

Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM100422\  
 Data File : BM036826.D  
 Acq On : 04 Oct 2022 11:09  
 Operator : CG/JU  
 Sample : PB147982BL  
 Misc :  
 ALS Vial : 3 Sample Multiplier: 1

Instrument :  
 BNA\_M  
 ClientSampleId :  
 PB147982BL

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\_M\Methods\8270-BM100322.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM036826.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         | 3.834       | 123           | 127         | 136          | rVB      | 236364         | 291793        | 1.32%           | 0.248%        |
| 2         | 4.452       | 227           | 232         | 242          | rBV      | 2717992        | 3413837       | 15.39%          | 2.901%        |
| 3         | 4.575       | 248           | 253         | 265          | rVB      | 141968         | 224844        | 1.01%           | 0.191%        |
| 4         | 5.069       | 331           | 337         | 353          | rVB      | 4310868        | 5898618       | 26.58%          | 5.013%        |
| 5         | 5.534       | 409           | 416         | 429          | rBV      | 9018878        | 12709760      | 57.28%          | 10.801%       |
| 6         | 6.151       | 516           | 521         | 528          | rVB      | 166174         | 239263        | 1.08%           | 0.203%        |
| 7         | 7.140       | 677           | 689         | 709          | rBV      | 8463158        | 13764326      | 62.03%          | 11.697%       |
| 8         | 7.975       | 822           | 831         | 841          | rBV      | 1425916        | 2244299       | 10.11%          | 1.907%        |
| 9         | 9.140       | 1021          | 1029        | 1039         | rBV      | 4942569        | 7986391       | 35.99%          | 6.787%        |
| 10        | 10.781      | 1300          | 1308        | 1318         | rBV      | 1972445        | 3218429       | 14.50%          | 2.735%        |
| 11        | 13.233      | 1717          | 1725        | 1734         | rBV      | 12793930       | 18309086      | 82.51%          | 15.560%       |
| 12        | 14.598      | 1950          | 1957        | 1967         | rBV      | 2962050        | 4143205       | 18.67%          | 3.521%        |
| 13        | 16.080      | 2202          | 2209        | 2235         | rBV      | 8638615        | 12537415      | 56.50%          | 10.655%       |
| 14        | 17.333      | 2416          | 2422        | 2437         | rBV      | 3193141        | 4605322       | 20.75%          | 3.914%        |
| 15        | 19.956      | 2861          | 2868        | 2882         | rBV      | 17031804       | 22189288      | 100.00%         | 18.857%       |
| 16        | 21.509      | 3127          | 3132        | 3140         | rBV      | 2639064        | 3503772       | 15.79%          | 2.978%        |
| 17        | 23.921      | 3536          | 3542        | 3555         | rVB2     | 1194079        | 2389884       | 10.77%          | 2.031%        |

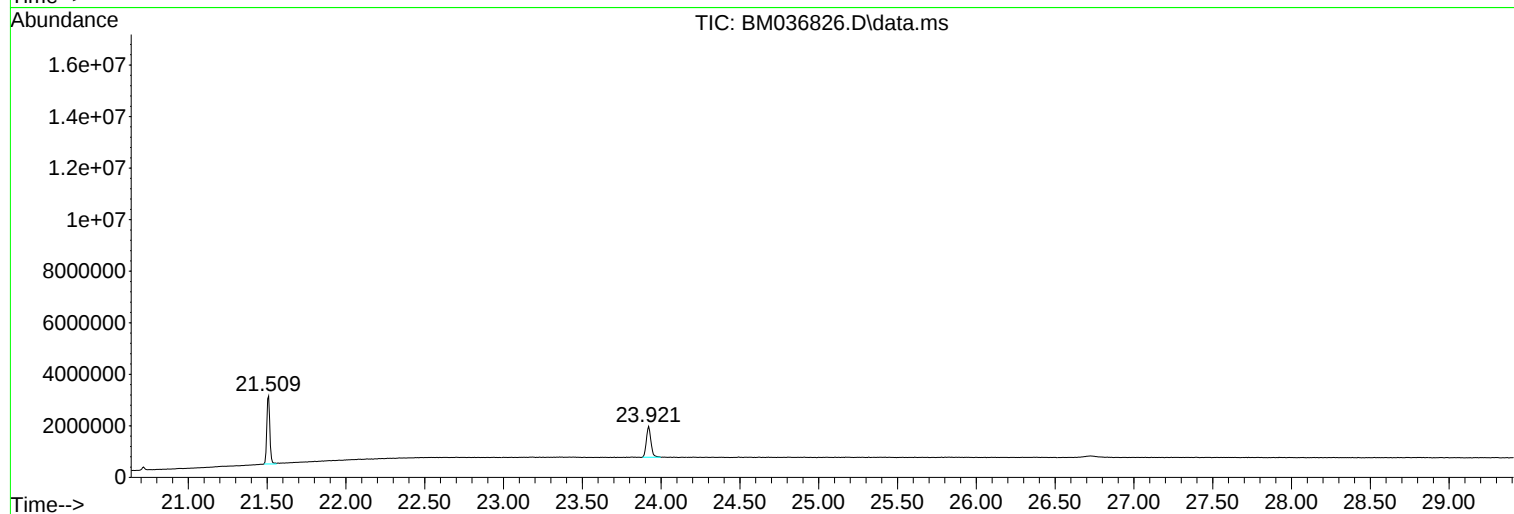
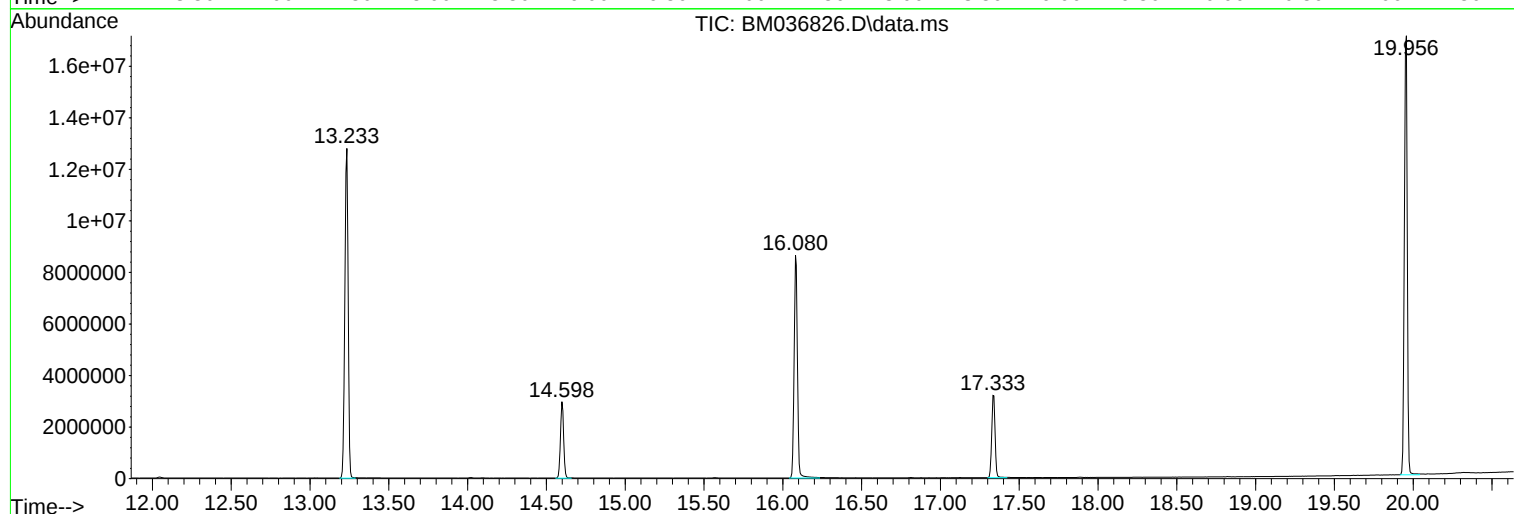
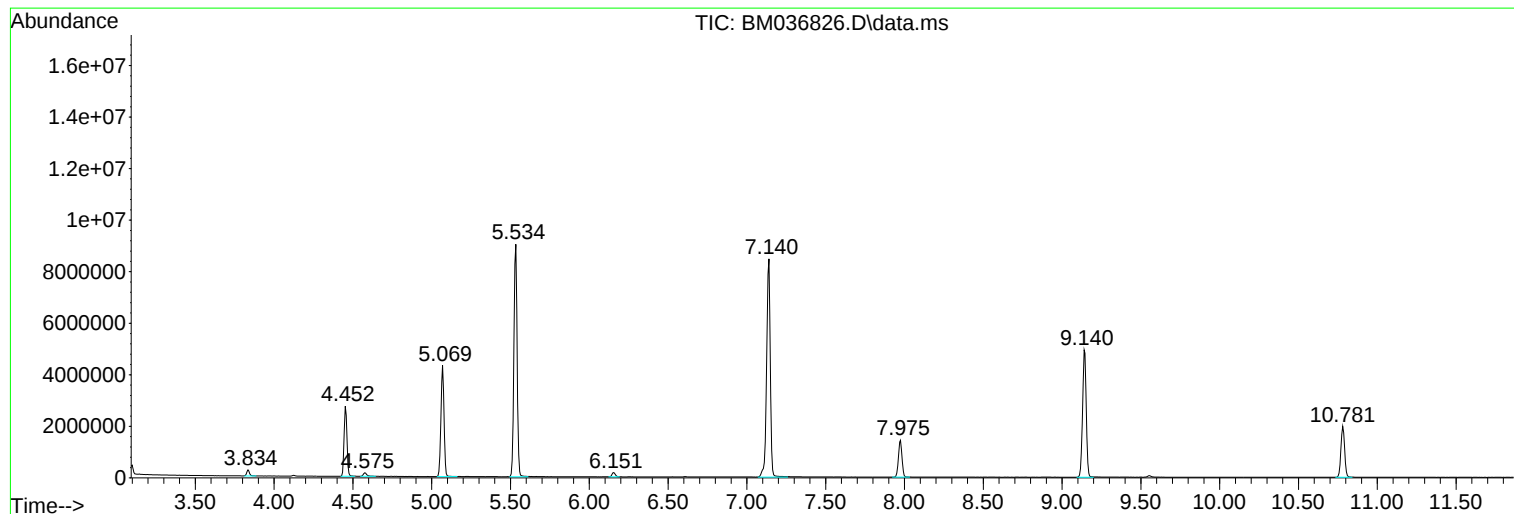
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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM100322.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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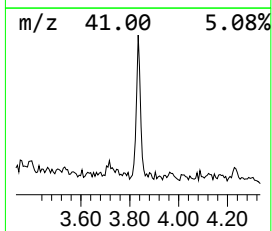
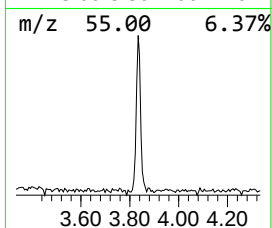
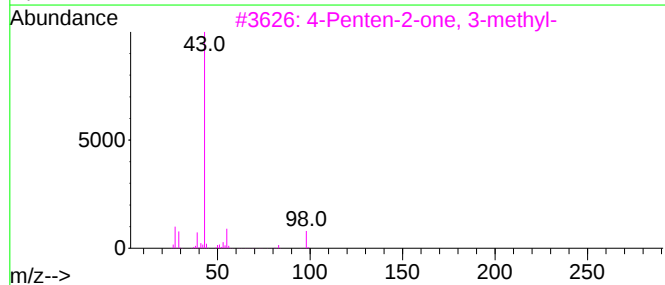
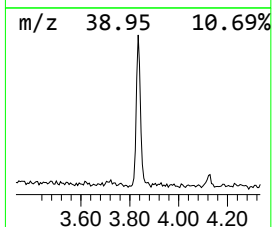
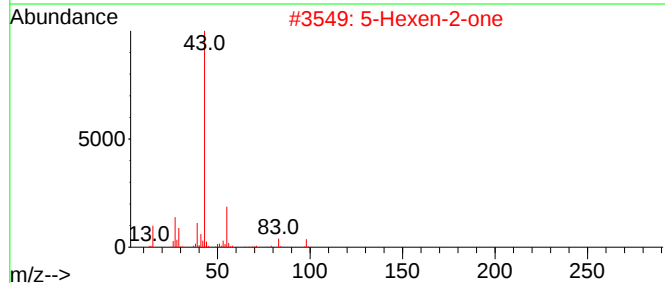
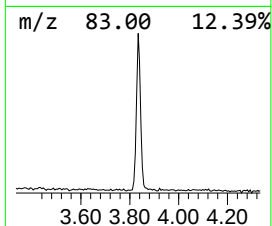
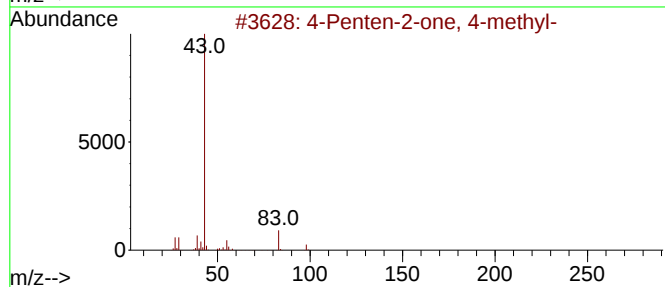
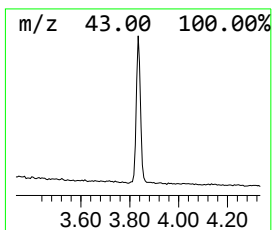
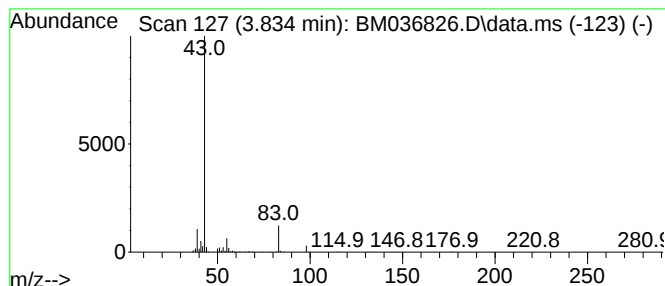
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM100322.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

| R.T.  | EstConc | Area   | Relative to ISTD       | R.T.  |
|-------|---------|--------|------------------------|-------|
| 3.834 | 2.60 ng | 291793 | 1,4-Dichlorobenzene-d4 | 7.975 |

| Hit# | of | 5 | Tentative ID                      | MW  | MolForm | CAS#        | Qual |
|------|----|---|-----------------------------------|-----|---------|-------------|------|
| 1    |    |   | 4-Penten-2-one, 4-methyl-         | 98  | C6H10O  | 003744-02-3 | 80   |
| 2    |    |   | 5-Hexen-2-one                     | 98  | C6H10O  | 000109-49-9 | 43   |
| 3    |    |   | 4-Penten-2-one, 3-methyl-         | 98  | C6H10O  | 000758-87-2 | 25   |
| 4    |    |   | Methyl 1-methylcyclopropyl ketone | 98  | C6H10O  | 001567-75-5 | 9    |
| 5    |    |   | 2-Vinylethyl acetate              | 114 | C6H10O2 | 001576-84-7 | 9    |



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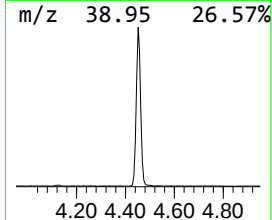
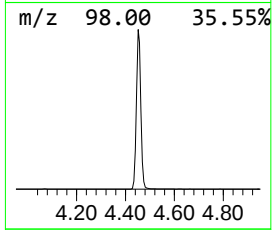
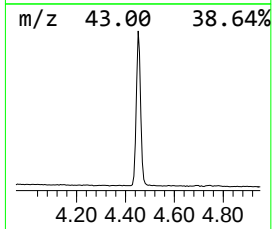
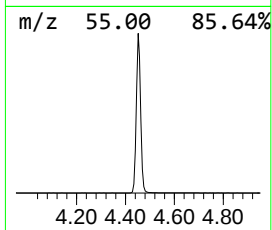
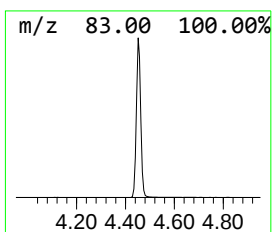
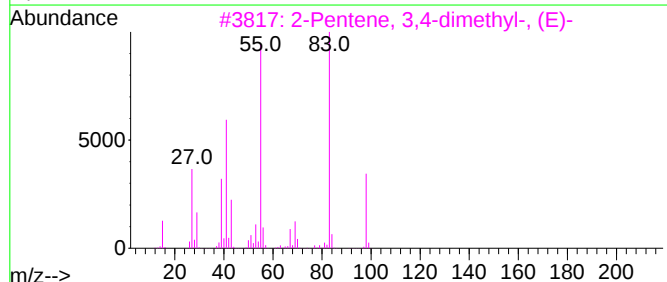
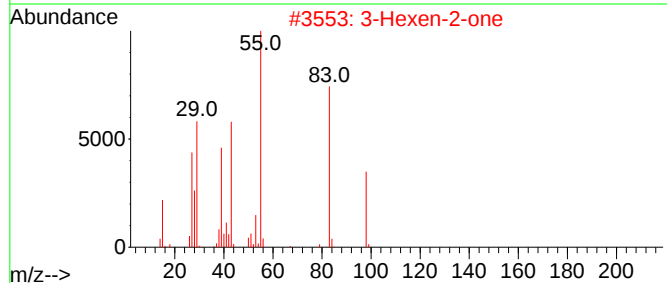
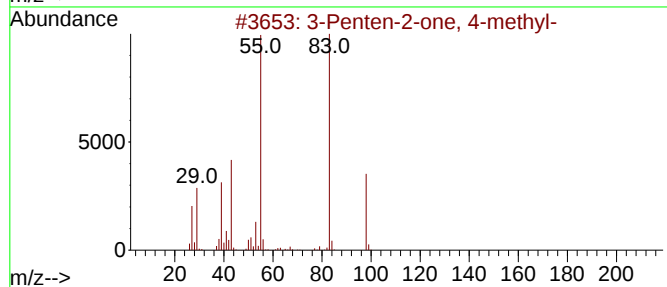
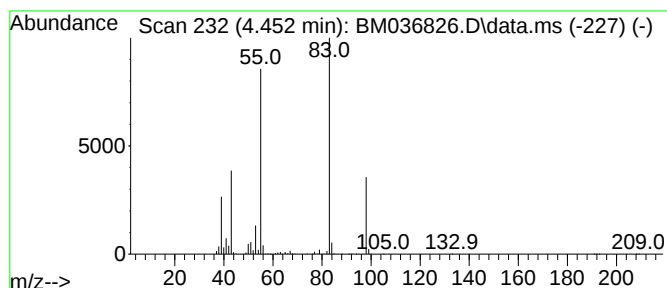
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM100322.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

| R.T.      | EstConc                        | Area    | Relative to ISTD       | R.T.        |      |
|-----------|--------------------------------|---------|------------------------|-------------|------|
| 4.452     | 30.42 ng                       | 3413840 | 1,4-Dichlorobenzene-d4 | 7.975       |      |
| Hit# of 5 | Tentative ID                   | MW      | MolForm                | CAS#        | Qual |
| 1         | 3-Penten-2-one, 4-methyl-      | 98      | C6H10O                 | 000141-79-7 | 94   |
| 2         | 3-Hexen-2-one                  | 98      | C6H10O                 | 000763-93-9 | 91   |
| 3         | 2-Pentene, 3,4-dimethyl-, (E)- | 98      | C7H14                  | 004914-92-5 | 90   |
| 4         | 2-Pentene, 3,4-dimethyl-, (Z)- | 98      | C7H14                  | 004914-91-4 | 86   |
| 5         | 2-Pentene, 2,4-dimethyl-       | 98      | C7H14                  | 000625-65-0 | 80   |



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Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
PB147982BL

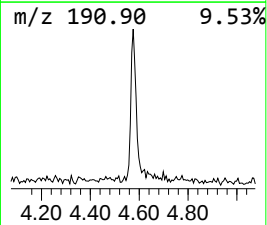
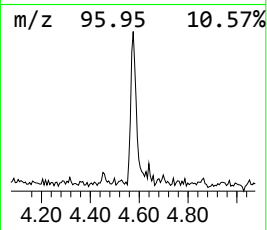
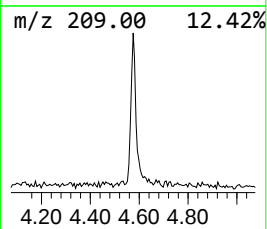
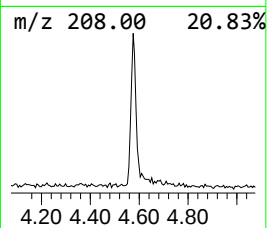
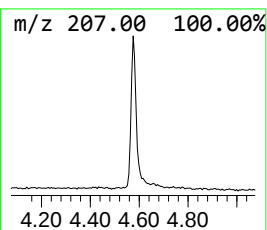
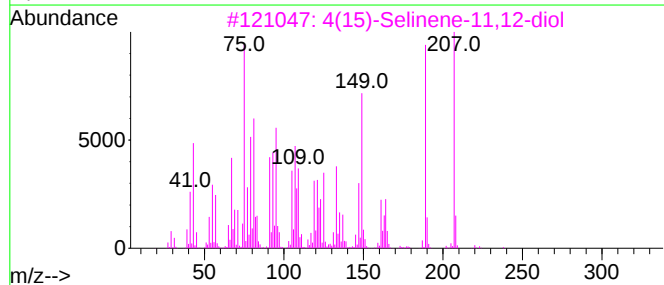
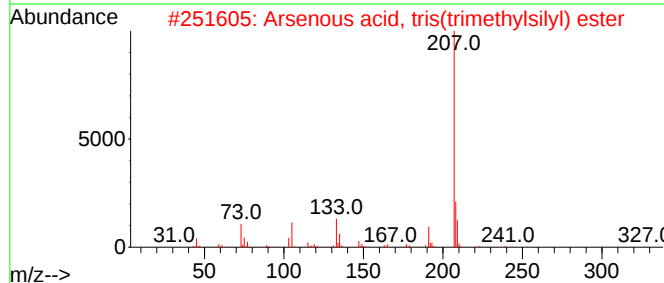
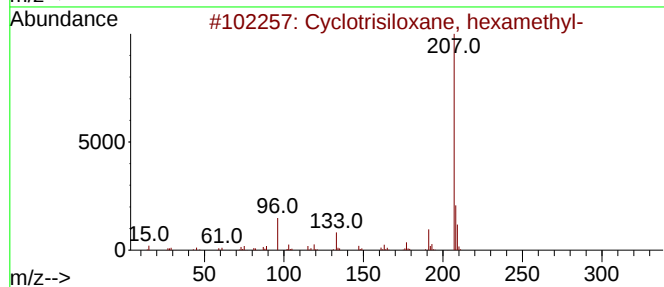
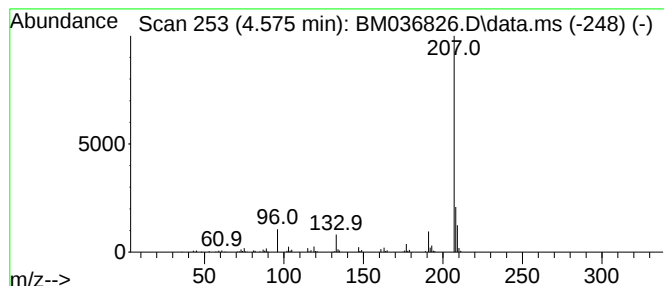
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM100322.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 3 Cyclotrisiloxane, hexamethyl- Concentration Rank 5

| R.T.  | EstConc | Area   | Relative to ISTD       | R.T.  |
|-------|---------|--------|------------------------|-------|
| 4.575 | 2.00 ng | 224844 | 1,4-Dichlorobenzene-d4 | 7.975 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm      | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|--------------|-------------|------|
| 1    |    |   | Cyclotrisiloxane, hexamethyl-       | 222 | C6H18O3Si3   | 000541-05-9 | 91   |
| 2    |    |   | Arsenous acid, tris(trimethylsil... | 342 | C9H27AsO3Si3 | 055429-29-3 | 56   |
| 3    |    |   | 4(15)-Selinene-11,12-diol           | 238 | C15H26O2     | 073035-82-2 | 50   |
| 4    |    |   | Benzo[h]quinoline, 2,4-dimethyl-    | 207 | C15H13N      | 000605-67-4 | 45   |
| 5    |    |   | 4-tert-Octylphenol, TMS derivative  | 278 | C17H30OSi    | 078721-87-6 | 39   |



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ALS Vial : 3 Sample Multiplier: 1

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BNA\_M  
ClientSampleId :  
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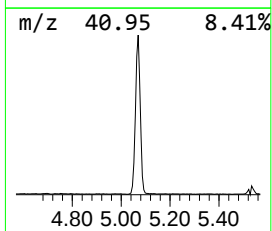
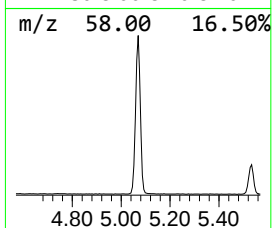
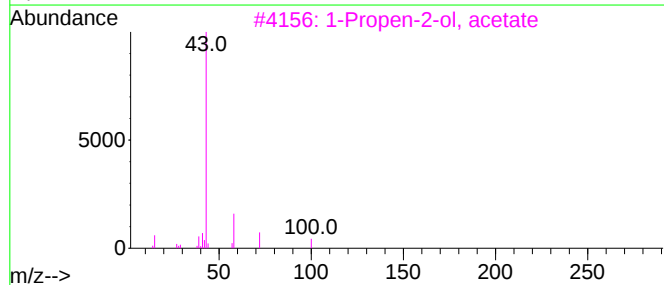
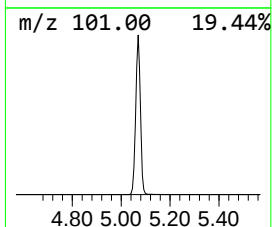
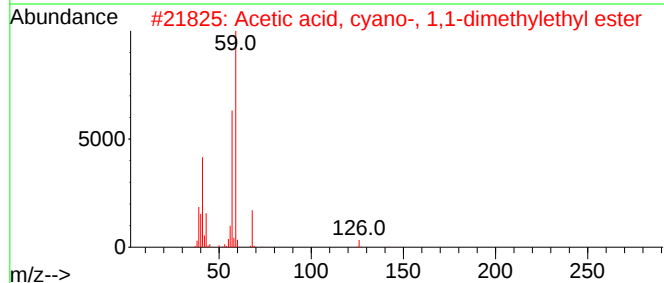
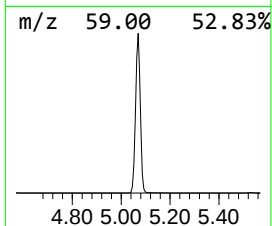
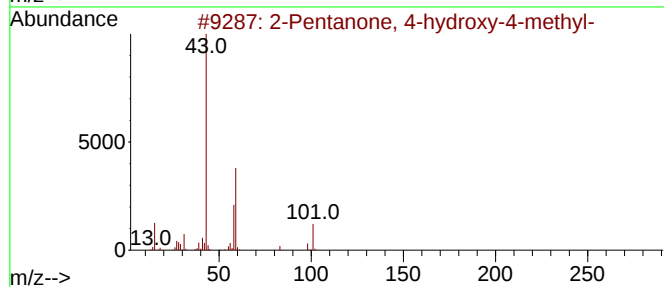
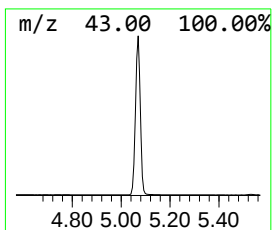
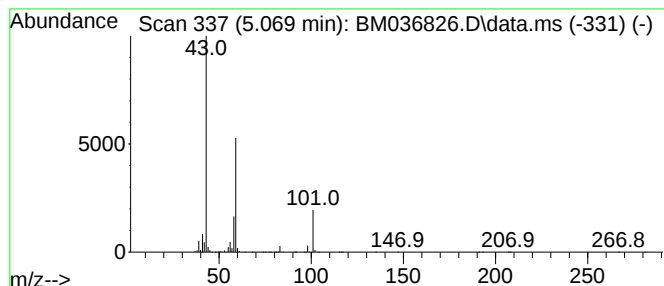
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM100322.M  
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TIC Library : C:\Database\NIST20.L  
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Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

| R.T.      | EstConc                             | Area    | Relative to ISTD       |          |             | R.T.  |
|-----------|-------------------------------------|---------|------------------------|----------|-------------|-------|
| 5.069     | 52.57 ng                            | 5898620 | 1,4-Dichlorobenzene-d4 |          |             | 7.975 |
| 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, cyano-, 1,1-dimethy... |         | 141                    | C7H11NO2 | 001116-98-9 | 23    |
| 3         | 1-Propen-2-ol, acetate              |         | 100                    | C5H8O2   | 000108-22-5 | 10    |
| 4         | 5-Hexen-2-one                       |         | 98                     | C6H10O   | 000109-49-9 | 9     |
| 5         | Morpholine, 4-methyl-               |         | 101                    | C5H11NO  | 000109-02-4 | 9     |



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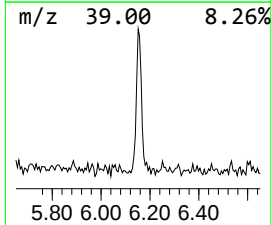
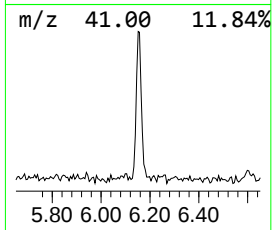
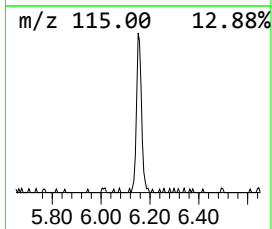
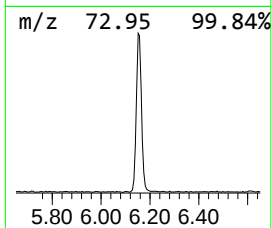
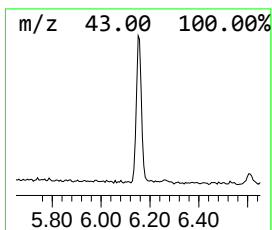
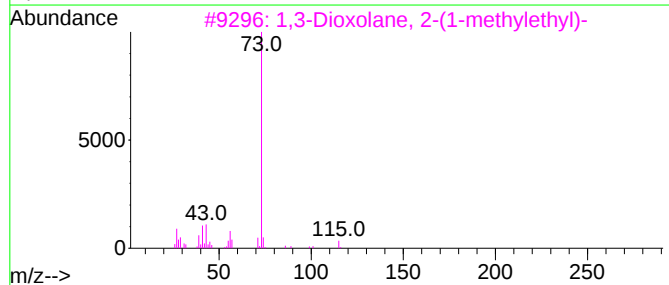
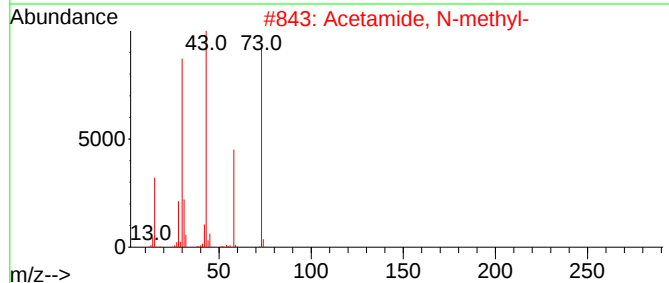
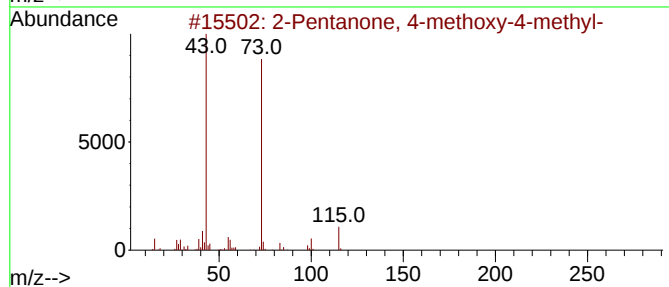
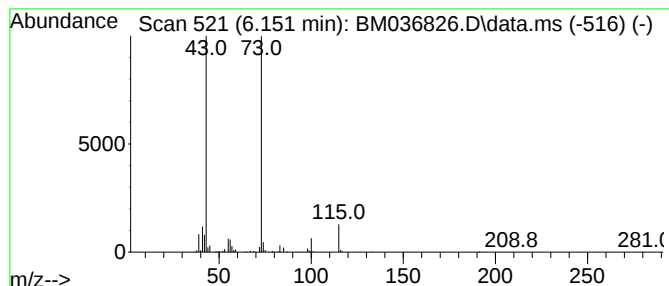
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 2-Pentanone, 4-methoxy-4-me... Concentration Rank 4

| R.T.  | EstConc | Area   | Relative to ISTD       | R.T.  |
|-------|---------|--------|------------------------|-------|
| 6.151 | 2.13 ng | 239263 | 1,4-Dichlorobenzene-d4 | 7.975 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|----------|--------------|------|
| 1    |    |   | 2-Pentanone, 4-methoxy-4-methyl-    | 130 | C7H14O2  | 000107-70-0  | 83   |
| 2    |    |   | Acetamide, N-methyl-                | 73  | C3H7NO   | 000079-16-3  | 33   |
| 3    |    |   | 1,3-Dioxolane, 2-(1-methylethyl)-   | 116 | C6H12O2  | 000822-83-3  | 32   |
| 4    |    |   | Isopropyl 5,11-dihydroxy-3,7,11-... | 314 | C18H34O4 | 1000223-34-1 | 17   |
| 5    |    |   | N-Ethylformamide                    | 73  | C3H7NO   | 000627-45-2  | 16   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM100422\  
Data File : BM036826.D  
Acq On : 04 Oct 2022 11:09  
Operator : CG/JU  
Sample : PB147982BL  
Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
PB147982BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM100322.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 |
| 4-Penten-2-one,... | 3.834 | 2.6     | ng    | 291793   | 1                     | 7.975 | 2244300 | 20.0 |
| 3-Penten-2-one,... | 4.452 | 30.4    | ng    | 3413840  | 1                     | 7.975 | 2244300 | 20.0 |
| Cyclotrisiloxan... | 4.575 | 2.0     | ng    | 224844   | 1                     | 7.975 | 2244300 | 20.0 |
| 2-Pentanone, 4-... | 5.069 | 52.6    | ng    | 5898620  | 1                     | 7.975 | 2244300 | 20.0 |
| 2-Pentanone, 4-... | 6.151 | 2.1     | ng    | 239263   | 1                     | 7.975 | 2244300 | 20.0 |