

Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG011823\  
 Data File : BG056337.D  
 Acq On : 18 Jan 2023 20:51  
 Operator : CG/JU  
 Sample : 01159-04  
 Misc :  
 ALS Vial : 9 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 MH-6

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-BG122722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG056337.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         | 3.317       | 3             | 5           | 15           | rVB      | 125976         | 151471        | 6.11%           | 1.441%        |
| 2         | 5.344       | 343           | 350         | 358          | rBB      | 88961          | 137969        | 5.57%           | 1.313%        |
| 3         | 5.826       | 424           | 432         | 445          | rBV      | 360901         | 591404        | 23.86%          | 5.627%        |
| 4         | 7.441       | 700           | 707         | 719          | rVB      | 377231         | 644380        | 26.00%          | 6.131%        |
| 5         | 8.305       | 847           | 854         | 863          | rBB      | 110293         | 186425        | 7.52%           | 1.774%        |
| 6         | 9.480       | 1046          | 1054        | 1064         | rBB      | 214035         | 387754        | 15.64%          | 3.690%        |
| 7         | 11.137      | 1328          | 1336        | 1346         | rBV      | 150375         | 263560        | 10.63%          | 2.508%        |
| 8         | 13.546      | 1739          | 1746        | 1753         | rBV      | 828730         | 1261621       | 50.90%          | 12.005%       |
| 9         | 14.921      | 1972          | 1980        | 1986         | rBV      | 290508         | 462360        | 18.65%          | 4.399%        |
| 10        | 16.255      | 2201          | 2207        | 2215         | rVB      | 197918         | 273269        | 11.02%          | 2.600%        |
| 11        | 16.396      | 2225          | 2231        | 2241         | rBV      | 691395         | 1052285       | 42.45%          | 10.013%       |
| 12        | 17.653      | 2439          | 2445        | 2452         | rBV      | 452825         | 683013        | 27.55%          | 6.499%        |
| 13        | 18.499      | 2585          | 2589        | 2599         | rBV2     | 89090          | 123680        | 4.99%           | 1.177%        |
| 14        | 19.756      | 2798          | 2803        | 2806         | rBV4     | 18500          | 26795         | 1.08%           | 0.255%        |
| 15        | 20.226      | 2877          | 2883        | 2889         | rBV      | 1869462        | 2478745       | 100.00%         | 23.586%       |
| 16        | 21.525      | 3100          | 3104        | 3111         | rBV      | 99682          | 148275        | 5.98%           | 1.411%        |
| 17        | 21.789      | 3145          | 3149        | 3156         | rVB      | 21135          | 37404         | 1.51%           | 0.356%        |
| 18        | 21.948      | 3169          | 3176        | 3188         | rVB2     | 451382         | 805057        | 32.48%          | 7.660%        |
| 19        | 25.379      | 3751          | 3760        | 3772         | rVB2     | 258790         | 793928        | 32.03%          | 7.554%        |

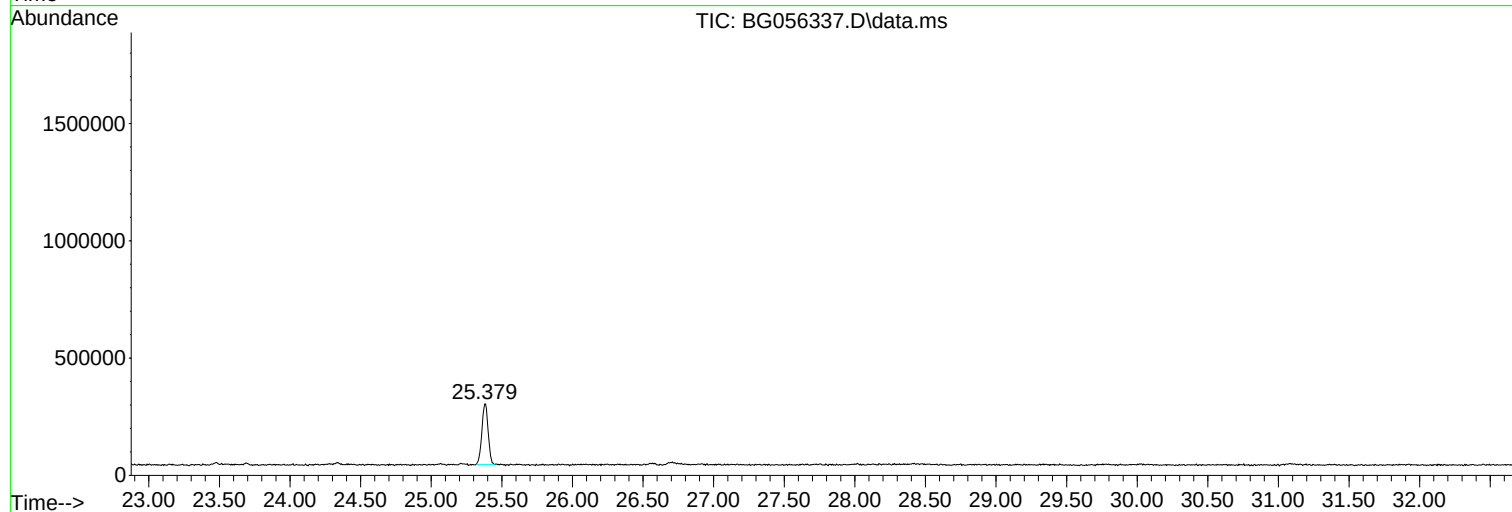
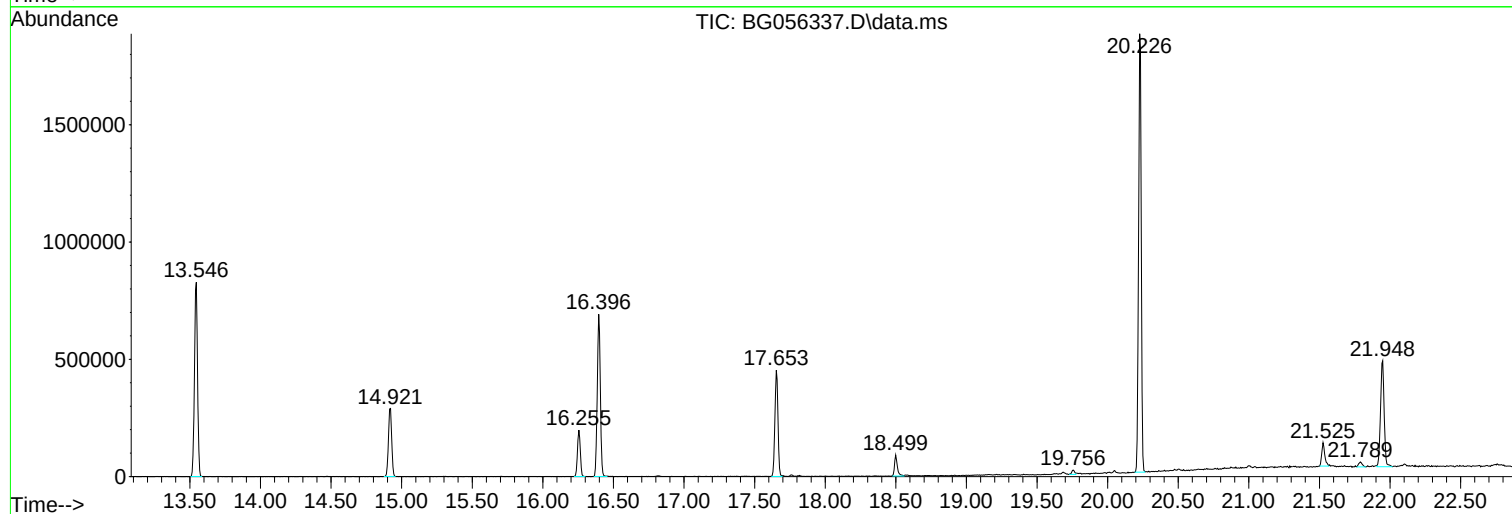
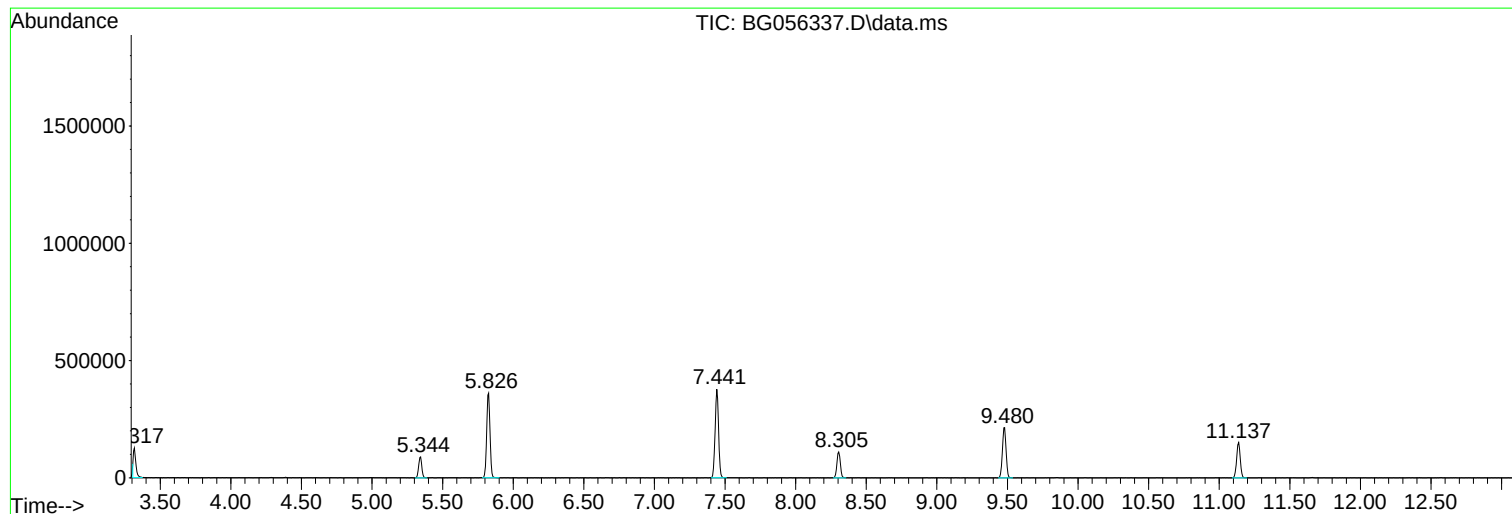
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ALS Vial : 9 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
MH-6

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG122722.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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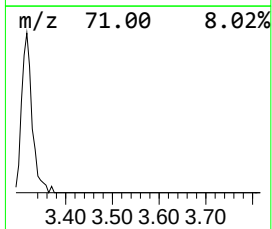
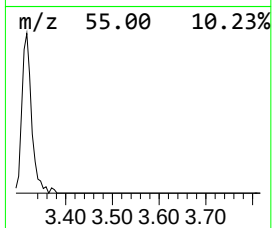
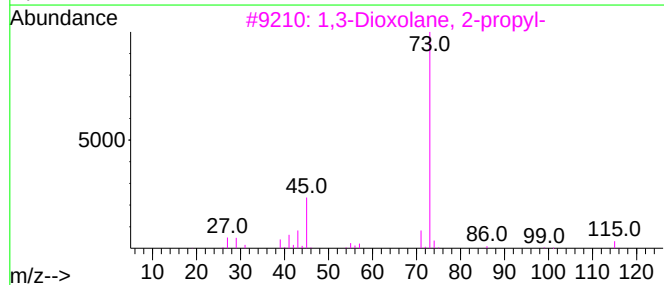
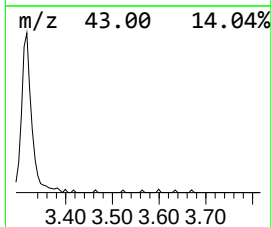
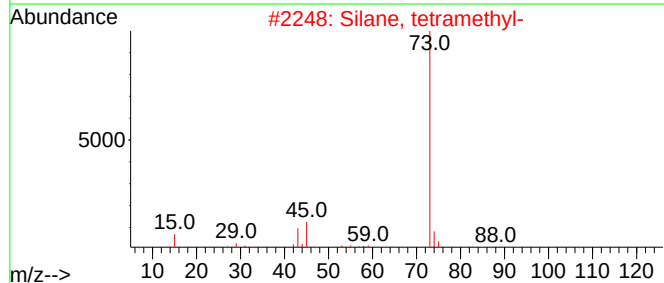
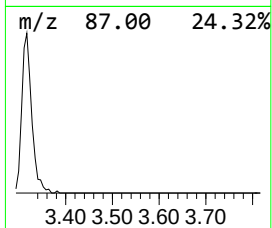
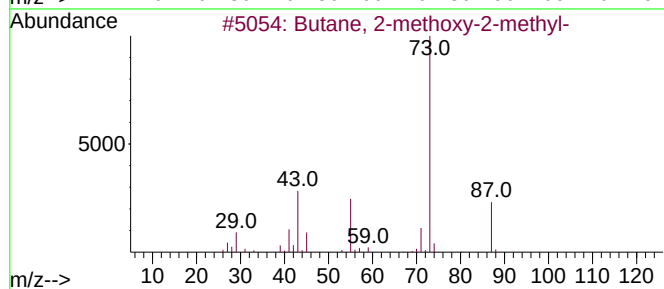
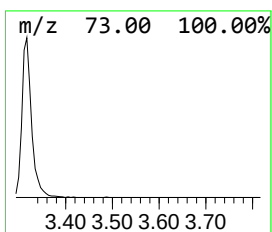
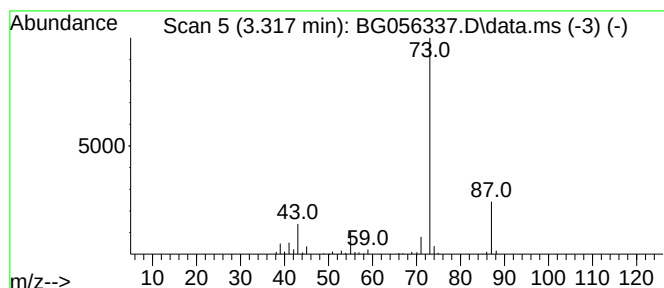
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TIC Integration Parameters: LSCINT.P

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Peak Number 1 unknown3.317 Concentration Rank 1

| R.T.  | EstConc  | Area   | Relative to ISTD       | R.T.  |
|-------|----------|--------|------------------------|-------|
| 3.317 | 16.25 ng | 151471 | 1,4-Dichlorobenzene-d4 | 8.305 |

| Hit# | of | 5 | Tentative ID                 | MW  | MolForm | CAS#        | Qual |
|------|----|---|------------------------------|-----|---------|-------------|------|
| 1    |    |   | Butane, 2-methoxy-2-methyl-  | 102 | C6H14O  | 000994-05-8 | 42   |
| 2    |    |   | Silane, tetramethyl-         | 88  | C4H12Si | 000075-76-3 | 9    |
| 3    |    |   | 1,3-Dioxolane, 2-propyl-     | 116 | C6H12O2 | 003390-13-4 | 9    |
| 4    |    |   | 3-Hexanol, 2,4-dimethyl-     | 130 | C8H18O  | 013432-25-2 | 9    |
| 5    |    |   | Propane, 2-methoxy-2-methyl- | 88  | C5H12O  | 001634-04-4 | 9    |



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Misc :  
ALS Vial : 9 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
MH-6

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG122722.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

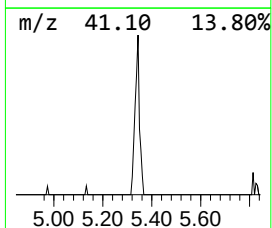
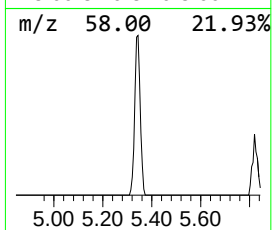
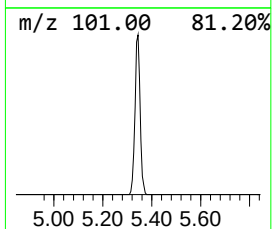
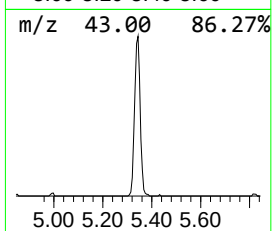
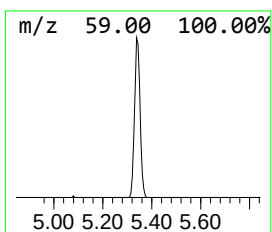
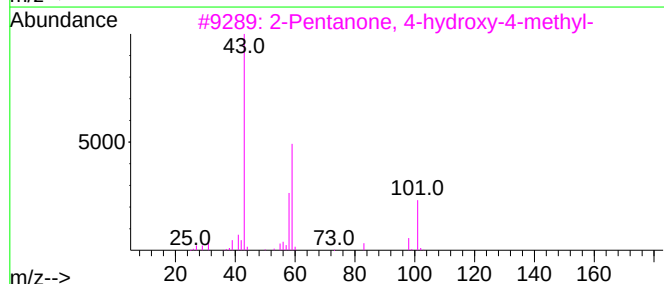
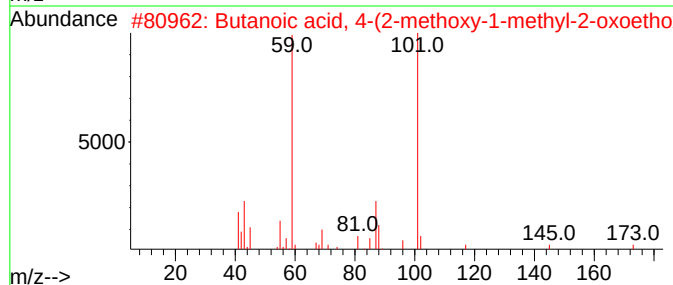
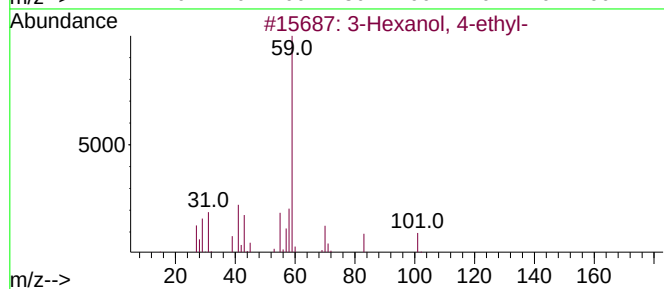
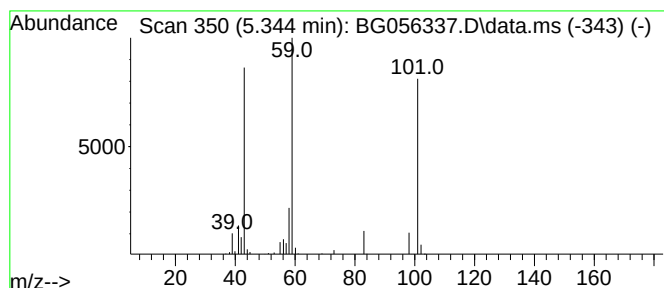
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 unknown5.344 Concentration Rank 2

| R.T.  | EstConc  | Area   | Relative to ISTD       | R.T.  |
|-------|----------|--------|------------------------|-------|
| 5.344 | 14.80 ng | 137969 | 1,4-Dichlorobenzene-d4 | 8.305 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|---------|-------------|------|
| 1    |    |   | 3-Hexanol, 4-ethyl-                 | 130 | C8H18O  | 019780-44-0 | 38   |
| 2    |    |   | Butanoic acid, 4-(2-methoxy-1-me... | 204 | C9H16O5 | 054966-46-0 | 36   |
| 3    |    |   | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2 | 000123-42-2 | 33   |
| 4    |    |   | Propane, 1-ethoxy-2-methyl-         | 102 | C6H14O  | 000627-02-1 | 25   |
| 5    |    |   | 4-Methoxy-1-pentene                 | 100 | C6H12O  | 098386-09-5 | 22   |



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ALS Vial : 9 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
MH-6

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG122722.M  
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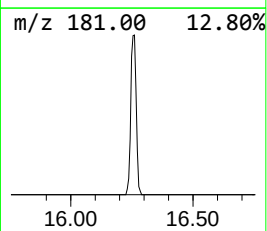
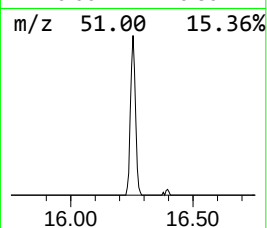
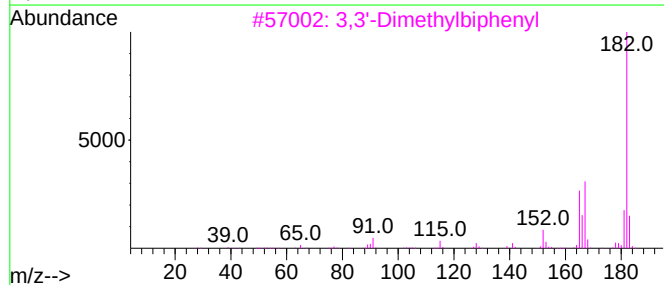
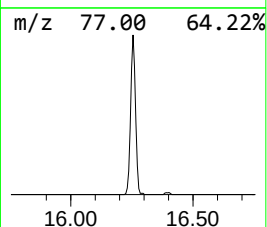
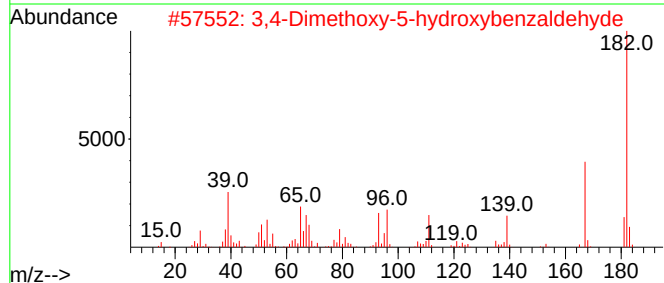
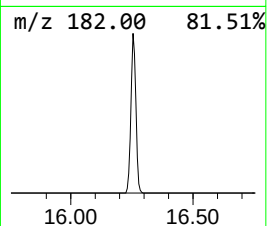
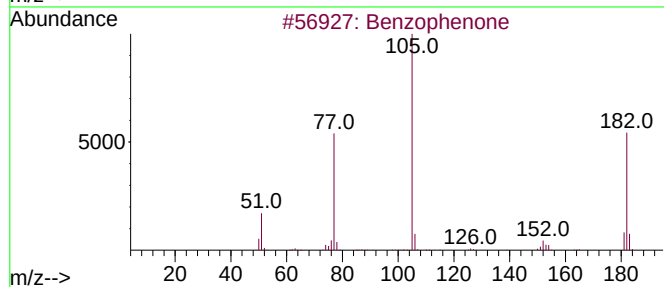
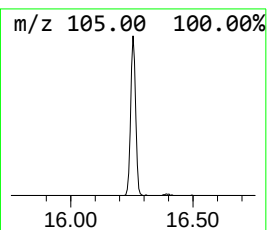
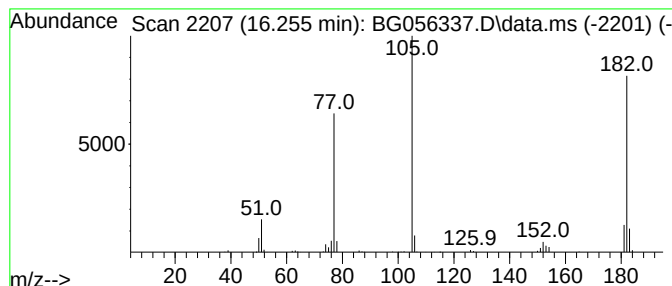
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 Benzophenone Concentration Rank 3

| R.T.   | EstConc  | Area   | Relative to ISTD | R.T.   |
|--------|----------|--------|------------------|--------|
| 16.255 | 11.82 ng | 273269 | Acenaphthene-d10 | 14.921 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm   | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|-----------|-------------|------|
| 1    |    |   | Benzophenone                        | 182 | C13H10O   | 000119-61-9 | 95   |
| 2    |    |   | 3,4-Dimethoxy-5-hydroxybenzaldehyde | 182 | C9H10O4   | 029865-90-5 | 47   |
| 3    |    |   | 3,3'-Dimethylbiphenyl               | 182 | C14H14    | 000612-75-9 | 43   |
| 4    |    |   | 2,4,6-Trimethoxytoluene             | 182 | C10H14O3  | 014107-97-2 | 43   |
| 5    |    |   | Benzilamide                         | 227 | C14H13NO2 | 004746-87-6 | 38   |



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ALS Vial : 9 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
MH-6

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG122722.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

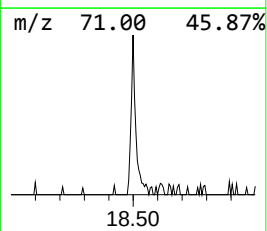
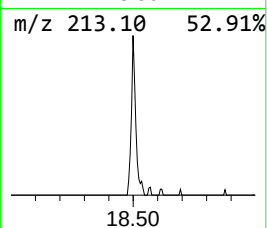
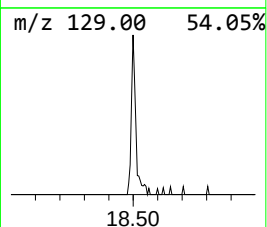
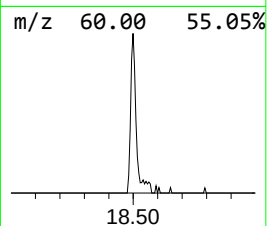
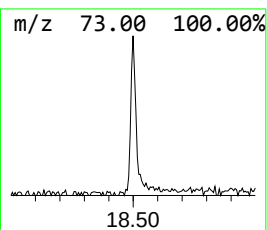
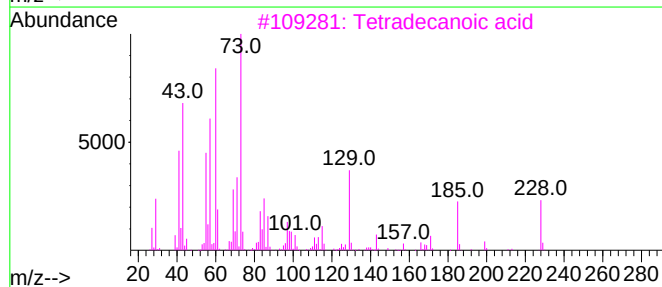
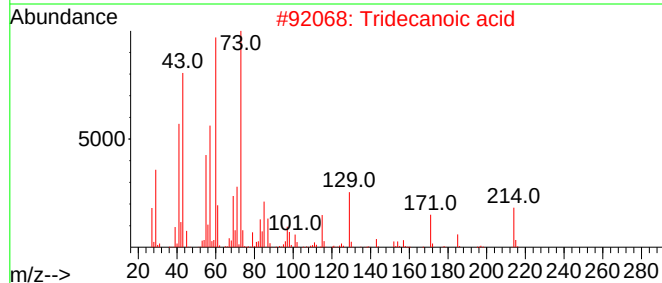
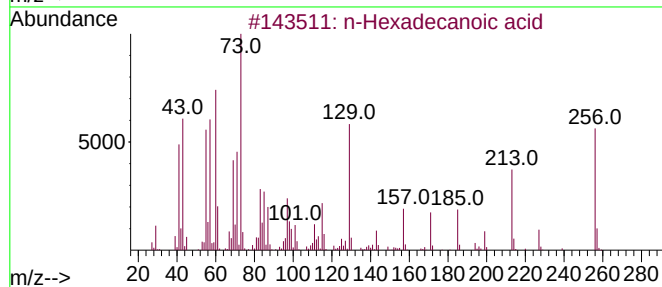
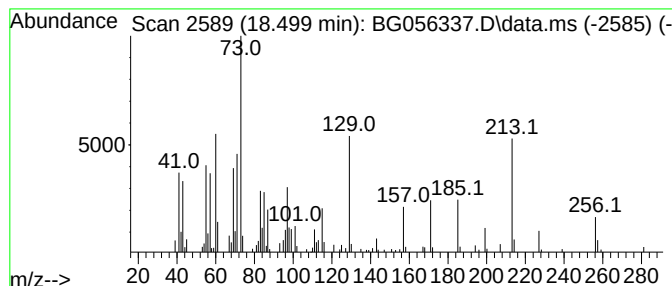
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 18.499 | 3.62 ng | 123680 | Phenanthrene-d10 | 17.653 |

| Hit# | of | 5 | Tentative ID                      | MW  | MolForm  | CAS#         | Qual |
|------|----|---|-----------------------------------|-----|----------|--------------|------|
| 1    |    |   | n-Hexadecanoic acid               | 256 | C16H32O2 | 000057-10-3  | 95   |
| 2    |    |   | Tridecanoic acid                  | 214 | C13H26O2 | 000638-53-9  | 93   |
| 3    |    |   | Tetradecanoic acid                | 228 | C14H28O2 | 000544-63-8  | 64   |
| 4    |    |   | Dodecanoic acid                   | 200 | C12H24O2 | 000143-07-7  | 64   |
| 5    |    |   | Adipic acid, hexyl isobutyl ester | 286 | C16H30O4 | 1000324-09-6 | 22   |



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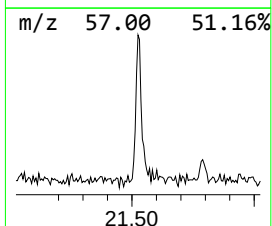
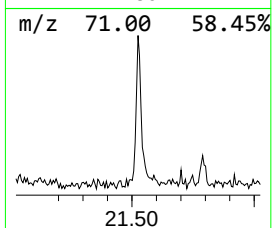
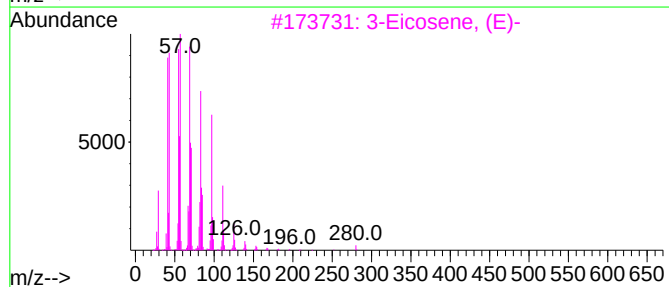
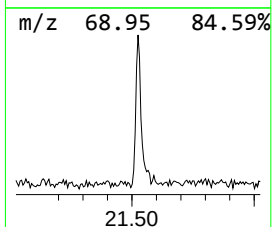
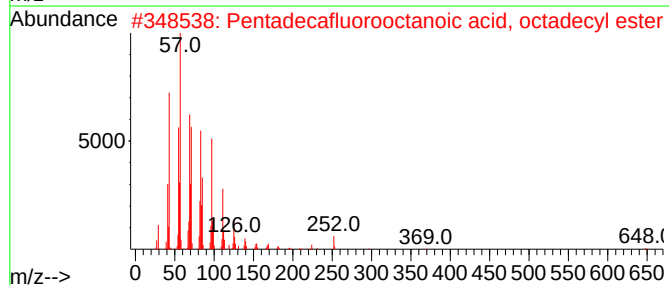
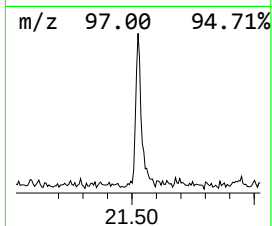
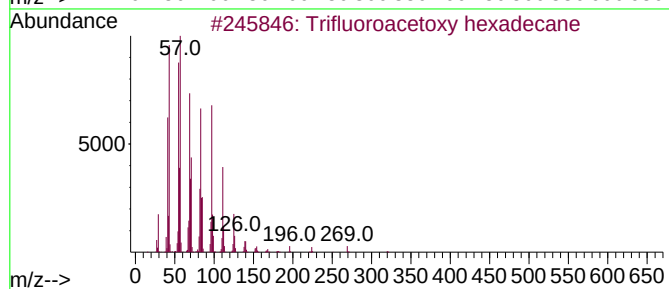
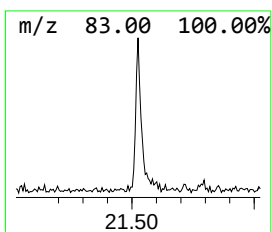
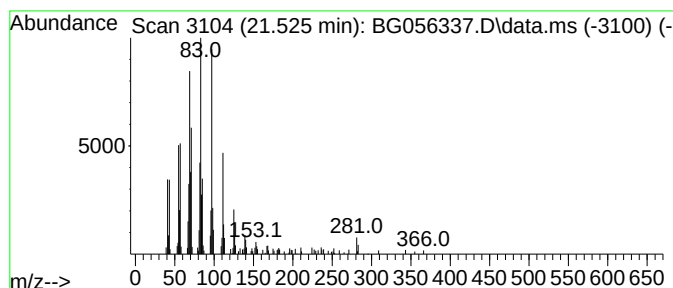
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 Trifluoroacetoxy hexadecane Concentration Rank 4

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 21.525 | 3.68 ng | 148275 | Chrysene-d12     | 21.948 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm     | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|-------------|--------------|------|
| 1    |    |   | Trifluoroacetoxy hexadecane         | 338 | C18H33F3O2  | 006222-03-3  | 91   |
| 2    |    |   | Pentadecafluorooctanoic acid, oc... | 666 | C26H37F15O2 | 1000406-04-8 | 90   |
| 3    |    |   | 3-Eicosene, (E)-                    | 280 | C20H40      | 074685-33-9  | 90   |
| 4    |    |   | 1-Heneicosyl formate                | 340 | C22H44O2    | 077899-03-7  | 87   |
| 5    |    |   | 1-Octadecanol                       | 270 | C18H38O     | 000112-92-5  | 87   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG011823\  
Data File : BG056337.D  
Acq On : 18 Jan 2023 20:51  
Operator : CG/JU  
Sample : 01159-04  
Misc :  
ALS Vial : 9 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
MH-6

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG122722.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 |
| unknown3.317       | 3.317  | 16.3    | ng    | 151471   | 1                     | 8.305  | 186425 | 20.0 |
| unknown5.344       | 5.344  | 14.8    | ng    | 137969   | 1                     | 8.305  | 186425 | 20.0 |
| Benzophenone       | 16.255 | 11.8    | ng    | 273269   | 3                     | 14.921 | 462360 | 20.0 |
| n-Hexadecanoic ... | 18.499 | 3.6     | ng    | 123680   | 4                     | 17.653 | 683013 | 20.0 |
| Trifluoroacetox... | 21.525 | 3.7     | ng    | 148275   | 5                     | 21.948 | 805057 | 20.0 |