

Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG062223\  
 Data File : BG057802.D  
 Acq On : 22 Jun 2023 9:19  
 Operator : CG/JU  
 Sample : PB153645BL  
 Misc :  
 ALS Vial : 3 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 PB153645BL

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-BG061923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057802.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         | 4.427       | 223           | 228         | 234          | rBV      | 34094          | 48546         | 1.48%           | 0.372%        |
| 2         | 5.026       | 322           | 330         | 338          | rBV      | 257294         | 371980        | 11.35%          | 2.847%        |
| 3         | 5.490       | 402           | 409         | 421          | rBV      | 727555         | 1132420       | 34.56%          | 8.667%        |
| 4         | 7.082       | 672           | 680         | 690          | rBV      | 725870         | 1210367       | 36.93%          | 9.264%        |
| 5         | 7.917       | 816           | 822         | 829          | rVB      | 111774         | 185389        | 5.66%           | 1.419%        |
| 6         | 9.080       | 1011          | 1020        | 1028         | rBV      | 402195         | 699288        | 21.34%          | 5.352%        |
| 7         | 10.725      | 1292          | 1300        | 1307         | rBV      | 163702         | 283958        | 8.67%           | 2.173%        |
| 8         | 13.181      | 1711          | 1718        | 1725         | rBV      | 1069455        | 1650763       | 50.37%          | 12.634%       |
| 9         | 14.556      | 1945          | 1952        | 1959         | rVB      | 280196         | 428649        | 13.08%          | 3.281%        |
| 10        | 16.042      | 2197          | 2205        | 2217         | rBV      | 989541         | 1486516       | 45.36%          | 11.377%       |
| 11        | 17.300      | 2412          | 2419        | 2425         | rBV      | 427159         | 624318        | 19.05%          | 4.778%        |
| 12        | 19.914      | 2858          | 2864        | 2870         | rBV      | 2498453        | 3277067       | 100.00%         | 25.081%       |
| 13        | 21.289      | 3093          | 3098        | 3104         | rVB      | 32974          | 48670         | 1.49%           | 0.373%        |
| 14        | 21.548      | 3136          | 3142        | 3152         | rBV2     | 476058         | 761799        | 23.25%          | 5.830%        |
| 15        | 24.697      | 3668          | 3678        | 3696         | rVB2     | 290505         | 856030        | 26.12%          | 6.552%        |

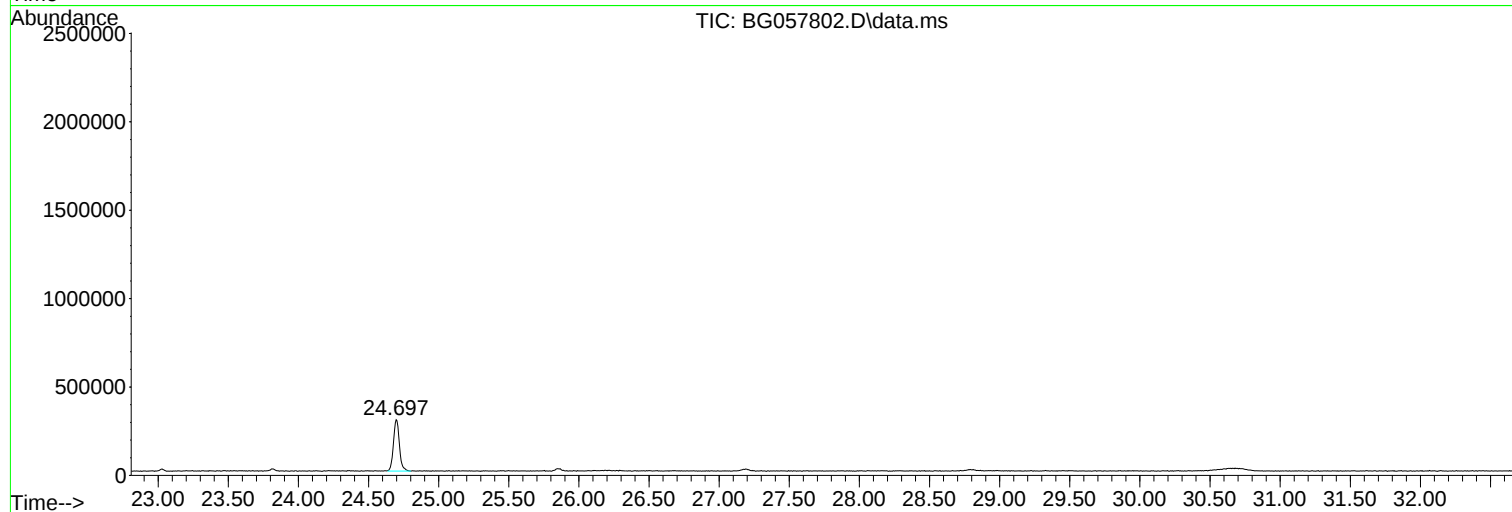
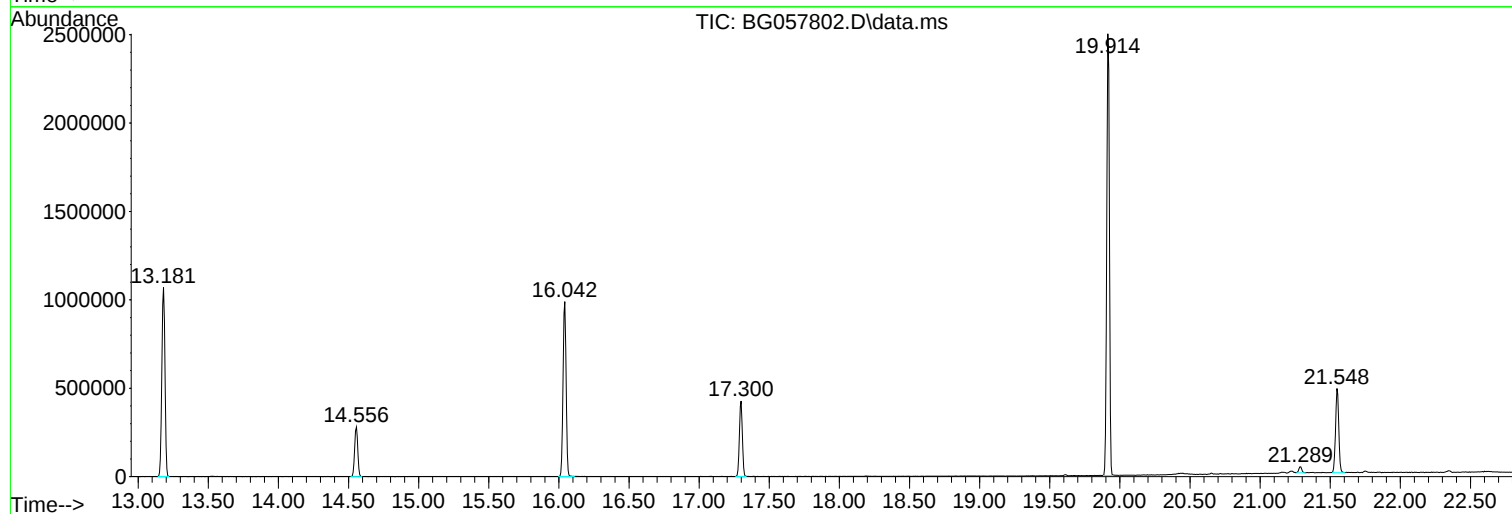
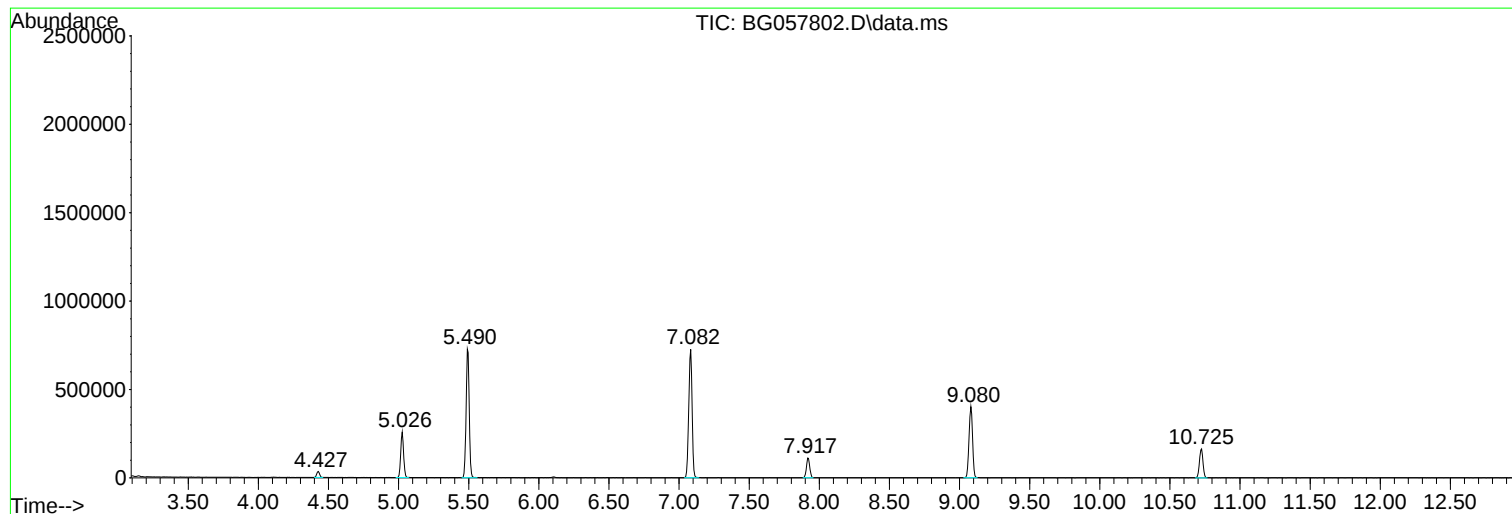
Sum of corrected areas: 13065760

Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG062223\  
Data File : BG057802.D  
Acq On : 22 Jun 2023 9:19  
Operator : CG/JU  
Sample : PB153645BL  
Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
PB153645BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG061923.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG062223\  
Data File : BG057802.D  
Acq On : 22 Jun 2023 9:19  
Operator : CG/JU  
Sample : PB153645BL  
Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
PB153645BL

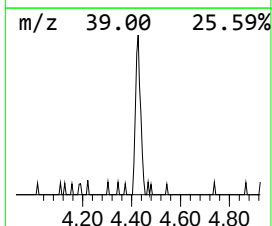
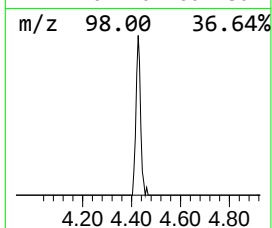
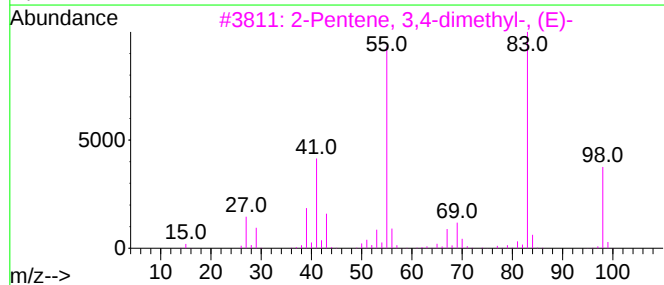
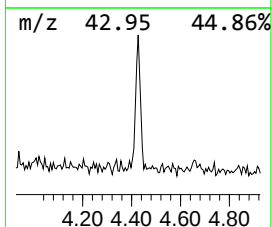
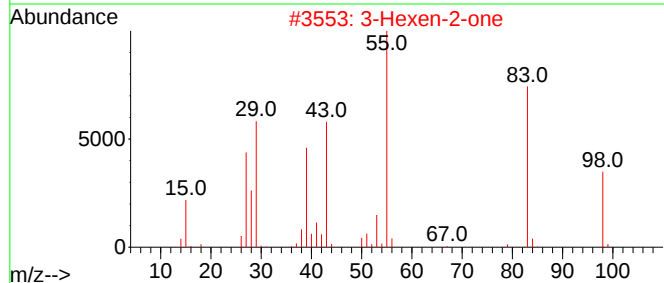
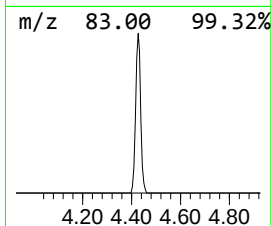
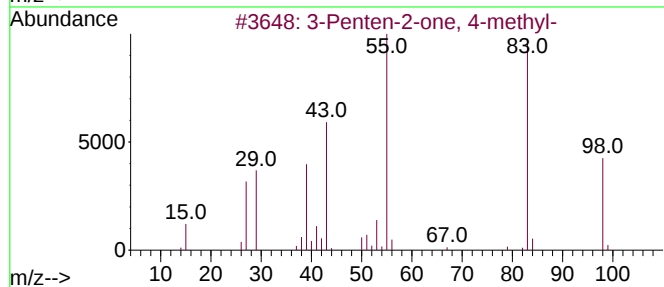
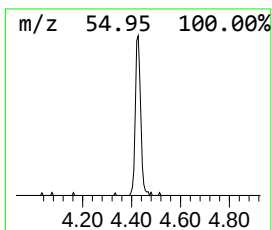
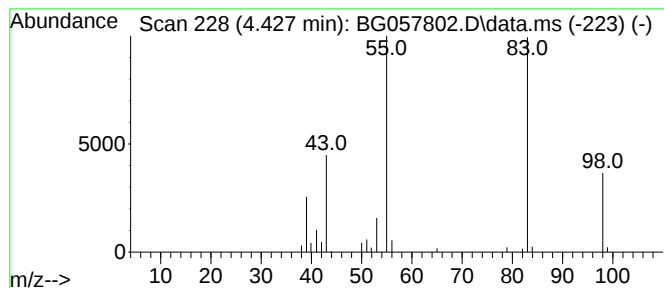
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG061923.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

| R.T.  | EstConc | Area  | Relative to ISTD       | R.T.  |
|-------|---------|-------|------------------------|-------|
| 4.427 | 5.24 ng | 48546 | 1,4-Dichlorobenzene-d4 | 7.922 |

| 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, 3,4-dimethyl-, (E)- | 98 | C7H14   | 004914-92-5 | 80   |
| 4    |      | 2-Pentene, 4,4-dimethyl-, (E)- | 98 | C7H14   | 000690-08-4 | 72   |
| 5    |      | 2-Pentene, 2,4-dimethyl-       | 98 | C7H14   | 000625-65-0 | 72   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG062223\  
Data File : BG057802.D  
Acq On : 22 Jun 2023 9:19  
Operator : CG/JU  
Sample : PB153645BL  
Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
PB153645BL

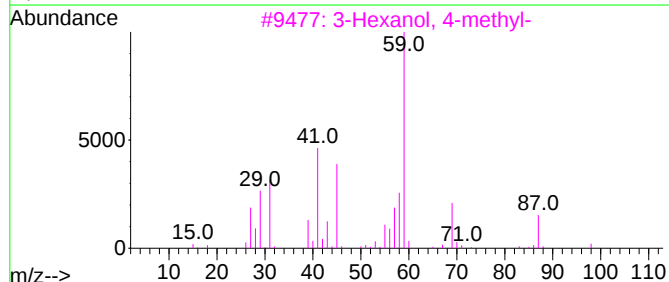
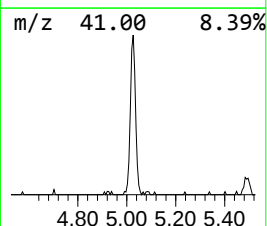
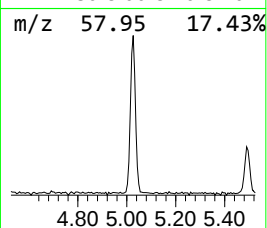
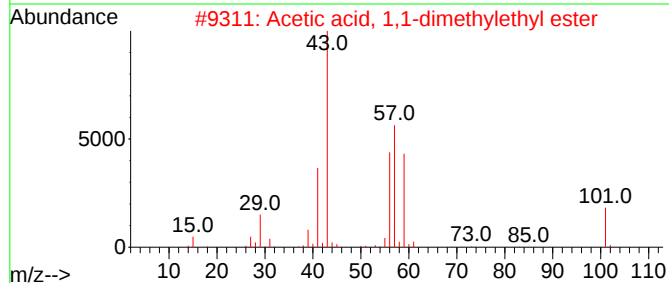
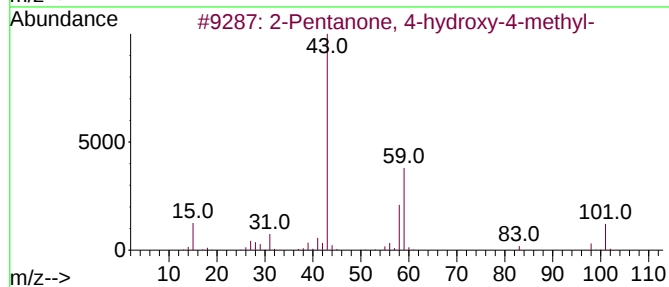
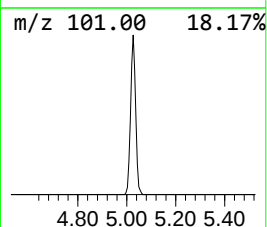
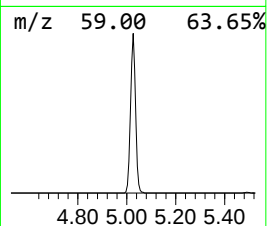
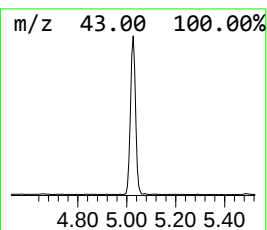
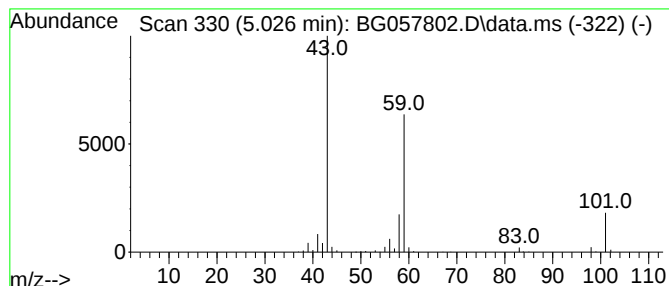
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG061923.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*

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

| R.T.      | EstConc                             | Area   | Relative to ISTD       |          |             | R.T.  |
|-----------|-------------------------------------|--------|------------------------|----------|-------------|-------|
| 5.026     | 40.13 ng                            | 371980 | 1,4-Dichlorobenzene-d4 |          |             | 7.922 |
| Hit# of 5 | Tentative ID                        |        | MW                     | MolForm  | CAS#        | Qual  |
| 1         | 2-Pentanone, 4-hydroxy-4-methyl-    |        | 116                    | C6H12O2  | 000123-42-2 | 53    |
| 2         | Acetic acid, 1,1-dimethylethyl e... |        | 116                    | C6H12O2  | 000540-88-5 | 39    |
| 3         | 3-Hexanol, 4-methyl-                |        | 116                    | C7H16O   | 000615-29-2 | 33    |
| 4         | 2-Hexanol, 2-methyl-                |        | 116                    | C7H16O   | 000625-23-0 | 28    |
| 5         | Acetic acid, cyano-, 1,1-dimethy... |        | 141                    | C7H11NO2 | 001116-98-9 | 23    |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG062223\  
Data File : BG057802.D  
Acq On : 22 Jun 2023 9:19  
Operator : CG/JU  
Sample : PB153645BL  
Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
PB153645BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG061923.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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-Penten-2-one,... | 4.427 | 5.2     | ng    | 48546    | 1                     | 7.922 | 185389 | 20.0 |
| 2-Pentanone, 4-... | 5.026 | 40.1    | ng    | 371980   | 1                     | 7.922 | 185389 | 20.0 |