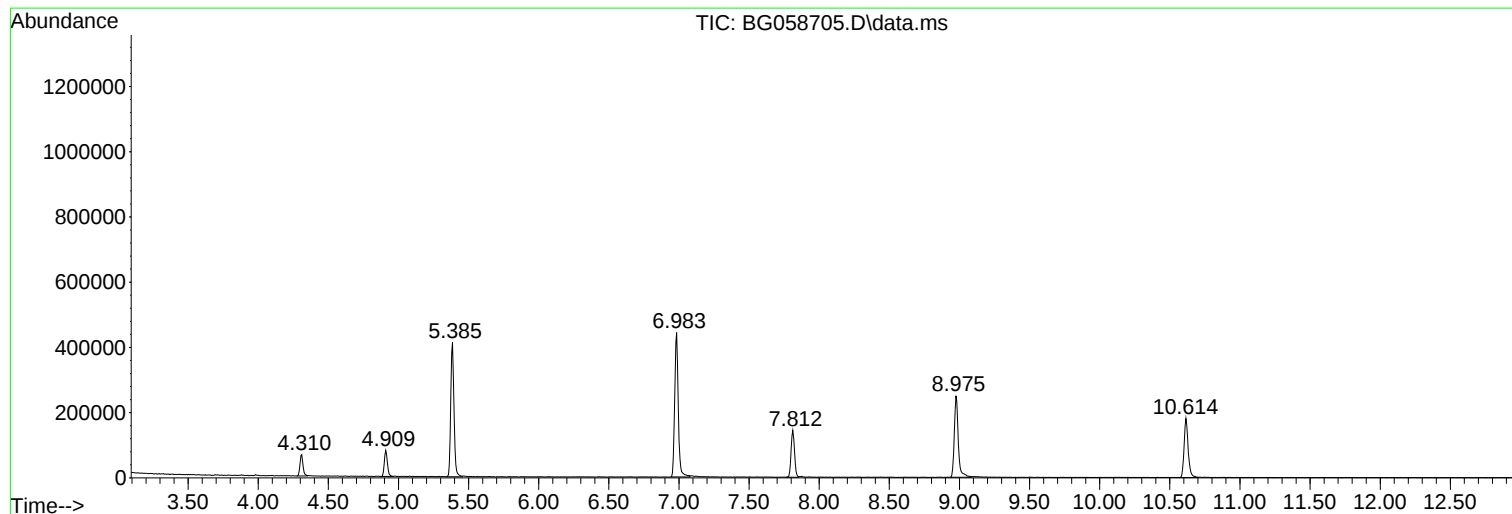
Sum of corrected areas: 9057162

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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG072823.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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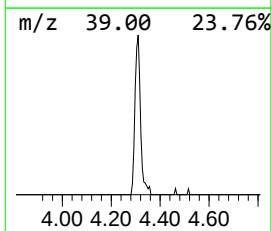
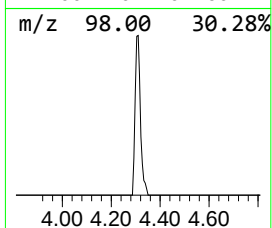
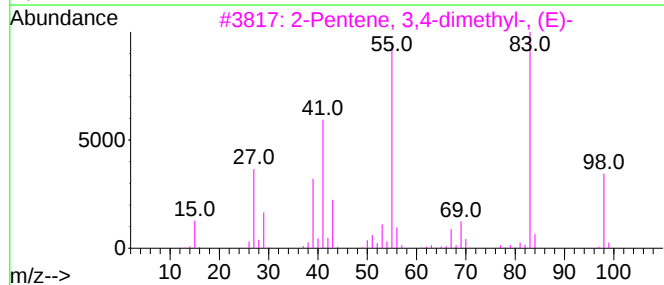
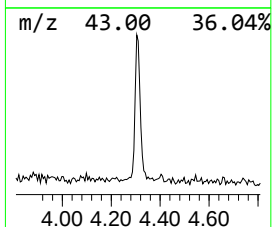
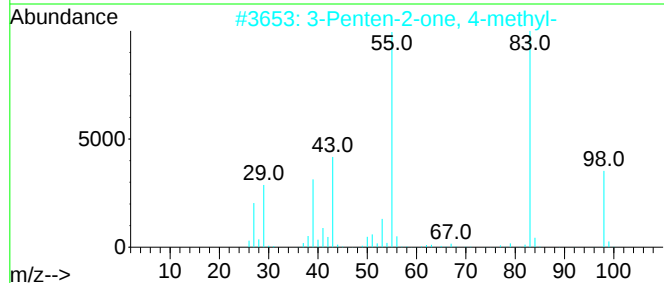
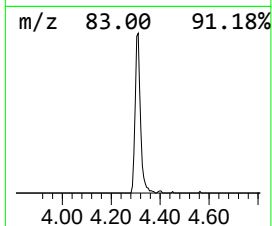
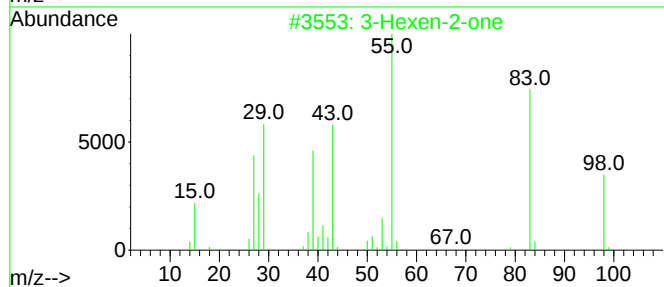
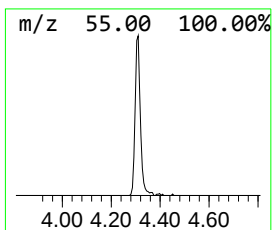
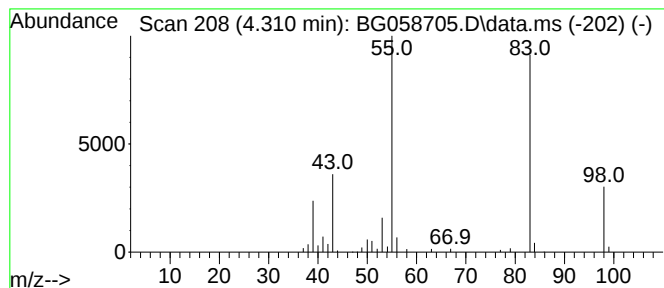
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG072823.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.  |
|-------|---------|-------|------------------------|-------|
| 4.310 | 8.16 ng | 98988 | 1,4-Dichlorobenzene-d4 | 7.812 |

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



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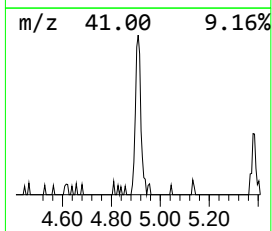
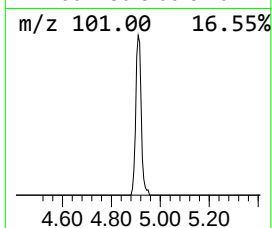
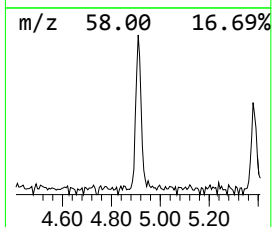
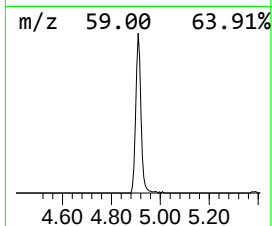
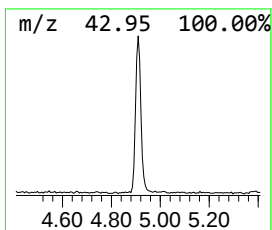
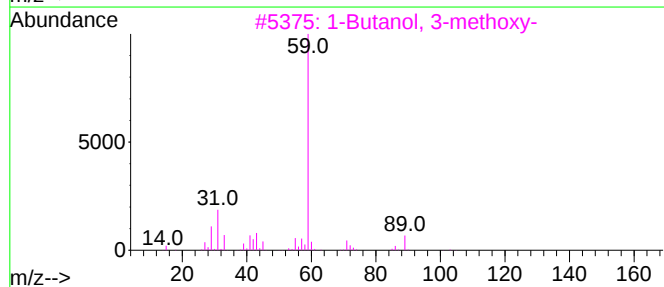
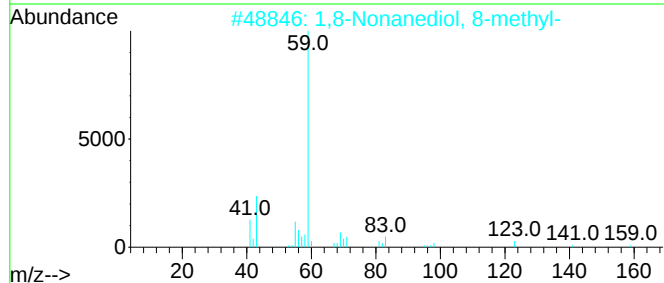
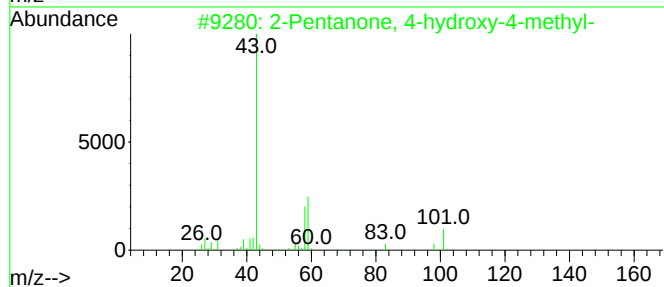
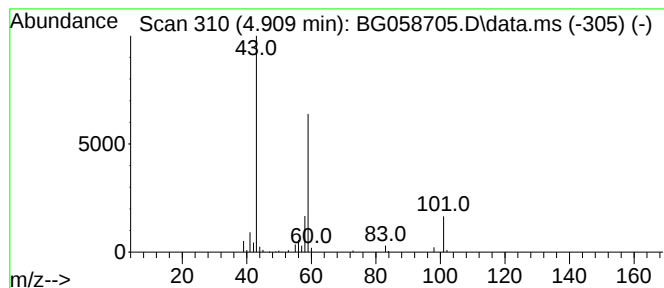
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TIC Integration Parameters: LSCINT.P

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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.  |
|-------|---------|--------|------------------------|-------|
| 4.909 | 9.89 ng | 119964 | 1,4-Dichlorobenzene-d4 | 7.812 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2  | 000123-42-2 | 59   |
| 2    |    |   | 1,8-Nonanediol, 8-methyl-           | 174 | C10H22O2 | 054725-73-4 | 37   |
| 3    |    |   | 1-Butanol, 3-methoxy-               | 104 | C5H12O2  | 002517-43-3 | 32   |
| 4    |    |   | 3-Hexanol, 4-methyl-                | 116 | C7H16O   | 000615-29-2 | 28   |
| 5    |    |   | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 25   |



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| TIC Top Hit name   | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|--------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                    |       |         |       |          | #                     | RT    | Resp   | Conc |
| 3-Hexen-2-one      | 4.310 | 8.2     | ng    | 98988    | 1                     | 7.812 | 242587 | 20.0 |
| 2-Pentanone, 4-... | 4.909 | 9.9     | ng    | 119964   | 1                     | 7.812 | 242587 | 20.0 |