

Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG111022\  
 Data File : BG055539.D  
 Acq On : 10 Nov 2022 14:29  
 Operator : CG/JU  
 Sample : N5474-02  
 Misc :  
 ALS Vial : 7 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 5592-4

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\_G\Methods\8270-BG110922.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055539.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         | 3.328       | 3             | 7           | 27           | rVB      | 791734         | 1380803       | 41.35%          | 9.263%        |
| 2         | 4.709       | 237           | 242         | 248          | rBV      | 33401          | 49409         | 1.48%           | 0.331%        |
| 3         | 5.326       | 340           | 347         | 355          | rVB      | 67925          | 108515        | 3.25%           | 0.728%        |
| 4         | 5.796       | 419           | 427         | 436          | rBV      | 399620         | 648313        | 19.42%          | 4.349%        |
| 5         | 7.400       | 692           | 700         | 710          | rBV      | 236997         | 405878        | 12.16%          | 2.723%        |
| 6         | 8.270       | 840           | 848         | 855          | rBV      | 164148         | 283642        | 8.50%           | 1.903%        |
| 7         | 9.439       | 1038          | 1047        | 1056         | rBV      | 555458         | 982727        | 29.43%          | 6.593%        |
| 8         | 11.102      | 1322          | 1330        | 1337         | rVB      | 215090         | 386129        | 11.56%          | 2.590%        |
| 9         | 13.517      | 1734          | 1741        | 1749         | rVB      | 1470805        | 2226179       | 66.67%          | 14.935%       |
| 10        | 14.886      | 1968          | 1974        | 1981         | rVB      | 339300         | 534754        | 16.02%          | 3.587%        |
| 11        | 16.366      | 2215          | 2226        | 2236         | rBV      | 1163536        | 1744088       | 52.24%          | 11.701%       |
| 12        | 17.629      | 2434          | 2441        | 2447         | rBV      | 466177         | 711102        | 21.30%          | 4.771%        |
| 13        | 18.493      | 2583          | 2588        | 2599         | rBV3     | 66655          | 132108        | 3.96%           | 0.886%        |
| 14        | 19.756      | 2798          | 2803        | 2809         | rBV6     | 33152          | 62430         | 1.87%           | 0.419%        |
| 15        | 20.215      | 2875          | 2881        | 2890         | rVB      | 2466279        | 3338918       | 100.00%         | 22.400%       |
| 16        | 21.537      | 3102          | 3106        | 3112         | rBV2     | 76479          | 115127        | 3.45%           | 0.772%        |
| 17        | 21.924      | 3166          | 3172        | 3179         | rBV2     | 502784         | 839894        | 25.15%          | 5.635%        |
| 18        | 23.722      | 3473          | 3478        | 3487         | rVB      | 81721          | 165377        | 4.95%           | 1.109%        |
| 19        | 25.350      | 3746          | 3755        | 3767         | rVB      | 272485         | 790681        | 23.68%          | 5.304%        |

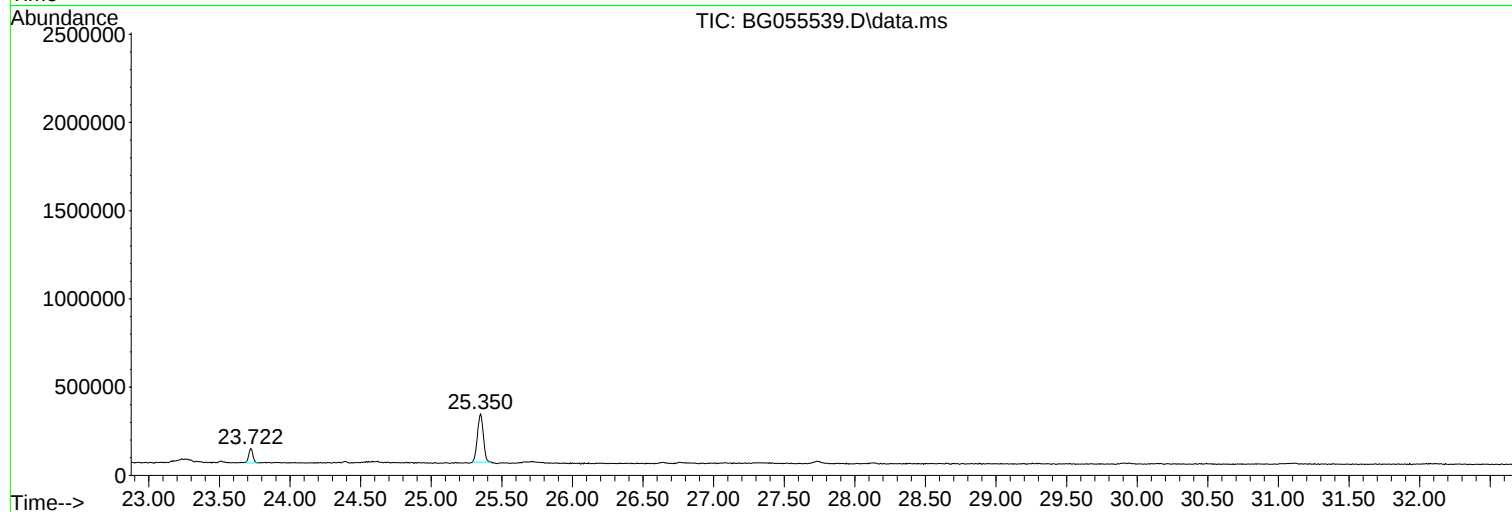
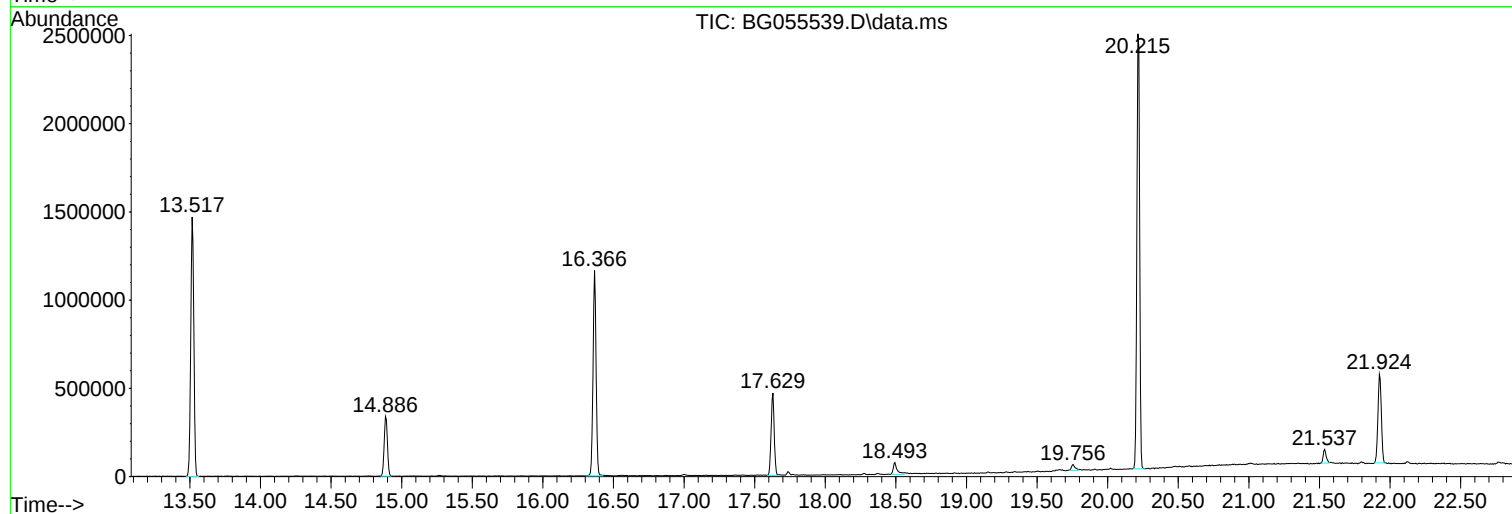
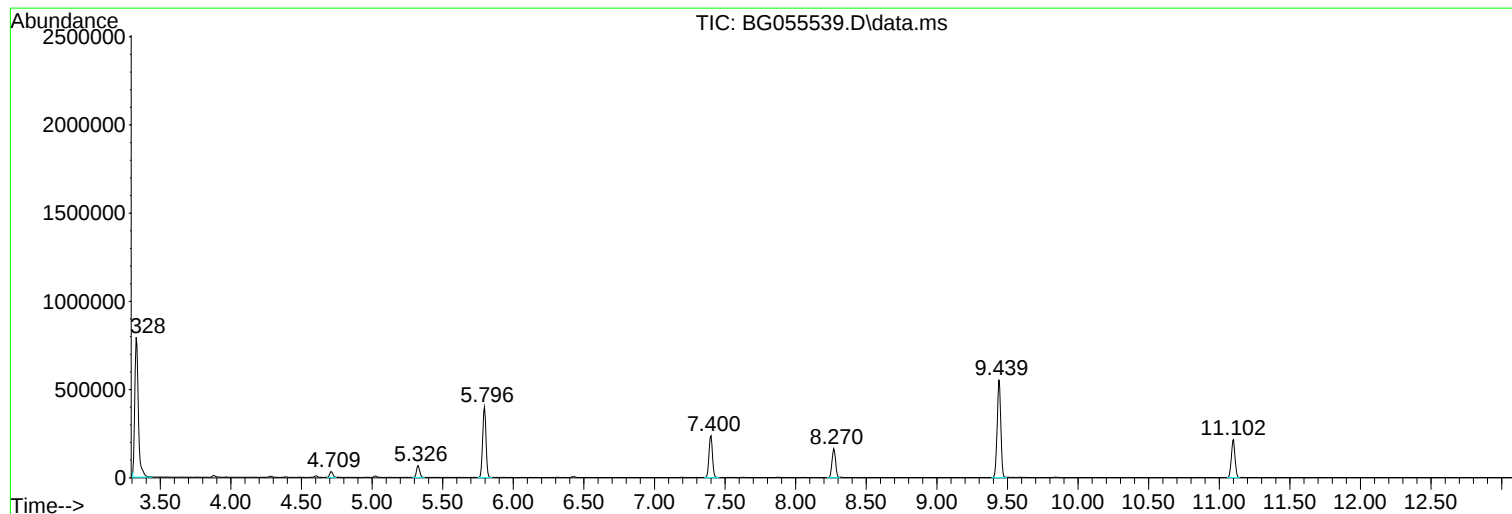
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ALS Vial : 7 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
5592-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG110922.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\BG111022\  
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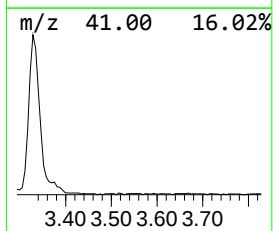
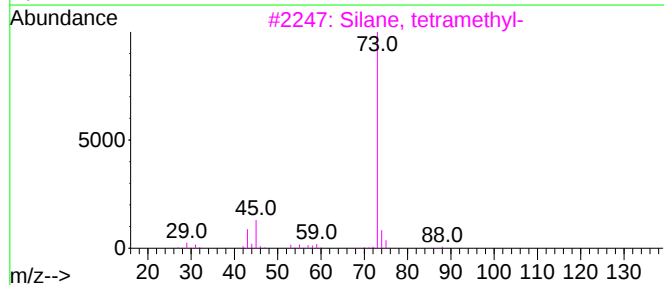
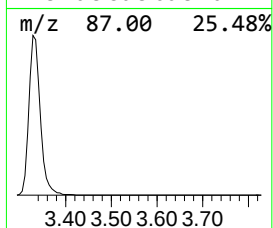
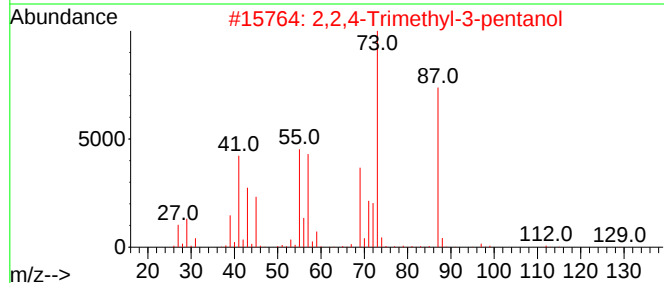
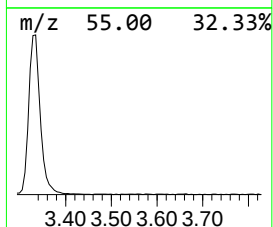
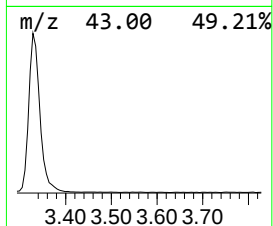
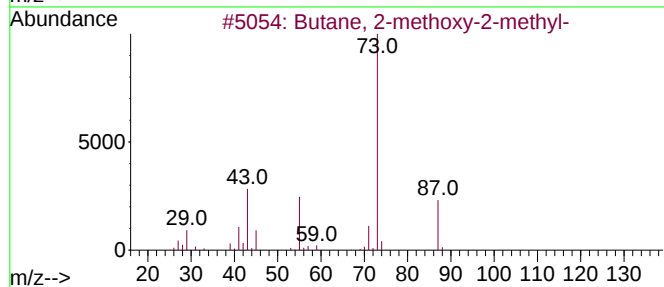
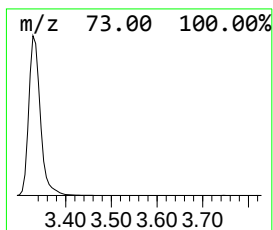
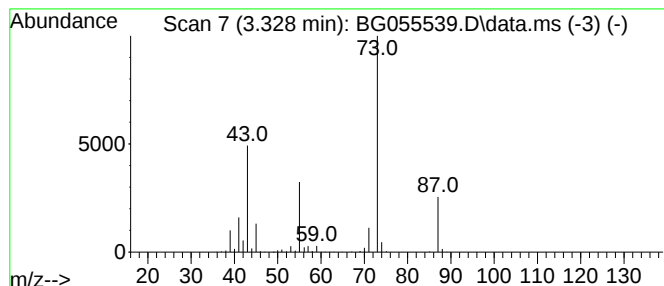
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

| R.T.  | EstConc  | Area    | Relative to ISTD       | R.T.  |
|-------|----------|---------|------------------------|-------|
| 3.328 | 97.36 ng | 1380800 | 1,4-Dichlorobenzene-d4 | 8.270 |

| Hit# | of | 5 | Tentative ID                | MW  | MolForm | CAS#        | Qual |
|------|----|---|-----------------------------|-----|---------|-------------|------|
| 1    |    |   | Butane, 2-methoxy-2-methyl- | 102 | C6H14O  | 000994-05-8 | 78   |
| 2    |    |   | 2,2,4-Trimethyl-3-pentanol  | 130 | C8H18O  | 005162-48-1 | 39   |
| 3    |    |   | Silane, tetramethyl-        | 88  | C4H12Si | 000075-76-3 | 25   |
| 4    |    |   | 1,3-Dioxolane, 2-methyl-    | 88  | C4H8O2  | 000497-26-7 | 25   |
| 5    |    |   | 1,3-Dioxolane, 2-propyl-    | 116 | C6H12O2 | 003390-13-4 | 23   |



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ALS Vial : 7 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
5592-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG110922.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

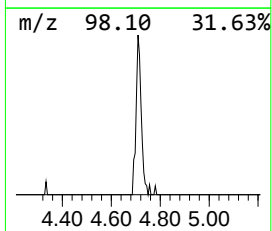
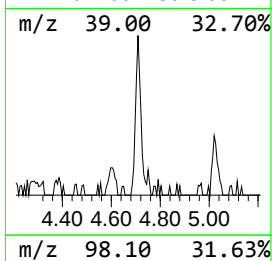
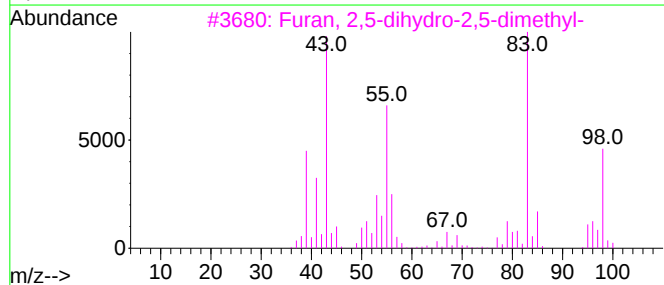
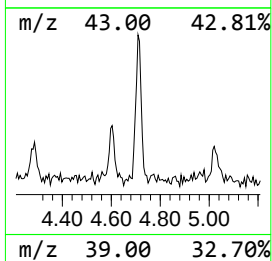
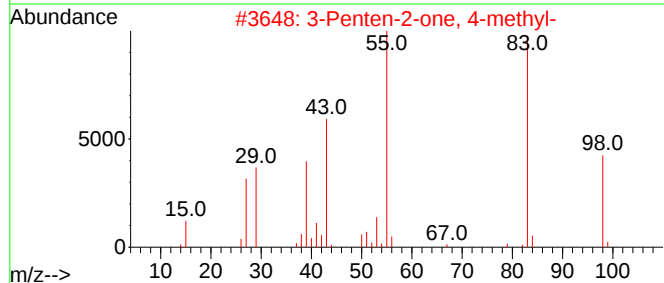
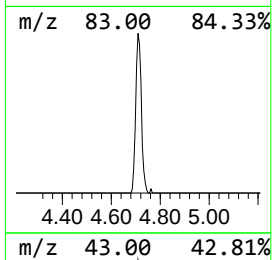
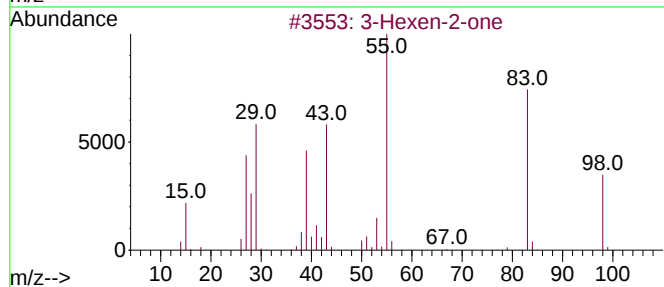
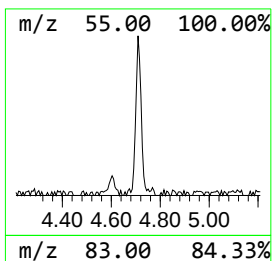
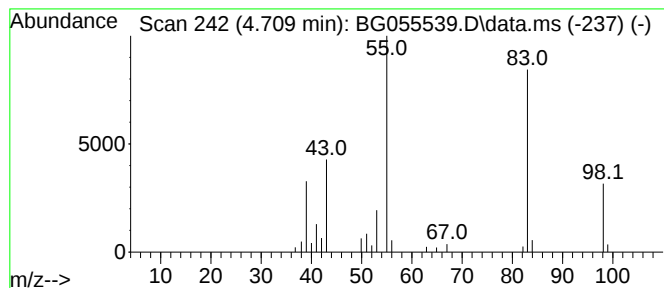
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 3-Hexen-2-one Concentration Rank 5

| R.T.  | EstConc | Area  | Relative to ISTD       | R.T.  |
|-------|---------|-------|------------------------|-------|
| 4.709 | 3.48 ng | 49409 | 1,4-Dichlorobenzene-d4 | 8.270 |

| 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 | 90   |
| 3    |    |   | Furan, 2,5-dihydro-2,5-dimethyl- | 98 | C6H10O  | 059242-27-2 | 80   |
| 4    |    |   | 2-Pentene, 3,4-dimethyl-, (E)-   | 98 | C7H14   | 004914-92-5 | 80   |
| 5    |    |   | 2-Pentene, 3,4-dimethyl-, (Z)-   | 98 | C7H14   | 004914-91-4 | 80   |



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Misc :  
ALS Vial : 7 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
5592-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG110922.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

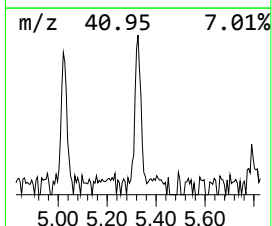
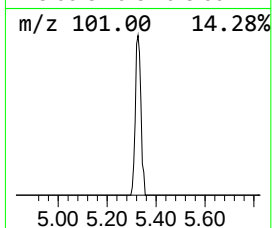
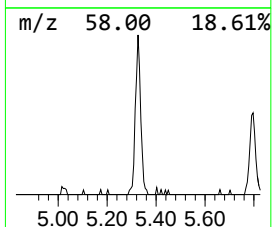
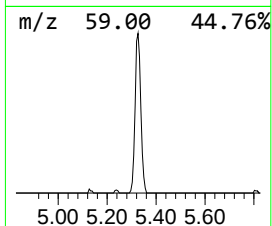
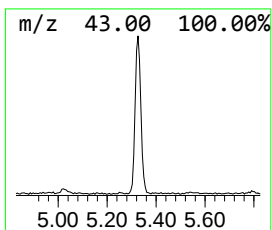
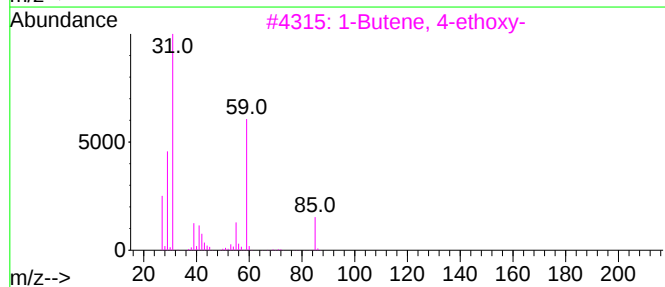
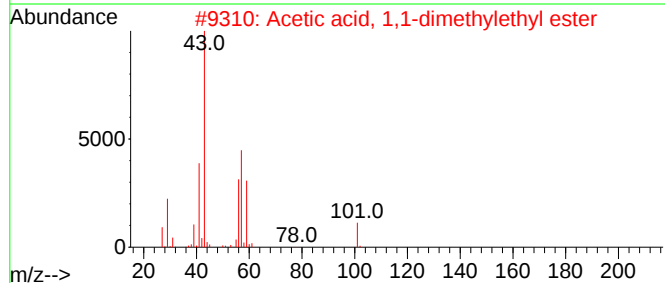
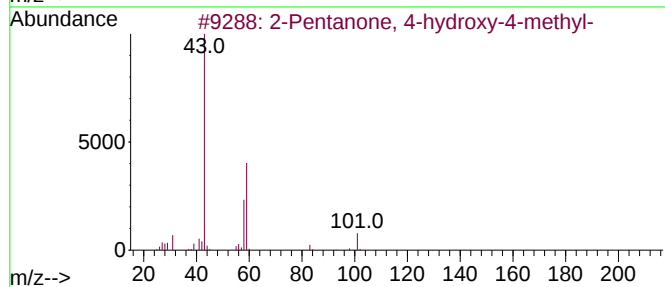
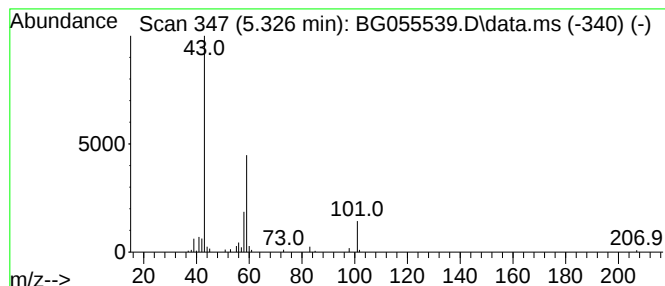
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

| R.T.  | EstConc | Area   | Relative to ISTD       | R.T.  |
|-------|---------|--------|------------------------|-------|
| 5.326 | 7.65 ng | 108515 | 1,4-Dichlorobenzene-d4 | 8.270 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|---------|-------------|------|
| 1    |    |   | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2 | 000123-42-2 | 78   |
| 2    |    |   | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 39   |
| 3    |    |   | 1-Butene, 4-ethoxy-                 | 100 | C6H12O  | 044611-46-3 | 23   |
| 4    |    |   | Acetone                             | 58  | C3H6O   | 000067-64-1 | 22   |
| 5    |    |   | 2,3-Butanedione, monooxime          | 101 | C4H7NO2 | 000057-71-6 | 16   |



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Misc :  
ALS Vial : 7 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
5592-4

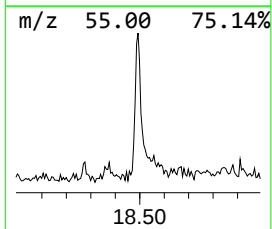
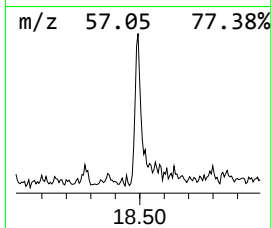
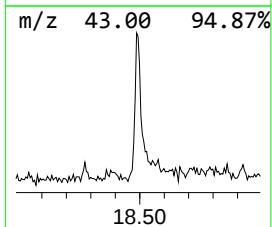
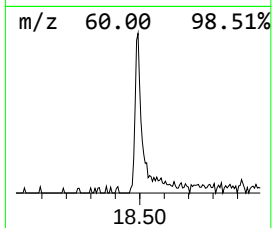
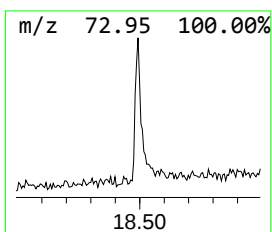
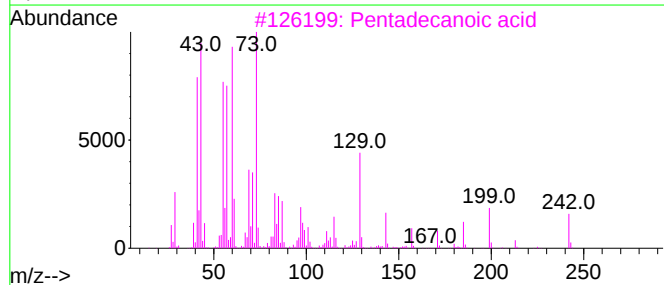
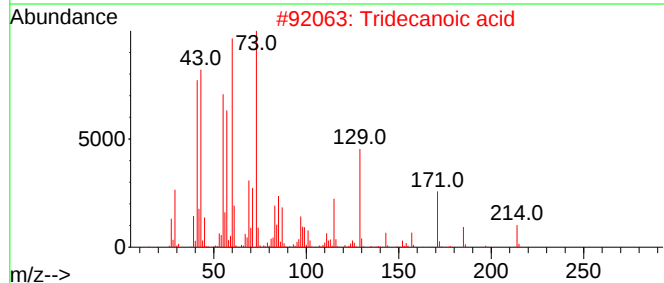
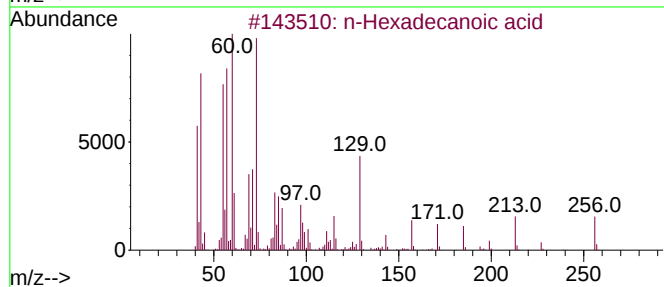
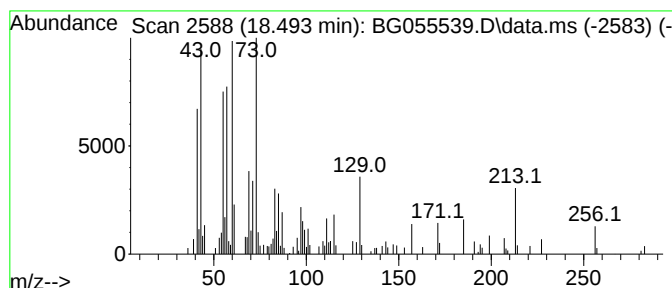
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG110922.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

| R.T.      | EstConc             | Area   | Relative to ISTD | R.T.        |      |
|-----------|---------------------|--------|------------------|-------------|------|
| 18.493    | 3.72 ng             | 132108 | Phenanthrene-d10 | 17.629      |      |
| Hit# of 5 | Tentative ID        | MW     | MolForm          | CAS#        | Qual |
| 1         | n-Hexadecanoic acid | 256    | C16H32O2         | 000057-10-3 | 99   |
| 2         | Tridecanoic acid    | 214    | C13H26O2         | 000638-53-9 | 95   |
| 3         | Pentadecanoic acid  | 242    | C15H30O2         | 001002-84-2 | 83   |
| 4         | Tetradecanoic acid  | 228    | C14H28O2         | 000544-63-8 | 72   |
| 5         | n-Decanoic acid     | 172    | C10H20O2         | 000334-48-5 | 70   |



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Instrument :  
BNA\_G  
ClientSampleId :  
5592-4

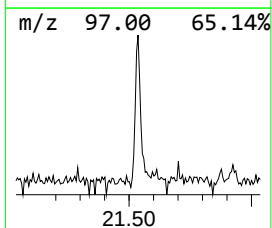
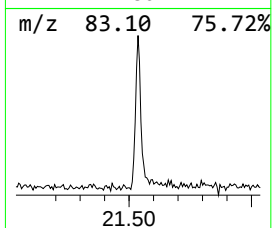
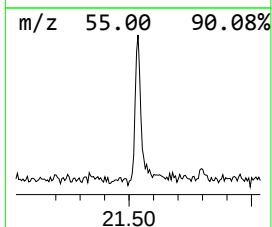
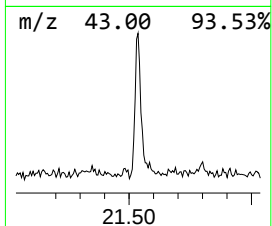
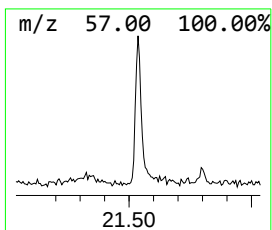
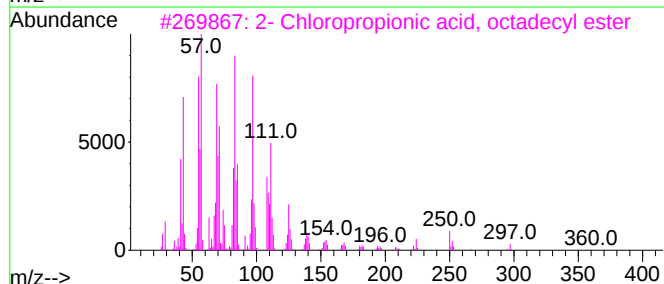
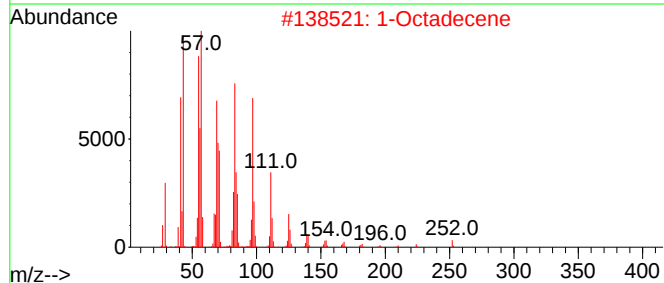
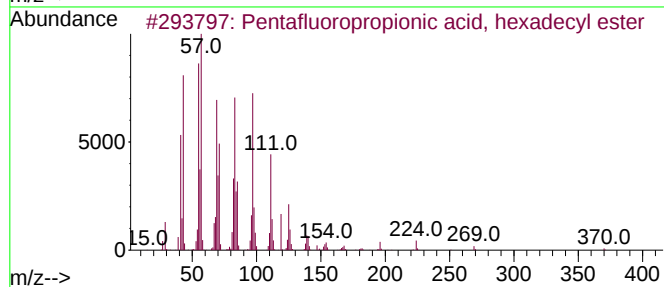
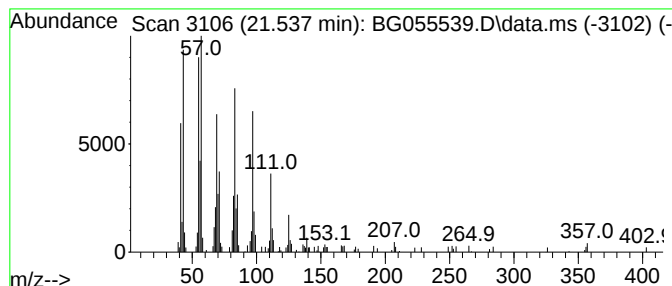
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG110922.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 5 Pentafluoropropionic acid, ... Concentration Rank 6

| R.T.      | EstConc                                                                  | Area   | Relative to ISTD | R.T.        |      |
|-----------|--------------------------------------------------------------------------|--------|------------------|-------------|------|
| 21.537    | 2.74 ng                                                                  | 115127 | Chrysene-d12     | 21.924      |      |
| Hit# of 5 | Tentative ID                                                             | MW     | MolForm          | CAS#        | Qual |
| 1         | Pentafluoropropionic acid, hexadecanoic acid, 2,2,3,3,4,4,4-heptafluoro- | 388    | C19H33F5O2       | 006222-07-7 | 91   |
| 2         | 1-Octadecene                                                             | 252    | C18H36           | 000112-88-9 | 91   |
| 3         | 2- Chloropropionic acid, octadecanoic acid, 2,2,3,3,4,4,4-heptafluoro-   | 360    | C21H41ClO2       | 088104-31-8 | 91   |
| 4         | Pentafluoropropionic acid, octadecanoic acid, 2,2,3,3,4,4,4-heptafluoro- | 416    | C21H37F5O2       | 959261-25-7 | 90   |
| 5         | 5-Eicosene, (E)-                                                         | 280    | C20H40           | 074685-30-6 | 87   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG111022\  
Data File : BG055539.D  
Acq On : 10 Nov 2022 14:29  
Operator : CG/JU  
Sample : N5474-02  
Misc :  
ALS Vial : 7 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
5592-4

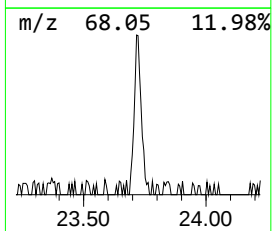
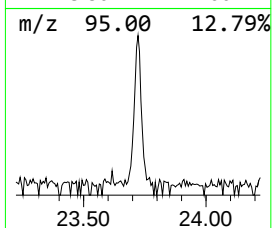
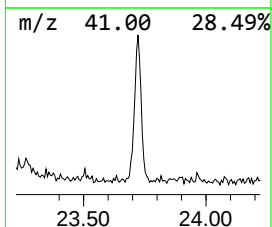
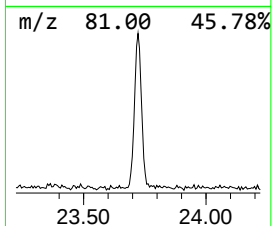
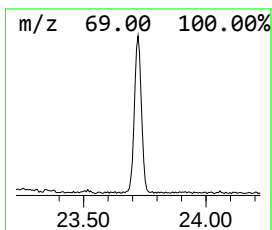
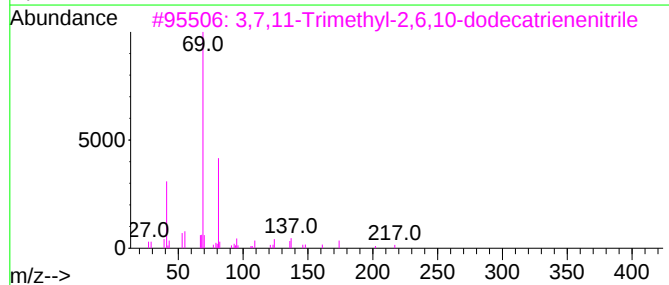
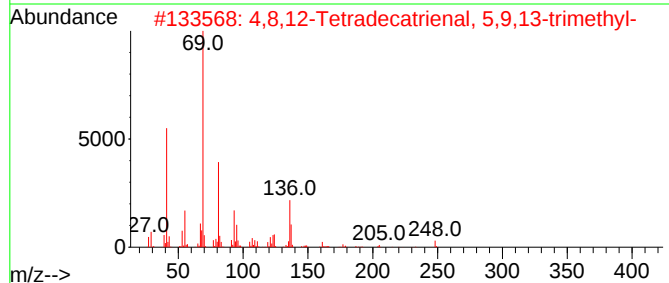
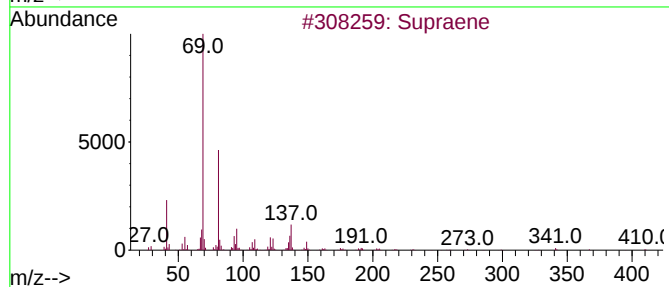
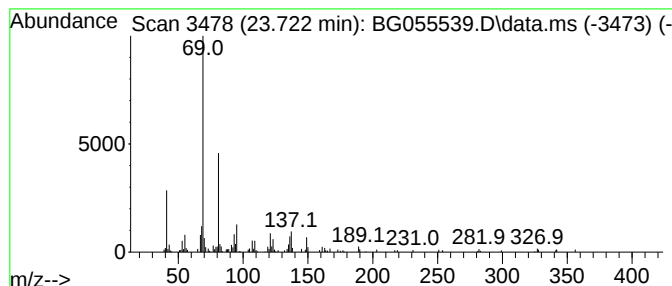
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 6 Supraene Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 23.722 | 4.18 ng | 165377 | Perylene-d12     | 25.350 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | Supraene                            | 410 | C30H50   | 007683-64-9 | 83   |
| 2    |    |   | 4,8,12-Tetradecatrienal, 5,9,13-... | 248 | C17H28O  | 066408-55-7 | 64   |
| 3    |    |   | 3,7,11-Trimethyl-2,6,10-dodecatr... | 217 | C15H23N  | 029789-67-1 | 64   |
| 4    |    |   | 3-Cyclohexene-1-carboxaldehyde, ... | 192 | C13H20O  | 052475-89-5 | 64   |
| 5    |    |   | 2,3,5-Trimethyl-2,3,5-hexanetric... | 203 | C12H17N3 | 003974-79-6 | 59   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG111022\  
Data File : BG055539.D  
Acq On : 10 Nov 2022 14:29  
Operator : CG/JU  
Sample : N5474-02  
Misc :  
ALS Vial : 7 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
5592-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG110922.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| Butane, 2-metho... | 3.328  | 97.4    | ng    | 1380800  | 1                     | 8.270  | 283642 | 20.0 |
| 3-Hexen-2-one      | 4.709  | 3.5     | ng    | 49409    | 1                     | 8.270  | 283642 | 20.0 |
| 2-Pentanone, 4-... | 5.326  | 7.7     | ng    | 108515   | 1                     | 8.270  | 283642 | 20.0 |
| n-Hexadecanoic ... | 18.493 | 3.7     | ng    | 132108   | 4                     | 17.629 | 711102 | 20.0 |
| Pentafluoroprop... | 21.537 | 2.7     | ng    | 115127   | 5                     | 21.924 | 839894 | 20.0 |
| Supraene           | 23.722 | 4.2     | ng    | 165377   | 6                     | 25.350 | 790681 | 20.0 |