

Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG111022\  
 Data File : BG055547.D  
 Acq On : 10 Nov 2022 20:16  
 Operator : CG/JU  
 Sample : N5474-01  
 Misc :  
 ALS Vial : 7 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 5592-3

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: BG055547.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         | 3.329       | 3             | 7           | 23           | rVB      | 581627         | 988483        | 40.14%          | 8.040%        |
| 2         | 4.710       | 237           | 242         | 249          | rBV      | 28165          | 39902         | 1.62%           | 0.325%        |
| 3         | 5.327       | 340           | 347         | 353          | rBV      | 65126          | 102882        | 4.18%           | 0.837%        |
| 4         | 5.791       | 419           | 426         | 435          | rVB      | 276328         | 452649        | 18.38%          | 3.682%        |
| 5         | 7.395       | 691           | 699         | 707          | rBV      | 183298         | 318249        | 12.92%          | 2.589%        |
| 6         | 8.270       | 841           | 848         | 861          | rVB      | 164481         | 277675        | 11.28%          | 2.259%        |
| 7         | 9.439       | 1039          | 1047        | 1058         | rBV      | 484391         | 862321        | 35.02%          | 7.014%        |
| 8         | 11.096      | 1319          | 1329        | 1337         | rBV      | 211092         | 381821        | 15.50%          | 3.106%        |
| 9         | 13.517      | 1734          | 1741        | 1748         | rVB      | 1223183        | 1852255       | 75.21%          | 15.066%       |
| 10        | 14.886      | 1966          | 1974        | 1981         | rVB      | 347801         | 534552        | 21.71%          | 4.348%        |
| 11        | 16.361      | 2218          | 2225        | 2234         | rBV      | 837858         | 1244291       | 50.53%          | 10.121%       |
| 12        | 17.624      | 2434          | 2440        | 2447         | rBV      | 463077         | 683589        | 27.76%          | 5.560%        |
| 13        | 18.488      | 2582          | 2587        | 2597         | rBV2     | 87489          | 147960        | 6.01%           | 1.203%        |
| 14        | 19.151      | 2697          | 2700        | 2704         | rBV4     | 22716          | 25272         | 1.03%           | 0.206%        |
| 15        | 19.751      | 2797          | 2802        | 2812         | rBV3     | 51372          | 94914         | 3.85%           | 0.772%        |
| 16        | 20.215      | 2875          | 2881        | 2888         | rVB      | 1834693        | 2462615       | 100.00%         | 20.031%       |
| 17        | 21.531      | 3101          | 3105        | 3110         | rBV3     | 55002          | 81792         | 3.32%           | 0.665%        |
| 18        | 21.919      | 3165          | 3171        | 3182         | rVB2     | 479024         | 820138        | 33.30%          | 6.671%        |
| 19        | 23.711      | 3472          | 3476        | 3482         | rVB2     | 40379          | 80522         | 3.27%           | 0.655%        |
| 20        | 25.338      | 3743          | 3753        | 3769         | rVB2     | 275468         | 842364        | 34.21%          | 6.852%        |

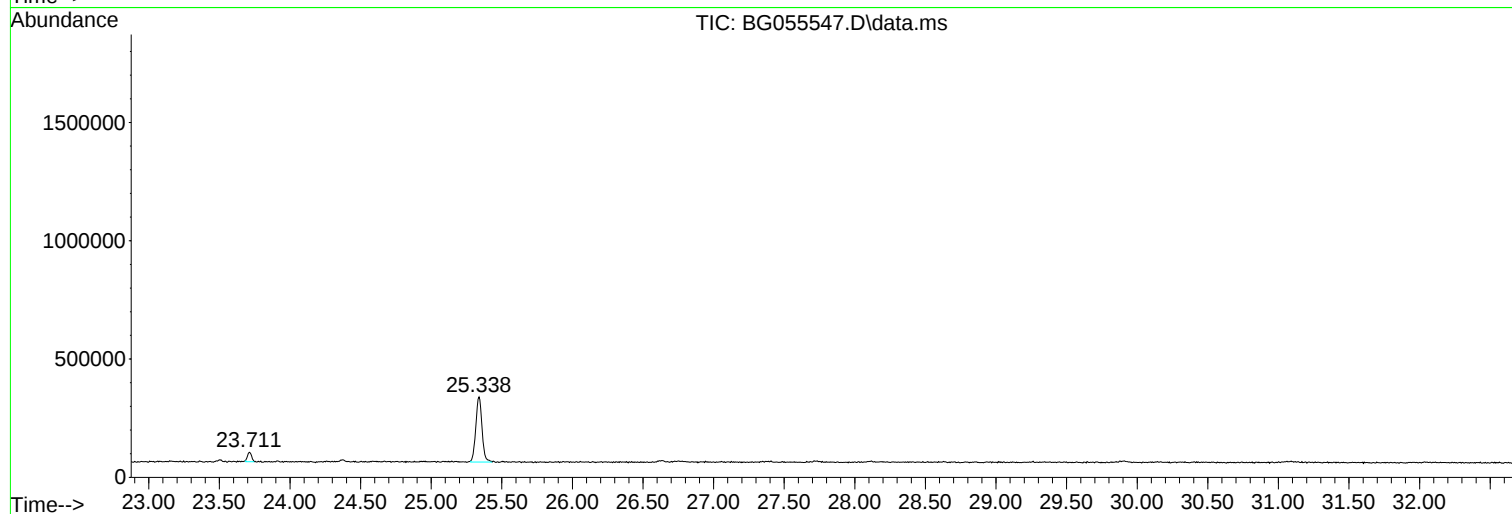
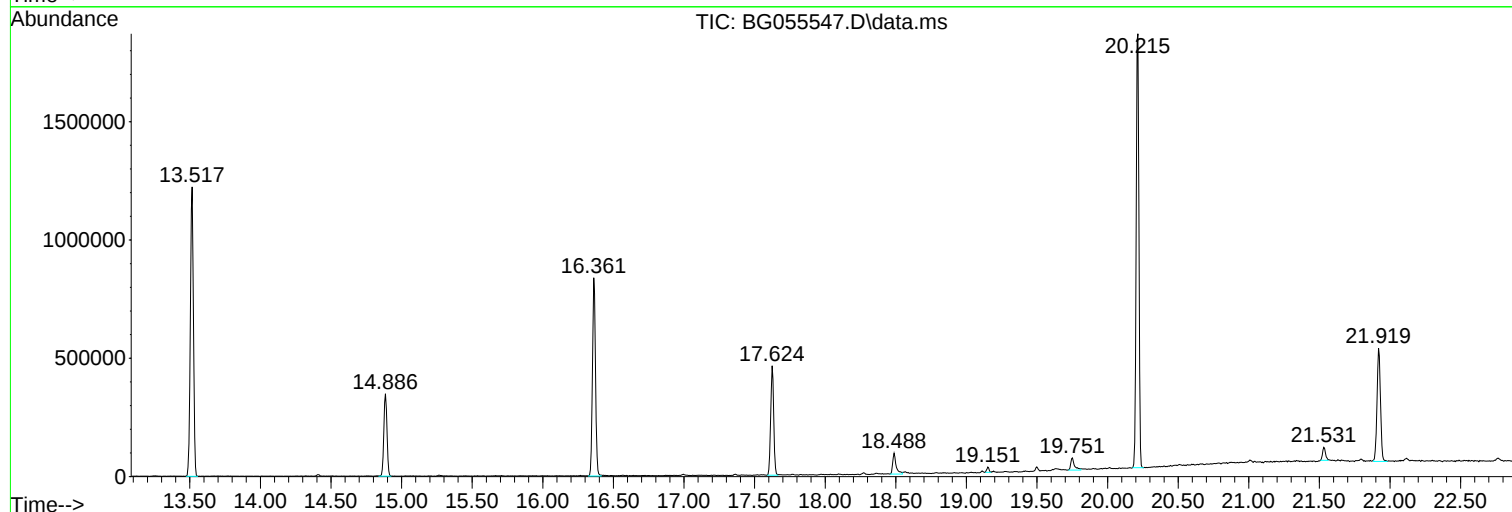
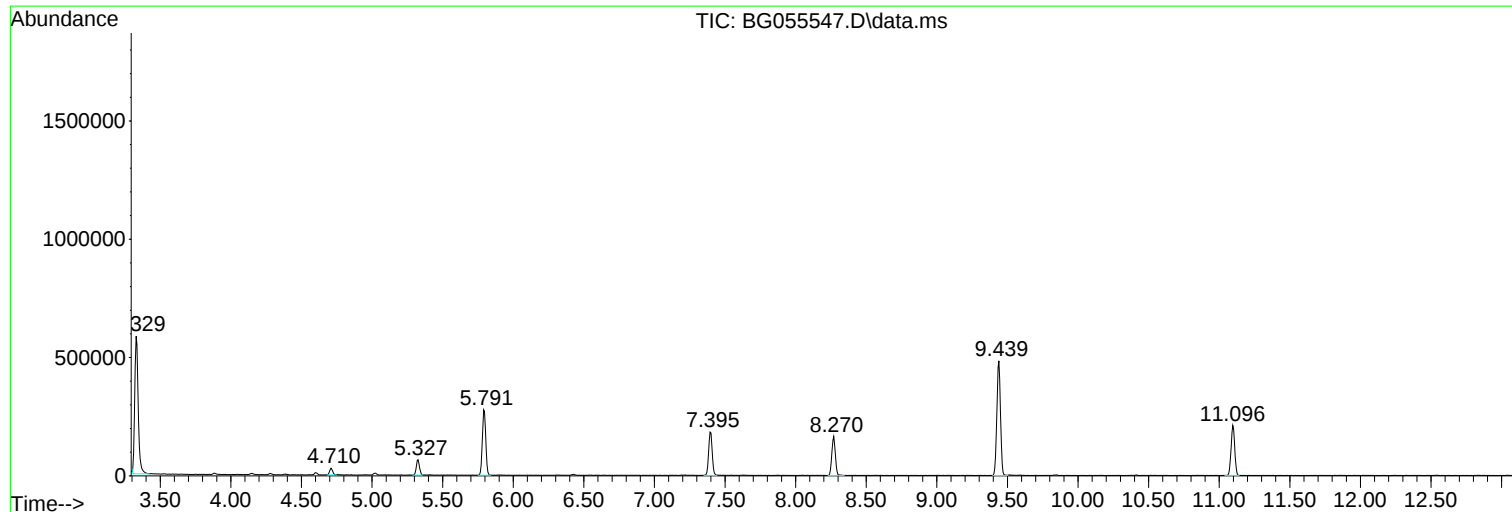
Sum of corrected areas: 12294246

Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG111022\  
Data File : BG055547.D  
Acq On : 10 Nov 2022 20:16  
Operator : CG/JU  
Sample : N5474-01  
Misc :  
ALS Vial : 7 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
5592-3

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\  
Data File : BG055547.D  
Acq On : 10 Nov 2022 20:16  
Operator : CG/JU  
Sample : N5474-01  
Misc :  
ALS Vial : 7 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
5592-3

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

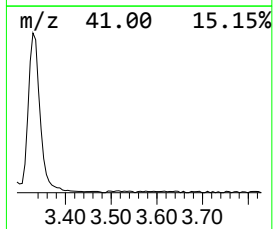
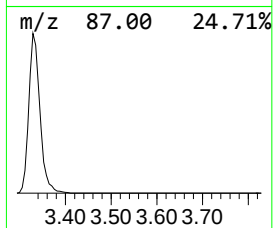
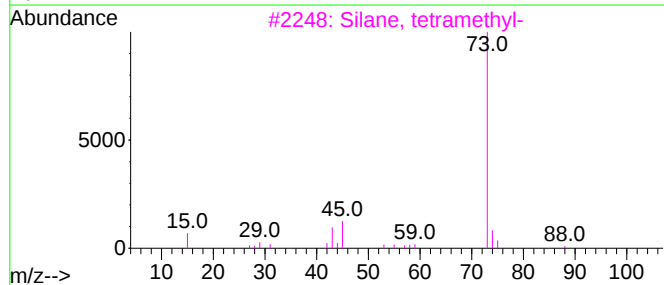
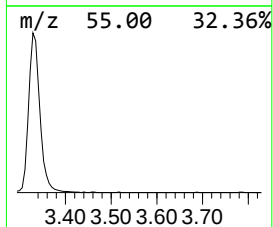
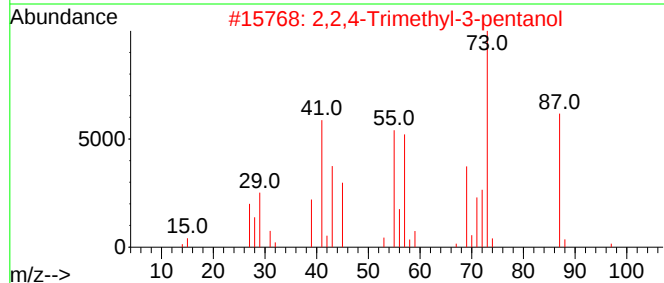
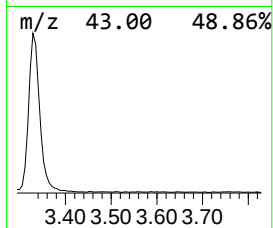
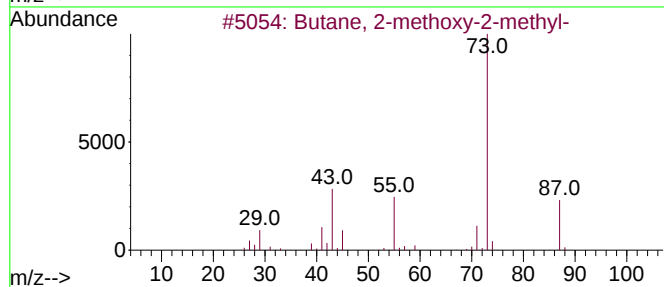
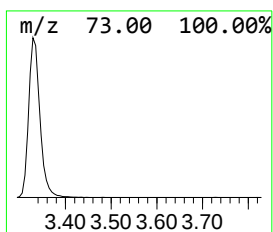
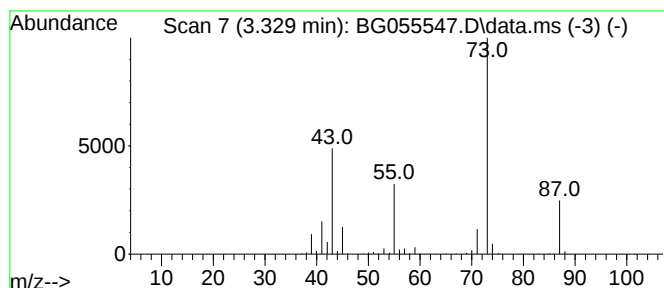
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*

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

| R.T.  | EstConc  | Area   | Relative to ISTD       | R.T.  |
|-------|----------|--------|------------------------|-------|
| 3.329 | 71.20 ng | 988483 | 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 | 17   |
| 4    |    |   | Pentane, 3-methoxy-         | 102 | C6H14O  | 036839-67-5 | 12   |
| 5    |    |   | 1,3-Dioxolane, 2-methyl-    | 88  | C4H8O2  | 000497-26-7 | 9    |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG111022\  
Data File : BG055547.D  
Acq On : 10 Nov 2022 20:16  
Operator : CG/JU  
Sample : N5474-01  
Misc :  
ALS Vial : 7 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
5592-3

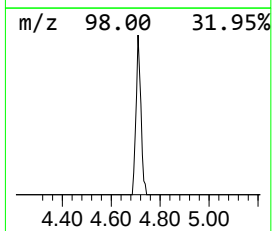
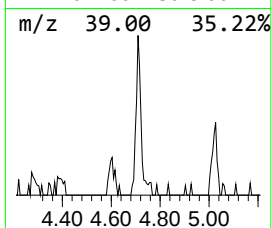
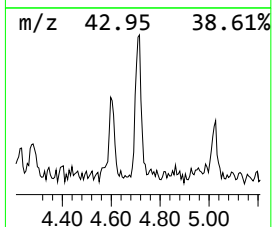
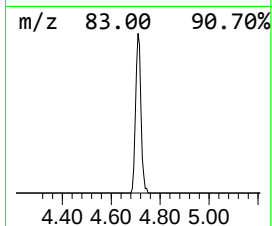
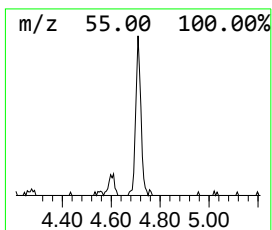
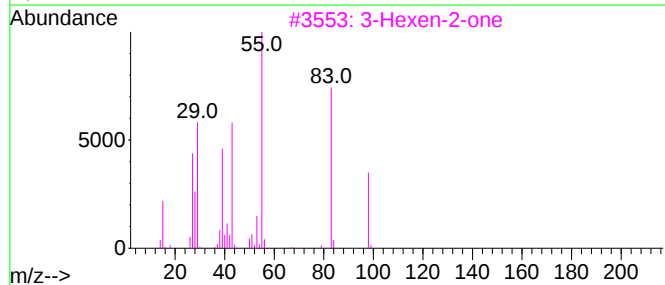
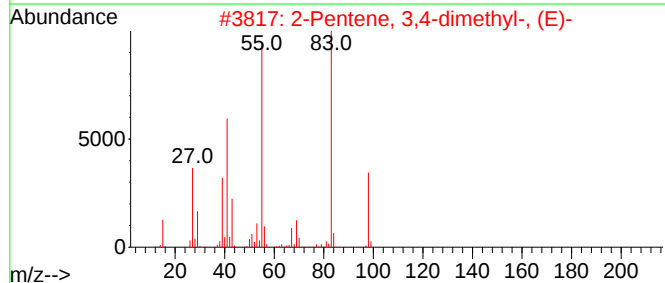
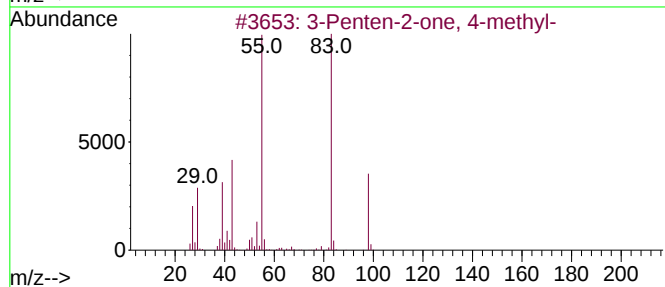
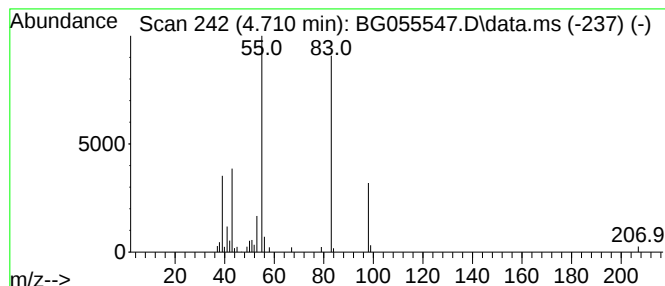
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG110922.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

| R.T.  | EstConc | Area  | Relative to ISTD       | R.T.  |
|-------|---------|-------|------------------------|-------|
| 4.710 | 2.87 ng | 39902 | 1,4-Dichlorobenzene-d4 | 8.270 |

| Hit# | of 5 | Tentative ID                   | MW | MolForm | CAS#        | Qual |
|------|------|--------------------------------|----|---------|-------------|------|
| 1    |      | 3-Penten-2-one, 4-methyl-      | 98 | C6H10O  | 000141-79-7 | 91   |
| 2    |      | 2-Pentene, 3,4-dimethyl-, (E)- | 98 | C7H14   | 004914-92-5 | 90   |
| 3    |      | 3-Hexen-2-one                  | 98 | C6H10O  | 000763-93-9 | 90   |
| 4    |      | 2-Pentene, 4,4-dimethyl-, (E)- | 98 | C7H14   | 000690-08-4 | 90   |
| 5    |      | 2-Pentene, 2,4-dimethyl-       | 98 | C7H14   | 000625-65-0 | 86   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG111022\  
Data File : BG055547.D  
Acq On : 10 Nov 2022 20:16  
Operator : CG/JU  
Sample : N5474-01  
Misc :  
ALS Vial : 7 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
5592-3

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

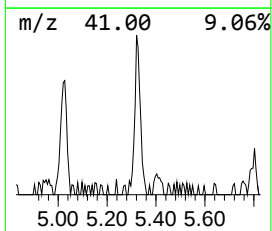
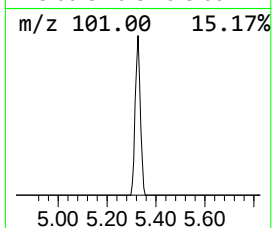
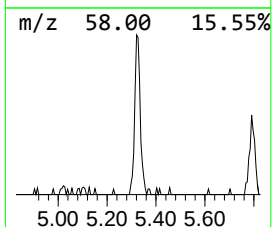
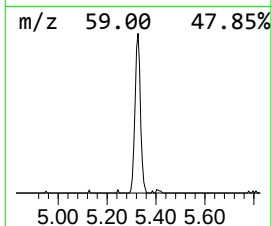
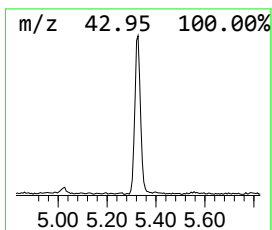
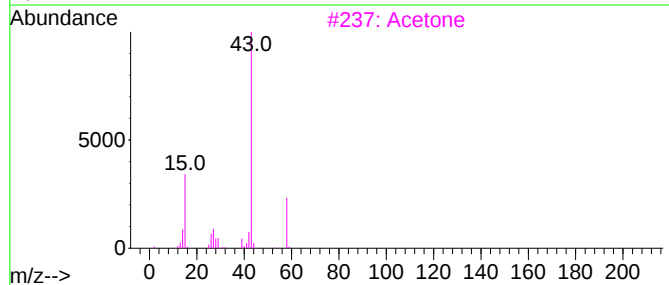
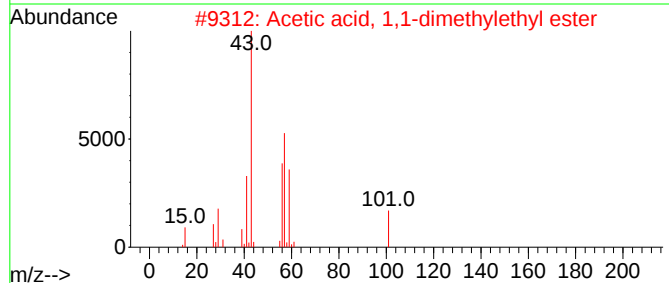
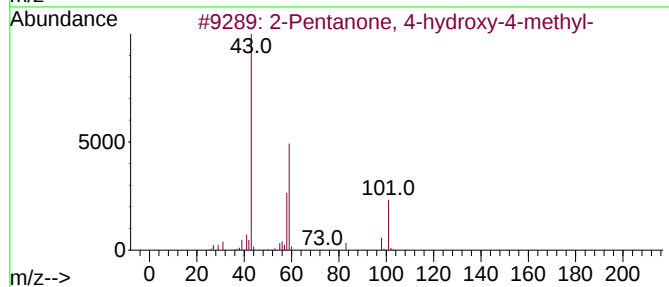
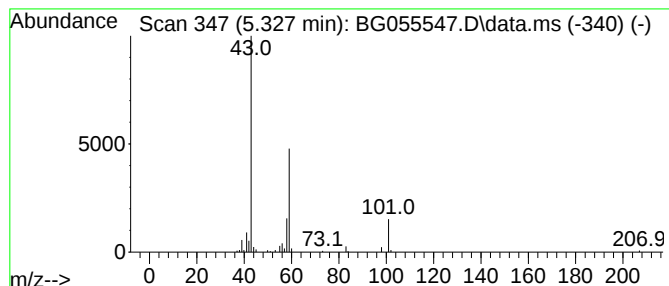
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*

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

| R.T.  | EstConc | Area   | Relative to ISTD       | R.T.  |
|-------|---------|--------|------------------------|-------|
| 5.327 | 7.41 ng | 102882 | 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 | 56   |
| 2    |    |   | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 38   |
| 3    |    |   | Acetone                             | 58  | C3H6O   | 000067-64-1 | 12   |
| 4    |    |   | 1-Propen-2-ol, acetate              | 100 | C5H8O2  | 000108-22-5 | 12   |
| 5    |    |   | Formamide, N,N-diethyl-             | 101 | C5H11NO | 000617-84-5 | 9    |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG111022\  
Data File : BG055547.D  
Acq On : 10 Nov 2022 20:16  
Operator : CG/JU  
Sample : N5474-01  
Misc :  
ALS Vial : 7 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
5592-3

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

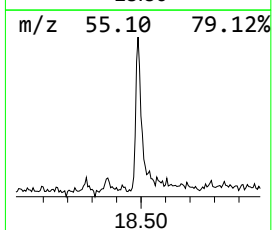
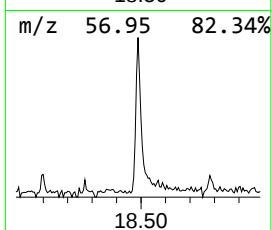
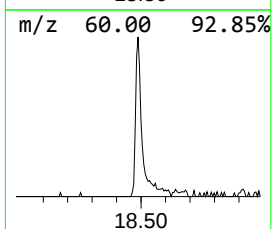
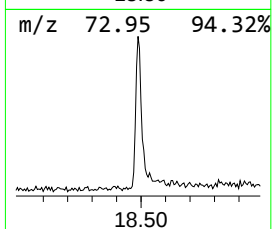
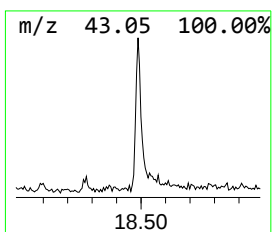
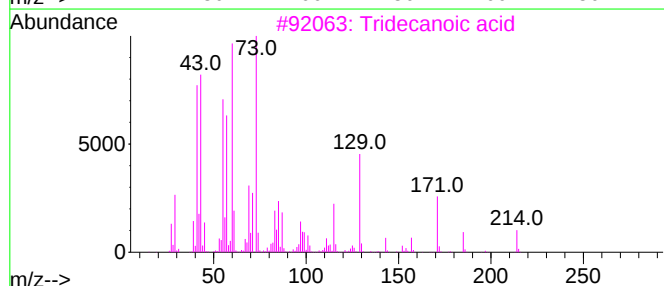
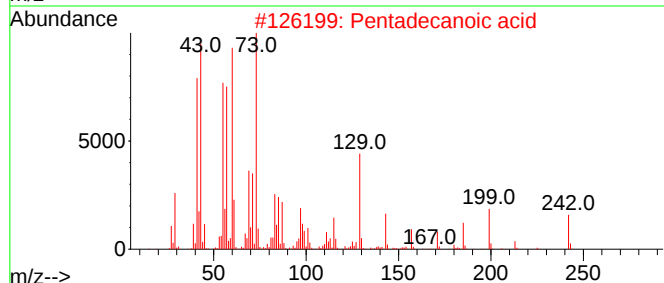
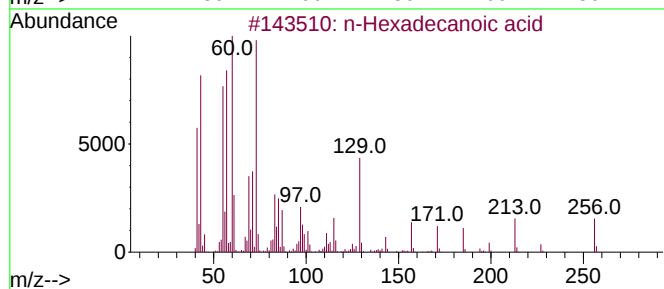
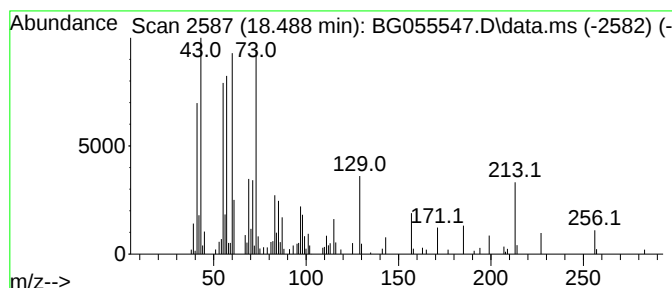
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 18.488 | 4.33 ng | 147960 | Phenanthrene-d10 | 17.624 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 99   |
| 2    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 74   |
| 3    |    |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 70   |
| 4    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 64   |
| 5    |    |   | Dodecanoic acid     | 200 | C12H24O2 | 000143-07-7 | 52   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG111022\  
Data File : BG055547.D  
Acq On : 10 Nov 2022 20:16  
Operator : CG/JU  
Sample : N5474-01  
Misc :  
ALS Vial : 7 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
5592-3

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

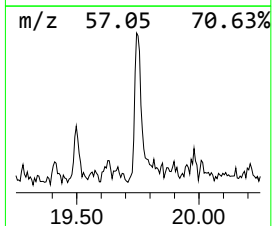
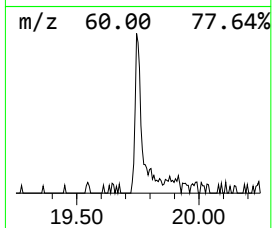
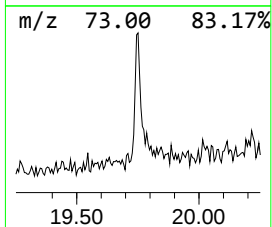
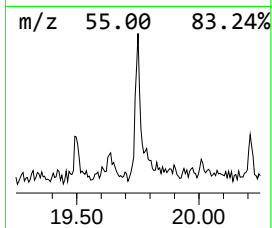
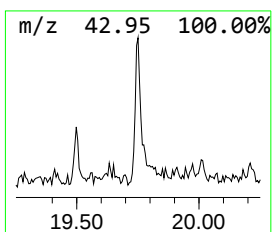
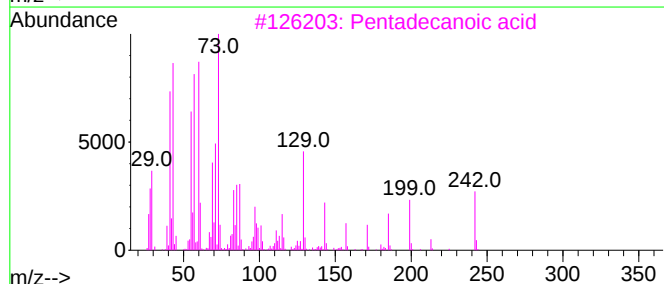
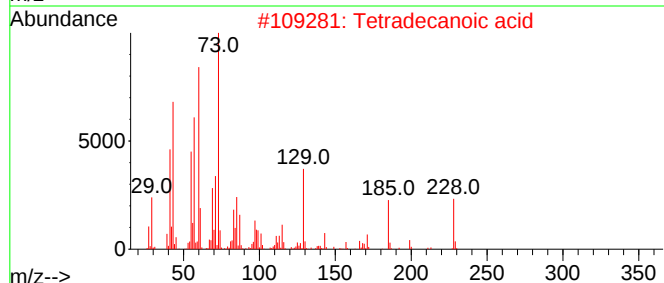
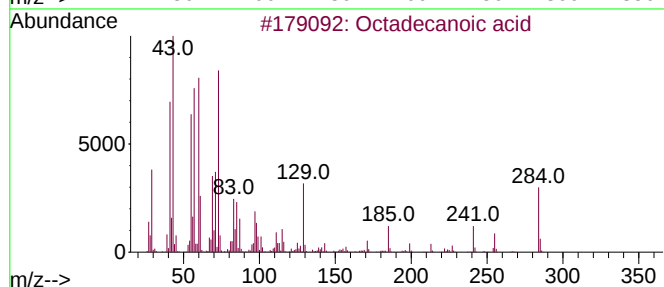
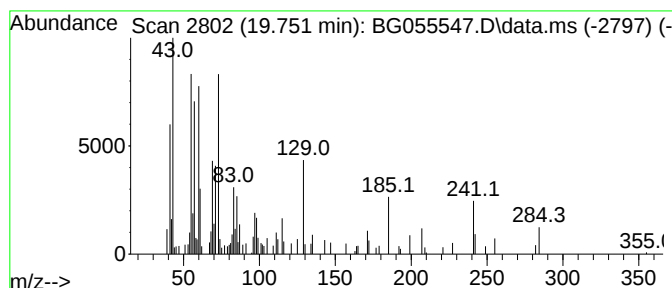
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*

Peak Number 5 Octadecanoic acid Concentration Rank 5

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 19.751 | 2.78 ng | 94914 | Phenanthrene-d10 | 17.624 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | Octadecanoic acid   | 284 | C18H36O2 | 000057-11-4 | 98   |
| 2    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 72   |
| 3    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 64   |
| 4    |    |   | n-Decanoic acid     | 172 | C10H20O2 | 000334-48-5 | 53   |
| 5    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 53   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG111022\  
Data File : BG055547.D  
Acq On : 10 Nov 2022 20:16  
Operator : CG/JU  
Sample : N5474-01  
Misc :  
ALS Vial : 7 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
5592-3

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

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| Butane, 2-metho... | 3.329  | 71.2    | ng    | 988483   | 1                     | 8.270  | 277675 | 20.0 |
| 3-Penten-2-one,... | 4.710  | 2.9     | ng    | 39902    | 1                     | 8.270  | 277675 | 20.0 |
| 2-Pentanone, 4-... | 5.327  | 7.4     | ng    | 102882   | 1                     | 8.270  | 277675 | 20.0 |
| n-Hexadecanoic ... | 18.488 | 4.3     | ng    | 147960   | 4                     | 17.624 | 683589 | 20.0 |
| Octadecanoic acid  | 19.751 | 2.8     | ng    | 94914    | 4                     | 17.624 | 683589 | 20.0 |