

Data Path : Z:\svoasrv\HPCHEM1\BNA\_P\Data\BP120321\  
 Data File : BP008210.D  
 Acq On : 03 Dec 2021 18:01  
 Operator : CG/JU  
 Sample : M4910-17  
 Misc :  
 ALS Vial : 9 Sample Multiplier: 1

Instrument :  
 BNA\_P  
 ClientSampleId :  
 SP-1-4

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\_P\Methods\8270E-BP112521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP008210.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         | 3.046       | 7             | 10          | 20           | rVB      | 53361          | 80855         | 2.27%           | 0.363%        |
| 2         | 4.922       | 322           | 329         | 343          | rBV      | 317698         | 450001        | 12.63%          | 2.022%        |
| 3         | 5.387       | 402           | 408         | 425          | rBV      | 1832603        | 2697483       | 75.73%          | 12.118%       |
| 4         | 5.993       | 505           | 511         | 517          | rBV      | 37863          | 54738         | 1.54%           | 0.246%        |
| 5         | 6.981       | 671           | 679         | 699          | rBV      | 1629016        | 2742294       | 76.99%          | 12.320%       |
| 6         | 7.793       | 810           | 817         | 826          | rBV      | 313002         | 494589        | 13.89%          | 2.222%        |
| 7         | 8.957       | 1005          | 1015        | 1028         | rBV      | 1064314        | 1780402       | 49.99%          | 7.998%        |
| 8         | 10.398      | 1253          | 1260        | 1273         | rBV      | 17455          | 48037         | 1.35%           | 0.216%        |
| 9         | 10.593      | 1282          | 1293        | 1302         | rBV      | 363029         | 635092        | 17.83%          | 2.853%        |
| 10        | 13.063      | 1706          | 1713        | 1731         | rBV      | 2245844        | 3446694       | 96.77%          | 15.484%       |
| 11        | 14.445      | 1941          | 1948        | 1966         | rBV      | 487836         | 791090        | 22.21%          | 3.554%        |
| 12        | 15.939      | 2194          | 2202        | 2223         | rBV      | 1546755        | 2558202       | 71.82%          | 11.493%       |
| 13        | 17.204      | 2411          | 2417        | 2427         | rBV      | 558775         | 852013        | 23.92%          | 3.828%        |
| 14        | 17.328      | 2434          | 2438        | 2445         | rVB5     | 36961          | 59033         | 1.66%           | 0.265%        |
| 15        | 18.104      | 2565          | 2570        | 2577         | rBV2     | 65285          | 100222        | 2.81%           | 0.450%        |
| 16        | 19.774      | 2848          | 2854        | 2865         | rBV      | 2928369        | 3561864       | 100.00%         | 16.002%       |
| 17        | 21.021      | 3062          | 3066        | 3074         | rBV      | 185044         | 255626        | 7.18%           | 1.148%        |
| 18        | 21.304      | 3110          | 3114        | 3120         | rBV      | 563542         | 771561        | 21.66%          | 3.466%        |
| 19        | 23.704      | 3516          | 3522        | 3531         | rVB      | 421412         | 879602        | 24.69%          | 3.952%        |

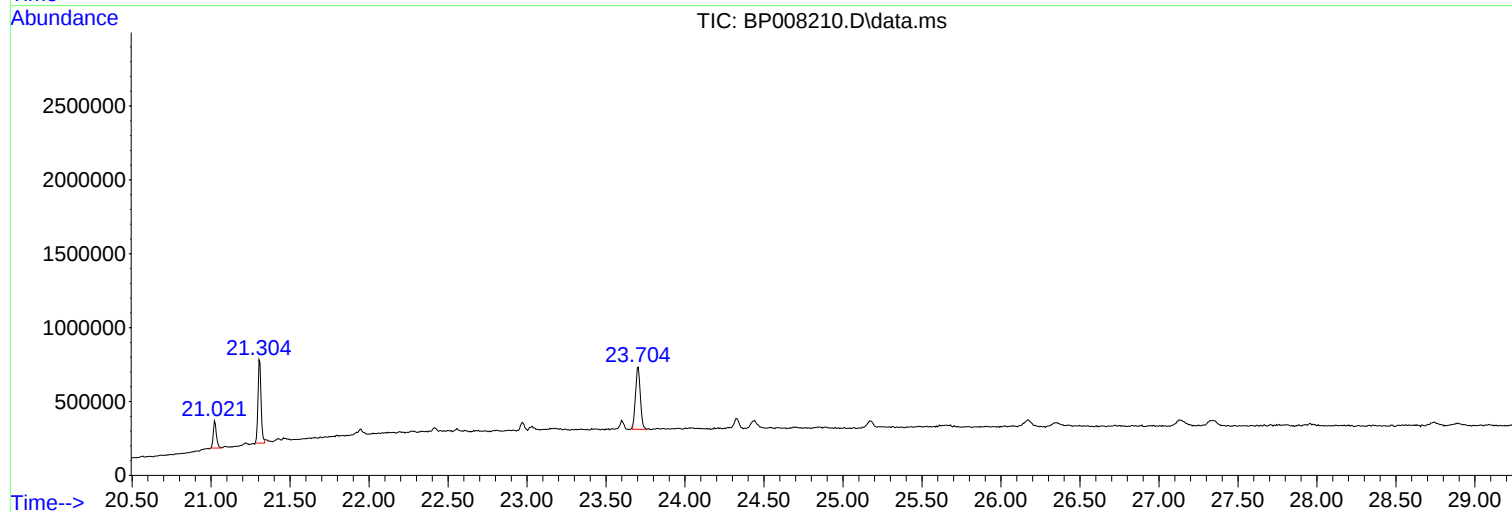
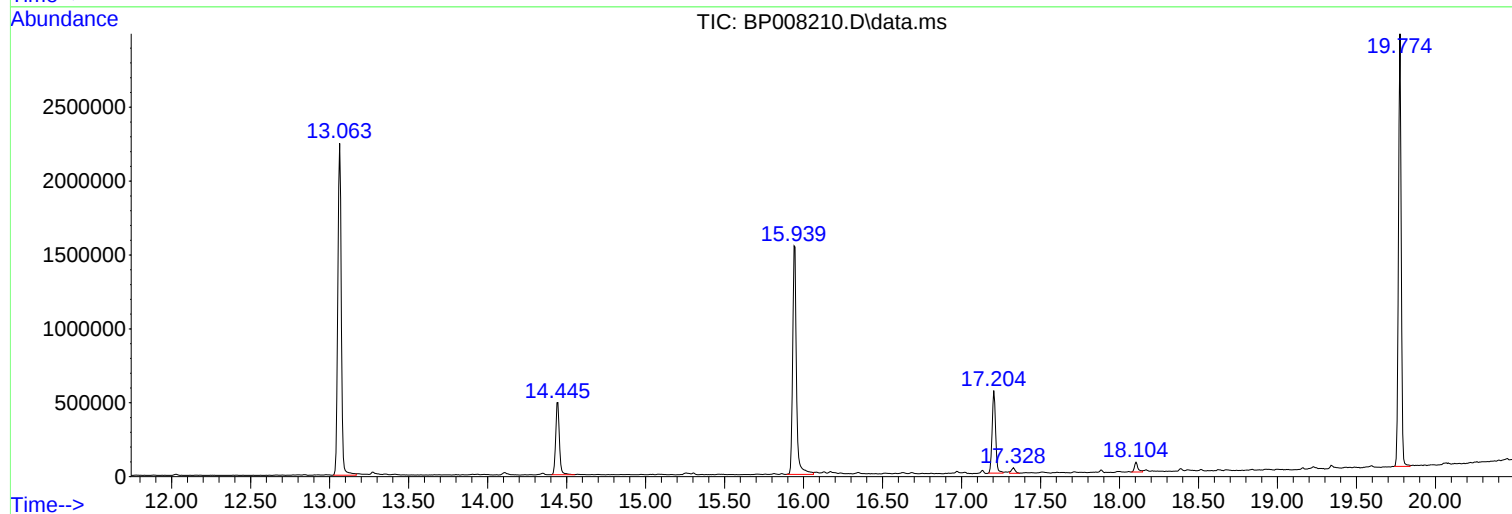
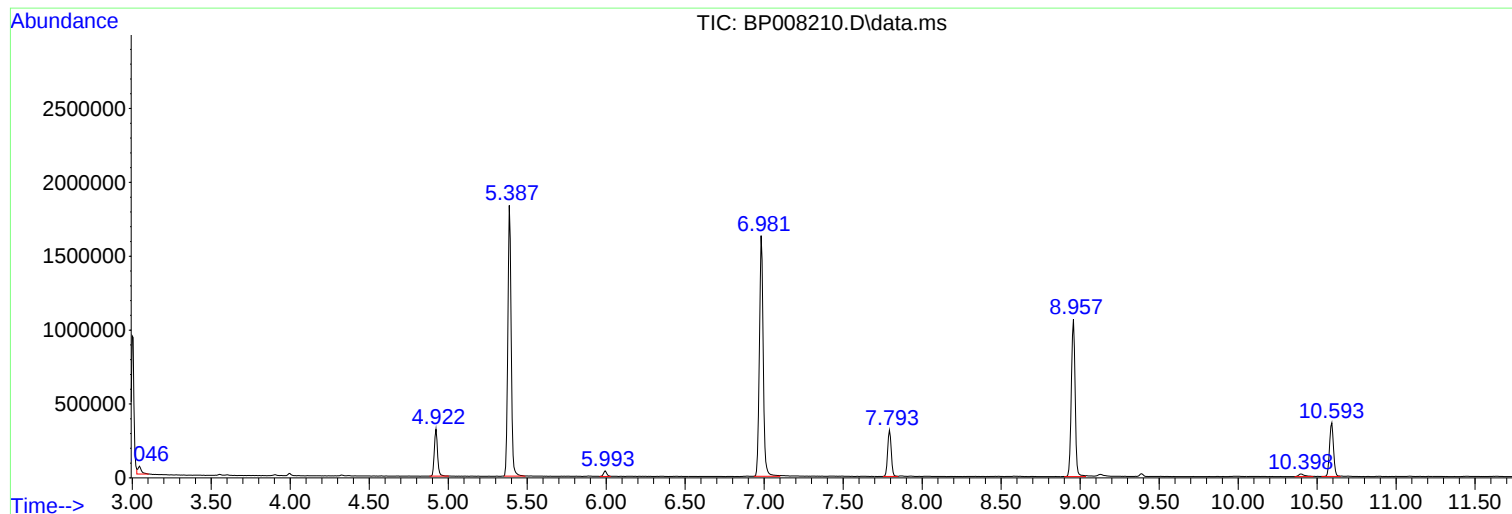
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Data Path : Z:\svoasrv\HPCHEM1\BNA\_P\Data\BP120321\  
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Misc :  
ALS Vial : 9 Sample Multiplier: 1

Instrument :  
BNA\_P  
ClientSampleId :  
SP-1-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_P\Methods\8270E-BP112521.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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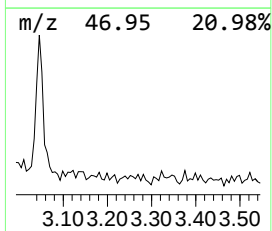
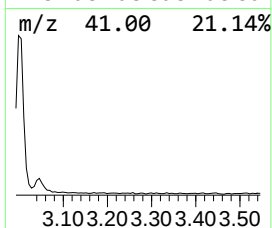
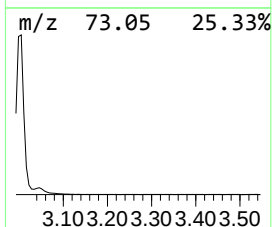
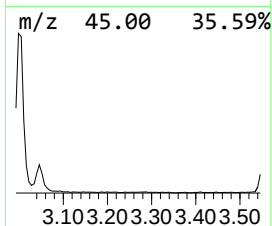
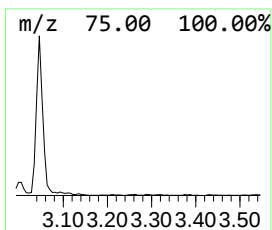
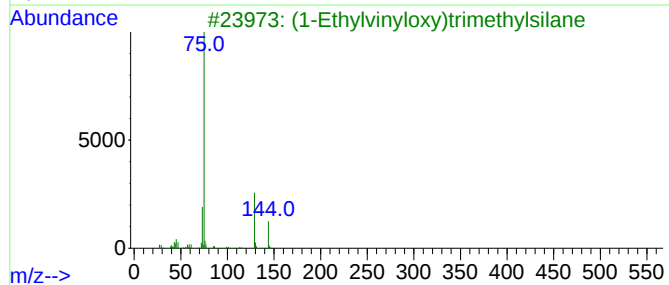
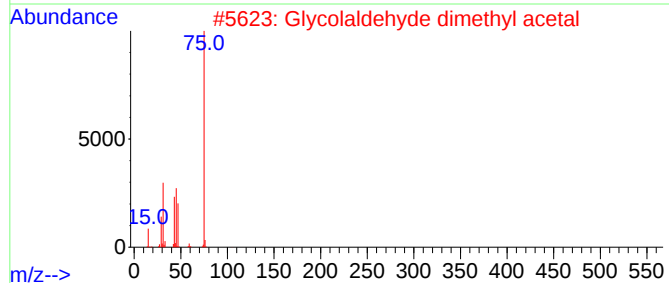
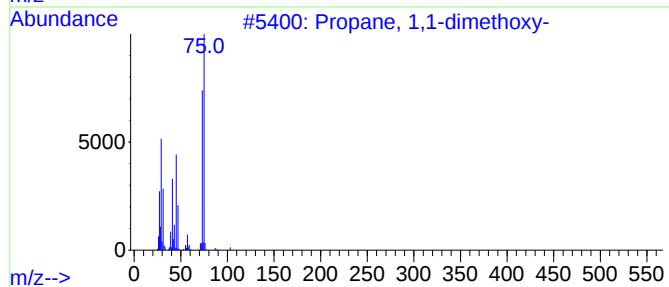
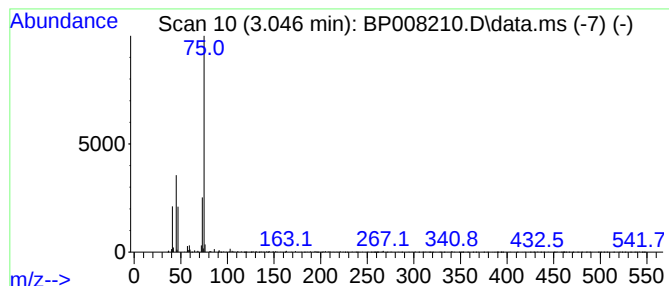
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 3

| R.T.  | EstConc | Area  | Relative to ISTD       | R.T.  |
|-------|---------|-------|------------------------|-------|
| 3.046 | 3.27 ng | 80855 | 1,4-Dichlorobenzene-d4 | 7.793 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm   | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|-----------|-------------|------|
| 1    |    |   | Propane, 1,1-dimethoxy-             | 104 | C5H12O2   | 004744-10-9 | 50   |
| 2    |    |   | Glycolaldehyde dimethyl acetal      | 106 | C4H10O3   | 030934-97-5 | 50   |
| 3    |    |   | (1-Ethylvinyl)oxy)trimethylsilane   | 144 | C7H16OSi  | 006651-40-7 | 42   |
| 4    |    |   | 3-Bromopropionaldehyde dimethyl ... | 182 | C5H11BrO2 | 036255-44-4 | 39   |
| 5    |    |   | Propane, 1,1-dimethoxy-2-methyl-    | 118 | C6H14O2   | 041632-89-7 | 36   |



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BNA\_P  
ClientSampleId :  
SP-1-4

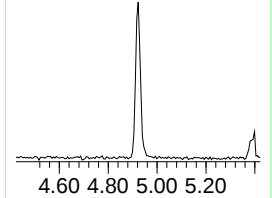
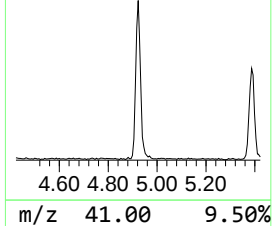
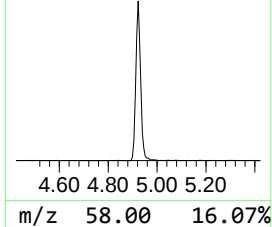
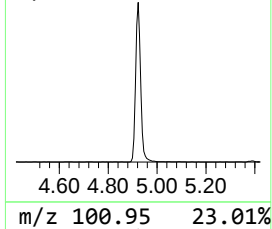
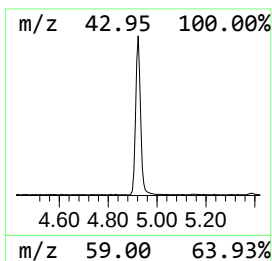
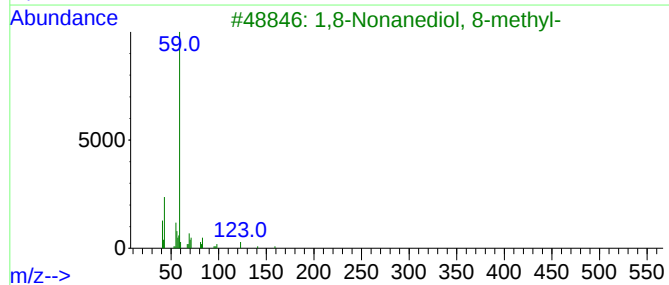
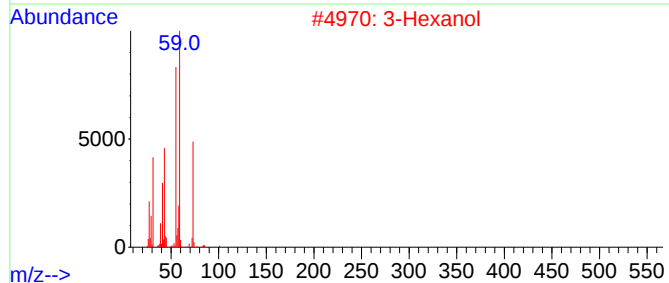
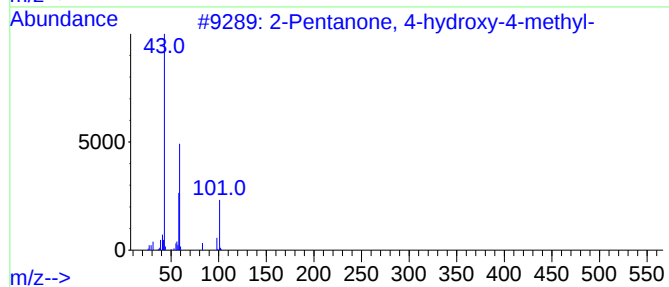
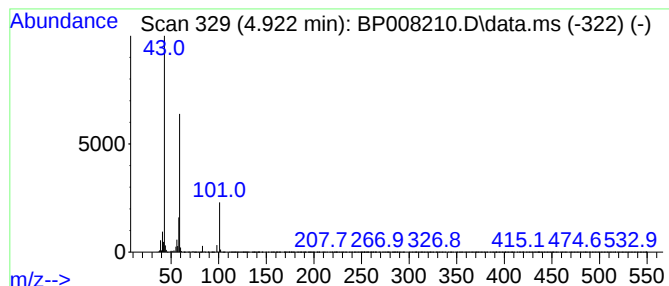
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_P\Methods\8270E-BP112521.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.  |
|-------|----------|--------|------------------------|-------|
| 4.922 | 18.20 ng | 450001 | 1,4-Dichlorobenzene-d4 | 7.793 |

| Hit# | of                                  | 5   | Tentative ID | MW          | MolForm | CAS# | Qual |
|------|-------------------------------------|-----|--------------|-------------|---------|------|------|
| 1    | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2      | 000123-42-2 | 56      |      |      |
| 2    | 3-Hexanol                           | 102 | C6H14O       | 000623-37-0 | 28      |      |      |
| 3    | 1,8-Nonanediol, 8-methyl-           | 174 | C10H22O2     | 054725-73-4 | 25      |      |      |
| 4    | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2     | 001116-98-9 | 17      |      |      |
| 5    | 2,3-Butanedione, monooxime          | 101 | C4H7NO2      | 000057-71-6 | 17      |      |      |



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ALS Vial : 9 Sample Multiplier: 1

Instrument :  
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SP-1-4

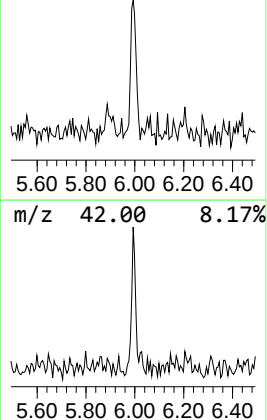
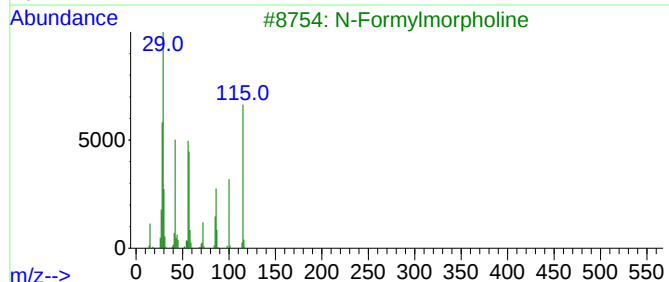
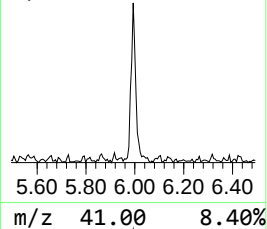
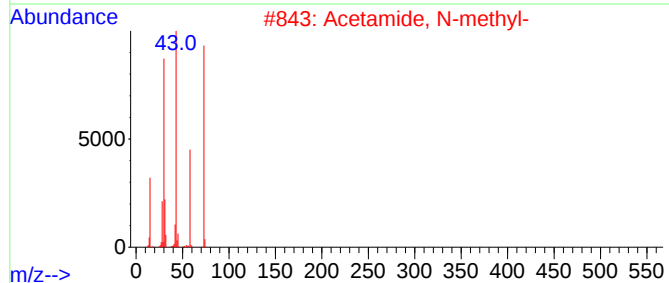
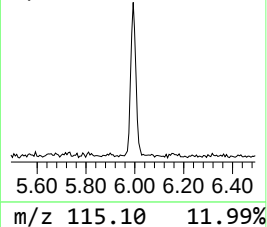
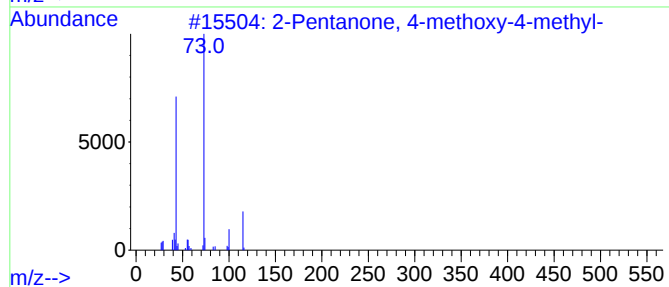
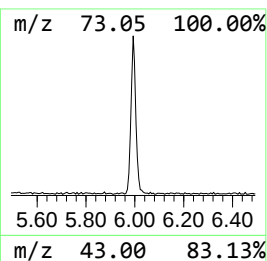
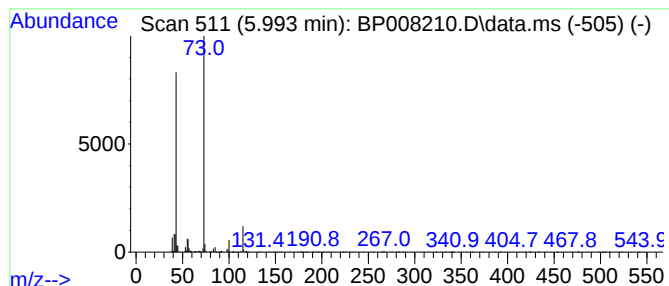
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_P\Methods\8270E-BP112521.M  
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TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 unknown5.993 Concentration Rank 5

| R.T.  | EstConc | Area  | Relative to ISTD       | R.T.  |
|-------|---------|-------|------------------------|-------|
| 5.993 | 2.21 ng | 54738 | 1,4-Dichlorobenzene-d4 | 7.793 |

| Hit# | of 5 | Tentative ID                        | MW  | MolForm   | CAS#        | Qual |
|------|------|-------------------------------------|-----|-----------|-------------|------|
| 1    |      | 2-Pentanone, 4-methoxy-4-methyl-    | 130 | C7H14O2   | 000107-70-0 | 59   |
| 2    |      | Acetamide, N-methyl-                | 73  | C3H7NO    | 000079-16-3 | 25   |
| 3    |      | N-Formylmorpholine                  | 115 | C5H9NO2   | 004394-85-8 | 9    |
| 4    |      | 1,3,5-Triacetoxy-hexahydro-1,3,5... | 261 | C9H15N3O6 | 058793-61-6 | 9    |
| 5    |      | Acetamide, N-butyl-                 | 115 | C6H13NO   | 001119-49-9 | 9    |



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Misc :  
ALS Vial : 9 Sample Multiplier: 1

Instrument :  
BNA\_P  
ClientSampleId :  
SP-1-4

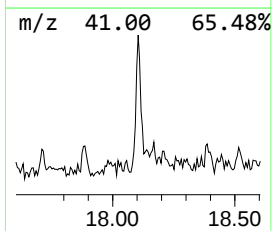
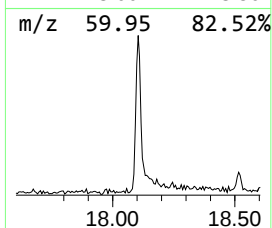
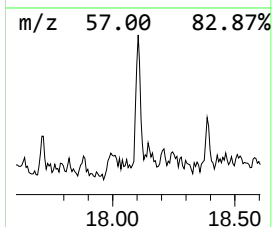
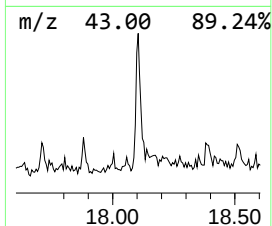
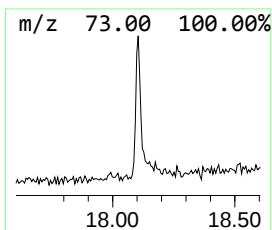
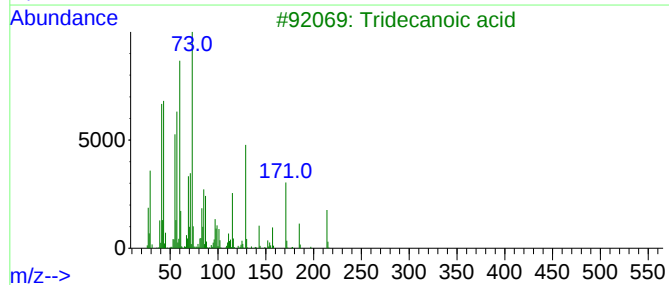
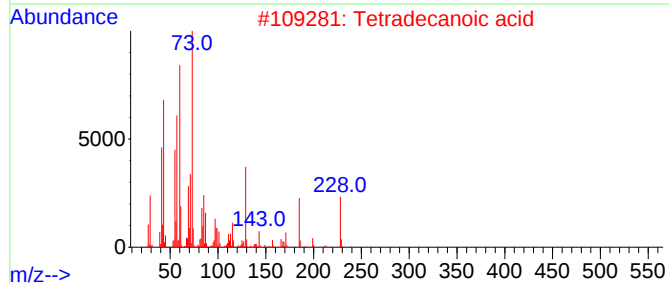
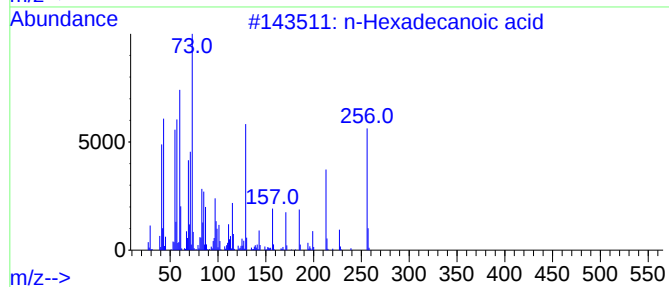
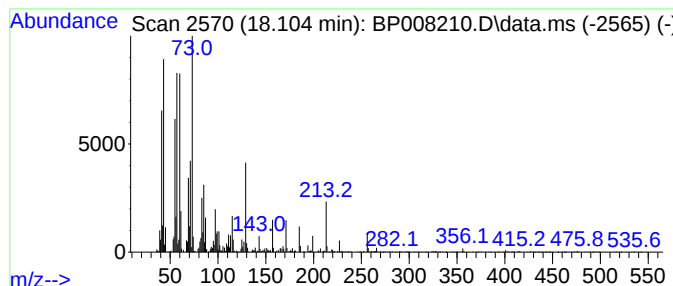
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TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 18.104 | 2.35 ng | 100222 | Phenanthrene-d10 | 17.204 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 98   |
| 2    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 87   |
| 3    |    |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 86   |
| 4    |    |   | Octadecanoic acid   | 284 | C18H36O2 | 000057-11-4 | 80   |
| 5    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 78   |



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SP-1-4

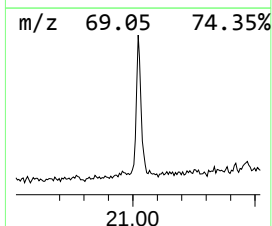
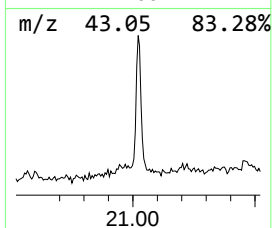
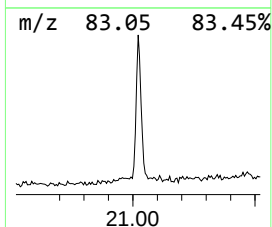
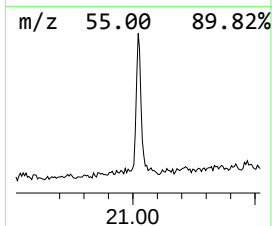
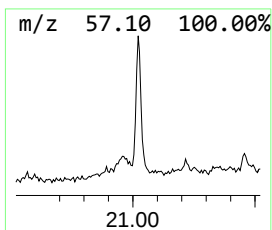
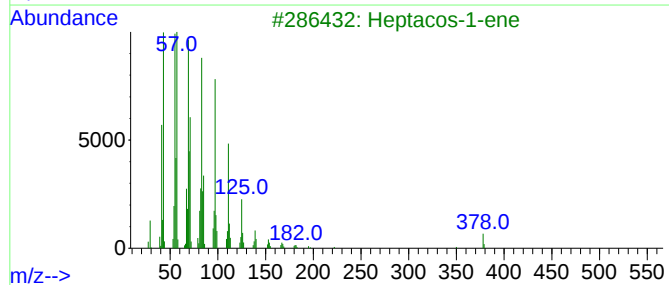
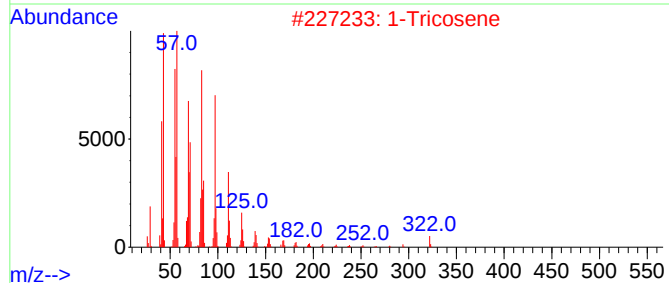
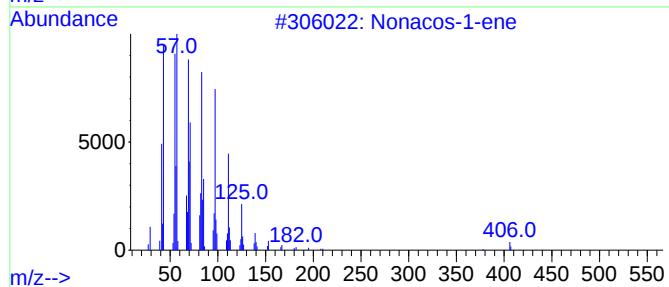
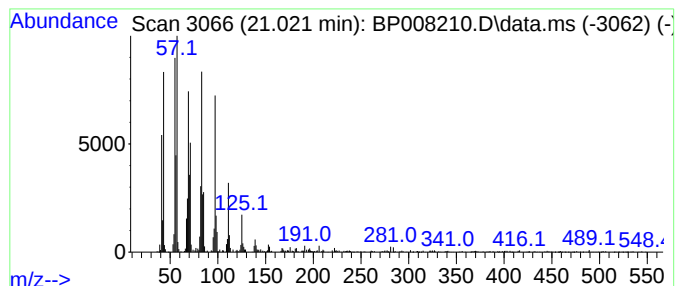
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_P\Methods\8270E-BP112521.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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Peak Number 5 Nonacos-1-ene Concentration Rank 2

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 21.022 | 6.63 ng | 255626 | Chrysene-d12     | 21.304 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm     | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|-------------|-------------|------|
| 1    |    |   | Nonacos-1-ene                       | 406 | C29H58      | 018835-35-3 | 96   |
| 2    |    |   | 1-Tricosene                         | 322 | C23H46      | 018835-32-0 | 95   |
| 3    |    |   | Heptacos-1-ene                      | 378 | C27H54      | 015306-27-1 | 94   |
| 4    |    |   | Trichloroacetic acid, hexadecyl ... | 386 | C18H33Cl3O2 | 074339-54-1 | 94   |
| 5    |    |   | Pentacos-1-ene                      | 350 | C25H50      | 016980-85-1 | 91   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_P\Data\BP120321\  
Data File : BP008210.D  
Acq On : 03 Dec 2021 18:01  
Operator : CG/JU  
Sample : M4910-17  
Misc :  
ALS Vial : 9 Sample Multiplier: 1

Instrument :  
BNA\_P  
ClientSampleId :  
SP-1-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_P\Methods\8270E-BP112521.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 |
| Propane, 1,1-di... | 3.046  | 3.3     | ng    | 80855    | 1                     | 7.793  | 494589 | 20.0 |
| 2-Pentanone, 4-... | 4.922  | 18.2    | ng    | 450001   | 1                     | 7.793  | 494589 | 20.0 |
| unknown5.993       | 5.993  | 2.2     | ng    | 54738    | 1                     | 7.793  | 494589 | 20.0 |
| n-Hexadecanoic ... | 18.104 | 2.4     | ng    | 100222   | 4                     | 17.204 | 852013 | 20.0 |
| Nonacos-1-ene      | 21.022 | 6.6     | ng    | 255626   | 5                     | 21.304 | 771561 | 20.0 |