

Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG082824\  
 Data File : BG062601.D  
 Acq On : 28 Aug 2024 18:41  
 Operator : MA/JU  
 Sample : P3767-01  
 Misc :  
 ALS Vial : 13 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 P-5-COMPOSITE

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-BG082724.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG062601.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         | 3.659       | 59            | 63          | 74           | rVB      | 45783          | 73026         | 1.83%           | 0.319%        |
| 2         | 5.051       | 295           | 300         | 309          | rVB      | 66630          | 102370        | 2.56%           | 0.448%        |
| 3         | 5.515       | 372           | 379         | 390          | rBV      | 921223         | 1446661       | 36.16%          | 6.328%        |
| 4         | 7.096       | 640           | 648         | 662          | rBV      | 919910         | 1591200       | 39.77%          | 6.961%        |
| 5         | 7.930       | 783           | 790         | 798          | rBV      | 270386         | 449590        | 11.24%          | 1.967%        |
| 6         | 9.082       | 978           | 986         | 994          | rBV      | 447416         | 788728        | 19.72%          | 3.450%        |
| 7         | 10.721      | 1257          | 1265        | 1273         | rBV      | 358063         | 652221        | 16.30%          | 2.853%        |
| 8         | 11.455      | 1382          | 1390        | 1398         | rBV2     | 57938          | 120129        | 3.00%           | 0.525%        |
| 9         | 13.177      | 1675          | 1683        | 1694         | rBV      | 1476522        | 2229959       | 55.74%          | 9.755%        |
| 10        | 14.552      | 1909          | 1917        | 1924         | rBV      | 627164         | 961597        | 24.04%          | 4.206%        |
| 11        | 14.751      | 1943          | 1951        | 1952         | rBV      | 62683          | 71380         | 1.78%           | 0.312%        |
| 12        | 14.769      | 1952          | 1954        | 1961         | rVB3     | 73946          | 103363        | 2.58%           | 0.452%        |
| 13        | 16.038      | 2163          | 2170        | 2180         | rBV      | 1281221        | 1956992       | 48.92%          | 8.561%        |
| 14        | 16.438      | 2233          | 2238        | 2244         | rVB4     | 24445          | 47455         | 1.19%           | 0.208%        |
| 15        | 16.696      | 2278          | 2282        | 2289         | rVB6     | 25462          | 46018         | 1.15%           | 0.201%        |
| 16        | 17.296      | 2378          | 2384        | 2389         | rBV      | 862597         | 1296113       | 32.40%          | 5.670%        |
| 17        | 17.337      | 2389          | 2391        | 2398         | rVB      | 133973         | 163251        | 4.08%           | 0.714%        |
| 18        | 18.189      | 2529          | 2536        | 2540         | rBV2     | 151439         | 256570        | 6.41%           | 1.122%        |
| 19        | 18.365      | 2561          | 2566        | 2570         | rBV3     | 34144          | 61215         | 1.53%           | 0.268%        |
| 20        | 19.088      | 2680          | 2689        | 2692         | rBV5     | 26535          | 52519         | 1.31%           | 0.230%        |
| 21        | 19.346      | 2728          | 2733        | 2741         | rBV      | 317853         | 467480        | 11.69%          | 2.045%        |
| 22        | 19.464      | 2749          | 2753        | 2762         | rVB3     | 57515          | 92731         | 2.32%           | 0.406%        |
| 23        | 19.593      | 2773          | 2775        | 2782         | rVB5     | 19901          | 40878         | 1.02%           | 0.179%        |
| 24        | 19.710      | 2785          | 2795        | 2803         | rBV      | 302684         | 571867        | 14.29%          | 2.502%        |
| 25        | 19.916      | 2823          | 2830        | 2840         | rVB      | 2972418        | 4000630       | 100.00%         | 17.501%       |
| 26        | 20.204      | 2876          | 2879        | 2881         | rBV2     | 33528          | 40494         | 1.01%           | 0.177%        |
| 27        | 20.357      | 2902          | 2905        | 2909         | rVB3     | 25465          | 42578         | 1.06%           | 0.186%        |
| 28        | 20.556      | 2935          | 2939        | 2943         | rBV3     | 49810          | 65566         | 1.64%           | 0.287%        |
| 29        | 20.603      | 2943          | 2947        | 2952         | rVV5     | 31169          | 48313         | 1.21%           | 0.211%        |
| 30        | 20.721      | 2963          | 2967        | 2971         | rBV3     | 49656          | 60762         | 1.52%           | 0.266%        |
| 31        | 21.214      | 3047          | 3051        | 3058         | rVB3     | 159398         | 246137        | 6.15%           | 1.077%        |
| 32        | 21.444      | 3087          | 3090        | 3095         | rVB      | 50867          | 62975         | 1.57%           | 0.275%        |
| 33        | 21.543      | 3099          | 3107        | 3112         | rVV2     | 916734         | 1766100       | 44.15%          | 7.726%        |
| 34        | 21.585      | 3112          | 3114        | 3122         | rVB      | 164834         | 235758        | 5.89%           | 1.031%        |
| 35        | 21.743      | 3137          | 3141        | 3145         | rBV3     | 64991          | 91294         | 2.28%           | 0.399%        |
| 36        | 22.331      | 3237          | 3241        | 3253         | rVB6     | 82259          | 177210        | 4.43%           | 0.775%        |

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Sample : P3767-01  
Misc :  
ALS Vial : 13 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
P-5-COMPOSITE

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-BG082724.M  
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

|    |        |      |      |      |      |        |         |        |        |
|----|--------|------|------|------|------|--------|---------|--------|--------|
| 37 | 23.653 | 3459 | 3466 | 3473 | rBV  | 106954 | 330507  | 8.26%  | 1.446% |
| 38 | 23.759 | 3480 | 3484 | 3490 | rVB2 | 81303  | 152288  | 3.81%  | 0.666% |
| 39 | 24.475 | 3600 | 3606 | 3616 | rVB2 | 88203  | 222217  | 5.55%  | 0.972% |
| 40 | 24.622 | 3622 | 3631 | 3648 | rBV3 | 562969 | 1673833 | 41.84% | 7.322% |

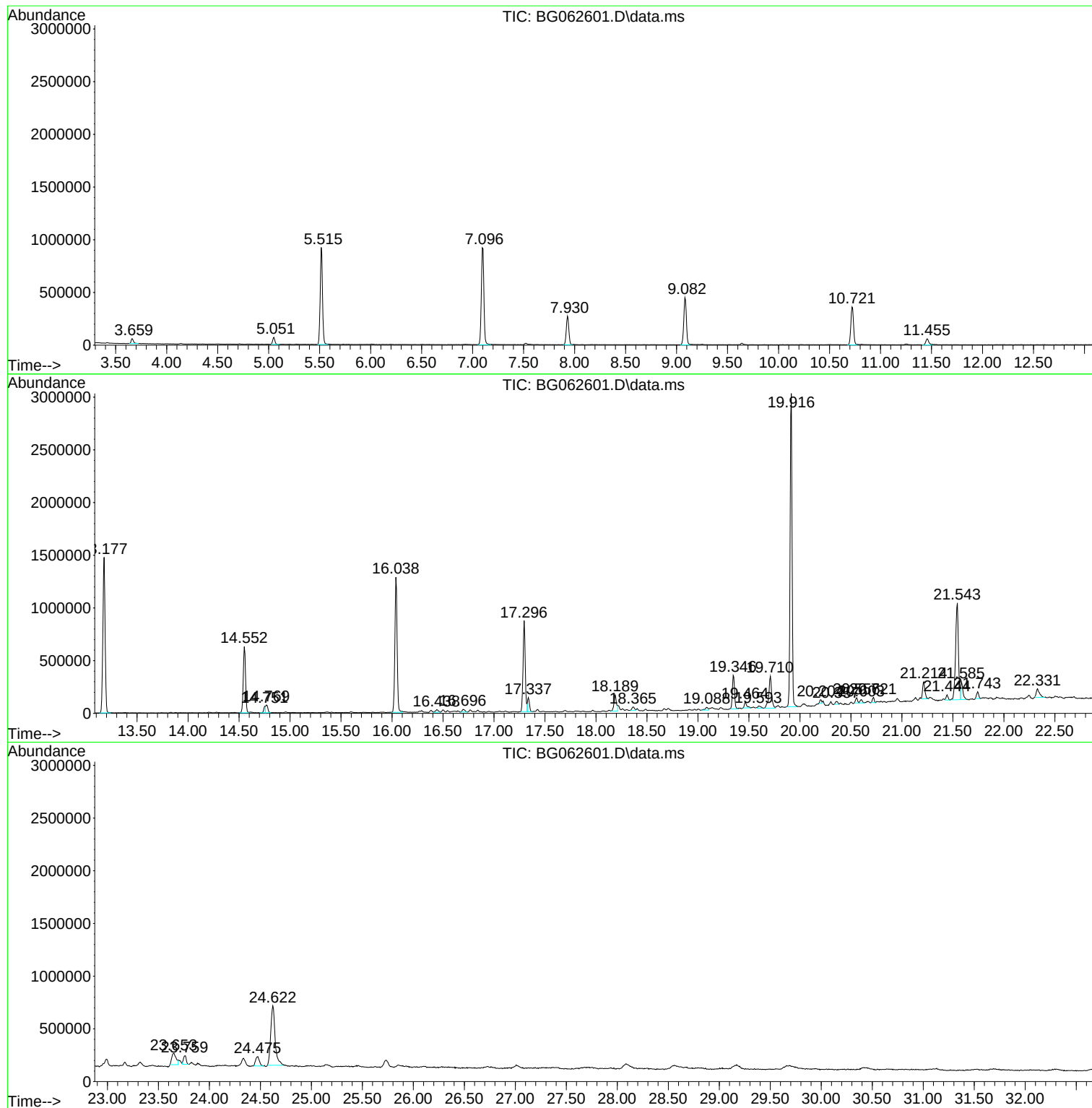
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Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG082824\  
Data File : BG062601.D  
Acq On : 28 Aug 2024 18:41  
Operator : MA/JU  
Sample : P3767-01  
Misc :  
ALS Vial : 13 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
P-5-COMPOSITE

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG082724.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\BG082824\  
Data File : BG062601.D  
Acq On : 28 Aug 2024 18:41  
Operator : MA/JU  
Sample : P3767-01  
Misc :  
ALS Vial : 13 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
P-5-COMPOSITE

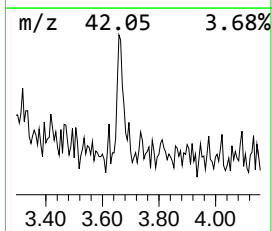
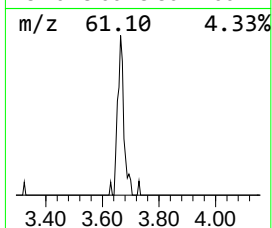
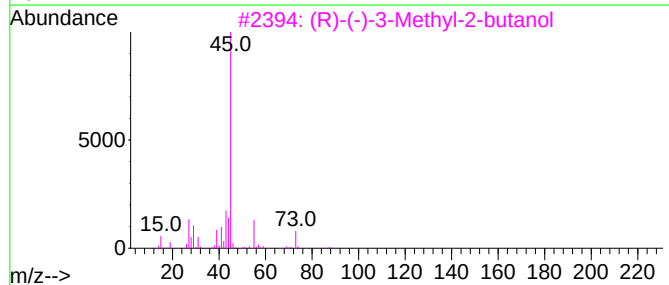
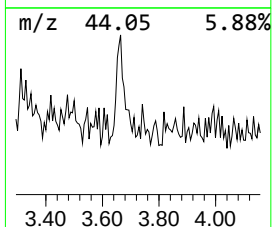
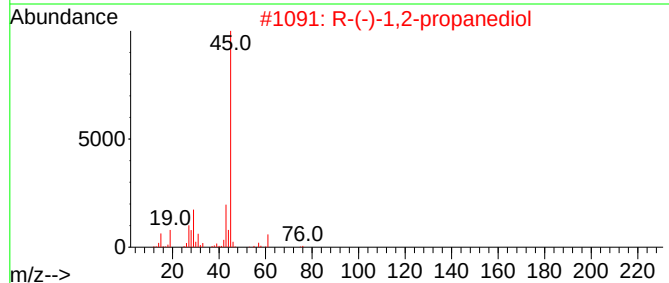
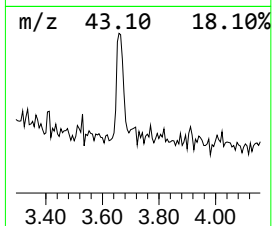
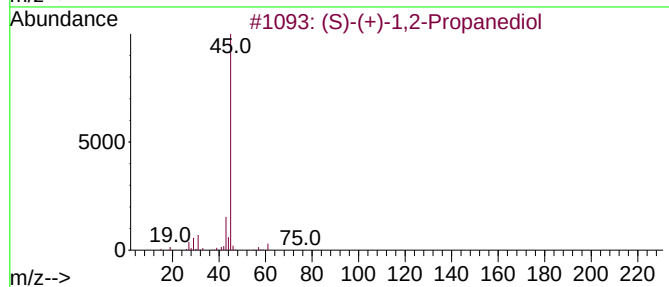
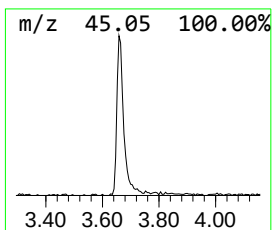
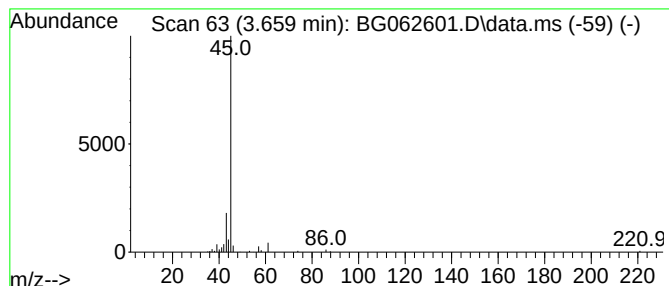
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG082724.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 (S)-(+)-1,2-Propanediol Concentration Rank 4

| R.T.  | EstConc | Area  | Relative to ISTD       | R.T.  |
|-------|---------|-------|------------------------|-------|
| 3.659 | 3.25 ng | 73026 | 1,4-Dichlorobenzene-d4 | 7.930 |

| Hit# | of                         | 5 | Tentative ID | MW | MolForm | CAS#        | Qual |
|------|----------------------------|---|--------------|----|---------|-------------|------|
| 1    | (S)-(+)-1,2-Propanediol    |   |              | 76 | C3H8O2  | 004254-15-3 | 56   |
| 2    | R-(-)-1,2-propanediol      |   |              | 76 | C3H8O2  | 004254-14-2 | 40   |
| 3    | (R)-(-)-3-Methyl-2-butanol |   |              | 88 | C5H12O  | 001572-93-6 | 9    |
| 4    | 2-Butanol, 3-methyl-       |   |              | 88 | C5H12O  | 000598-75-4 | 9    |
| 5    | 1-Butene, 4-methoxy        |   |              | 86 | C5H10O  | 004696-30-4 | 9    |



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Operator : MA/JU  
Sample : P3767-01  
Misc :  
ALS Vial : 13 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
P-5-COMPOSITE

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG082724.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

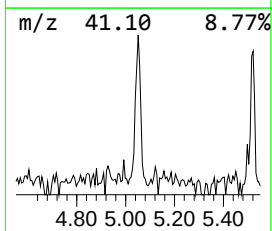
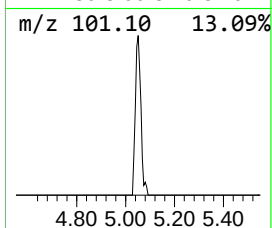
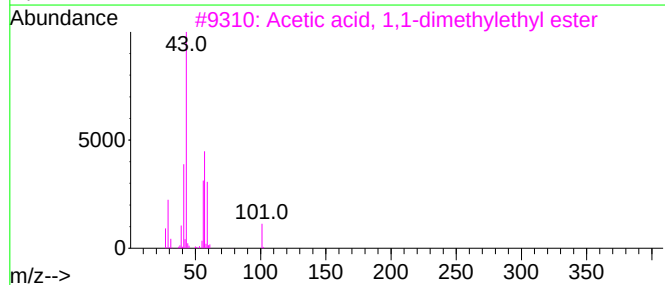
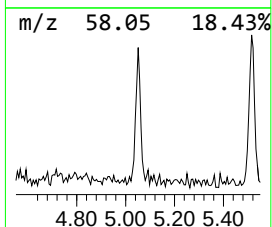
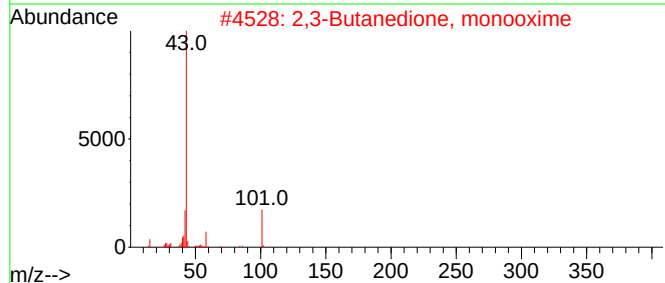
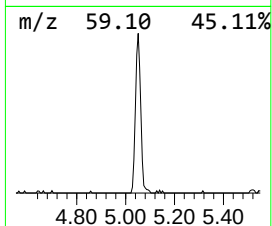
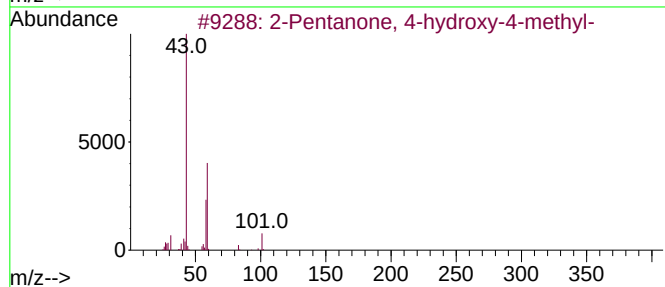
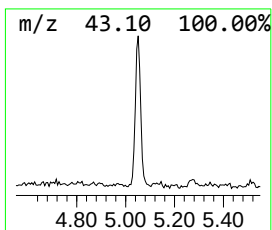
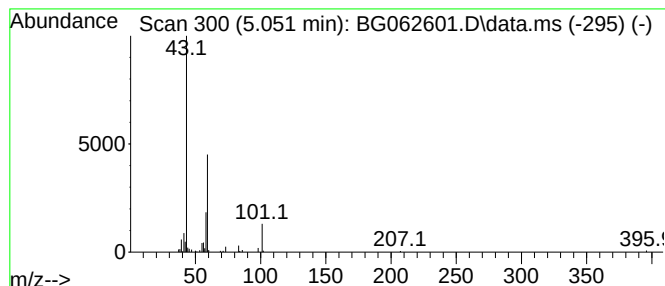
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

| R.T.  | EstConc | Area   | Relative to ISTD       | R.T.  |
|-------|---------|--------|------------------------|-------|
| 5.051 | 4.55 ng | 102370 | 1,4-Dichlorobenzene-d4 | 7.930 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|---------|-------------|------|
| 1    |    |   | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2 | 000123-42-2 | 78   |
| 2    |    |   | 2,3-Butanedione, monooxime          | 101 | C4H7NO2 | 000057-71-6 | 27   |
| 3    |    |   | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 25   |
| 4    |    |   | 4-Penten-2-one, 4-methyl-           | 98  | C6H10O  | 003744-02-3 | 9    |
| 5    |    |   | 2-Propyn-1-ol, acetate              | 98  | C5H6O2  | 000627-09-8 | 9    |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG082824\  
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Sample : P3767-01  
Misc :  
ALS Vial : 13 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
P-5-COMPOSITE

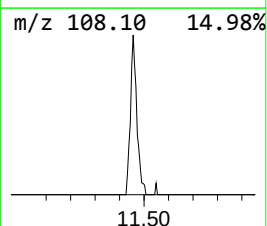
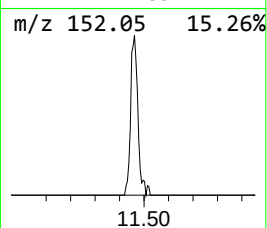
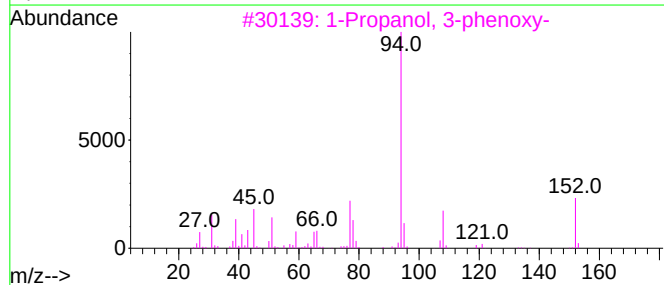
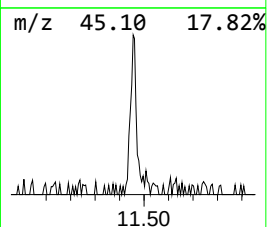
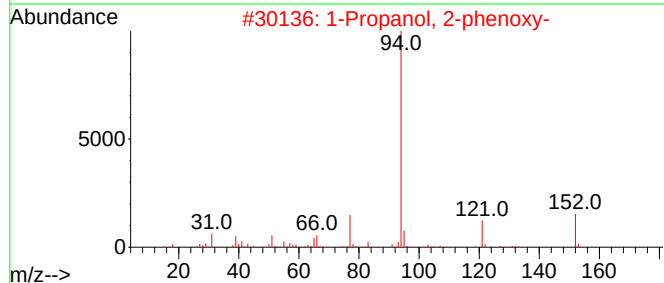
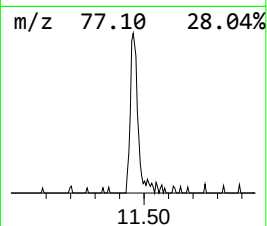
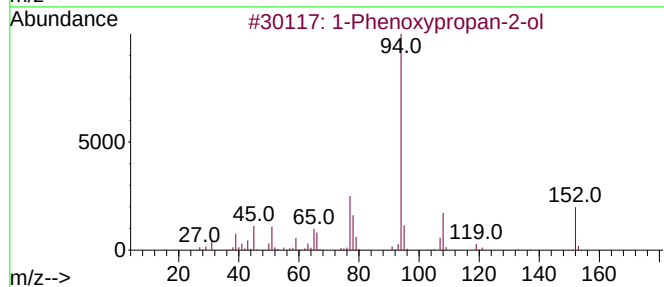
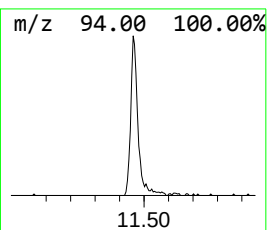
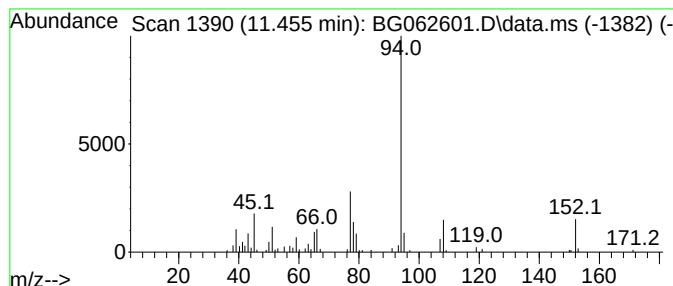
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG082724.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 3 1-Phenoxypropan-2-ol Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 11.455 | 3.68 ng | 120129 | Naphthalene-d8   | 10.721 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | 1-Phenoxypropan-2-ol                | 152 | C9H12O2  | 000770-35-4 | 96   |
| 2    |    |   | 1-Propanol, 2-phenoxy-              | 152 | C9H12O2  | 004169-04-4 | 64   |
| 3    |    |   | 1-Propanol, 3-phenoxy-              | 152 | C9H12O2  | 006180-61-6 | 60   |
| 4    |    |   | Carbonic acid, (3,4,4-trimethyl-... | 252 | C13H16O5 | 109123-69-5 | 59   |
| 5    |    |   | Benzene, propoxy-                   | 136 | C9H12O   | 000622-85-5 | 53   |



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Sample : P3767-01  
Misc :  
ALS Vial : 13 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
P-5-COMPOSITE

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG082724.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

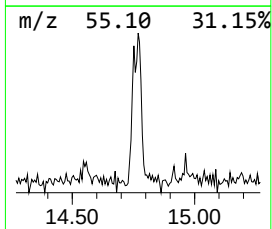
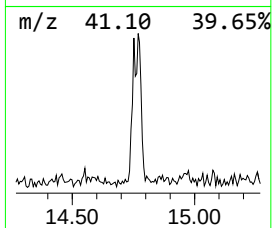
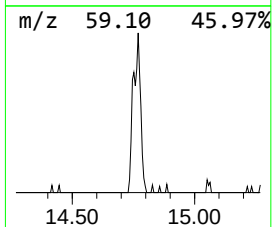
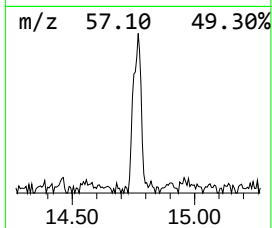
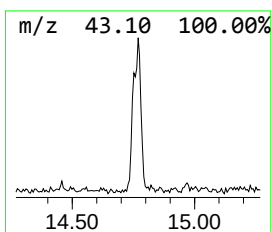
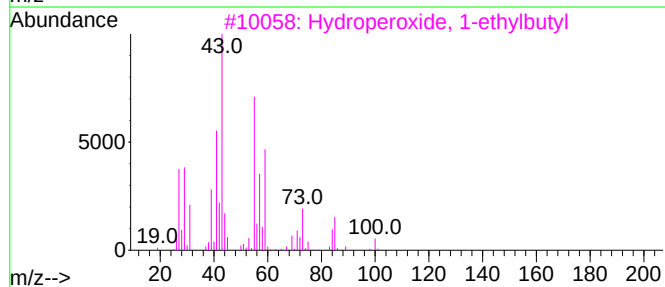
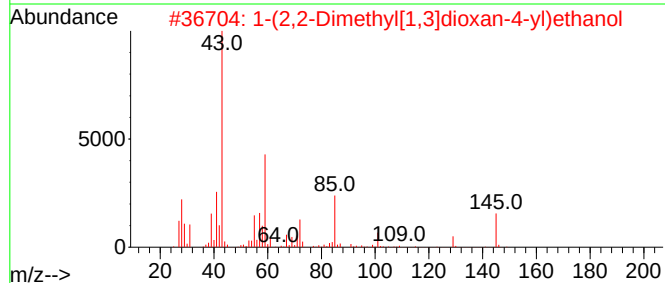
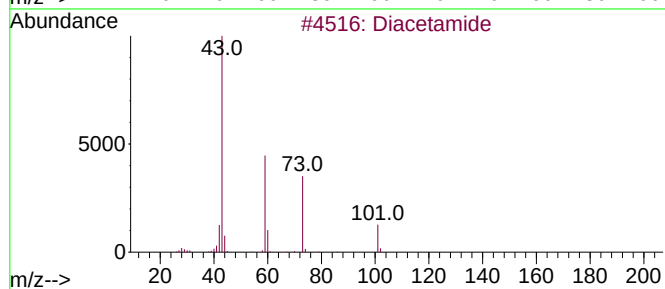
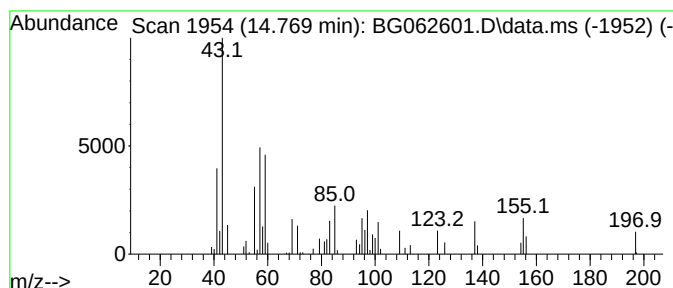
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 unknown14.769 Concentration Rank 6

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 14.769 | 2.15 ng | 103363 | Acenaphthene-d10 | 14.552 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|----------|--------------|------|
| 1    |    |   | Diacetamide                         | 101 | C4H7NO2  | 000625-77-4  | 22   |
| 2    |    |   | 1-(2,2-Dimethyl[1,3]dioxan-4-yl)... | 160 | C8H16O3  | 1000191-77-9 | 17   |
| 3    |    |   | Hydroperoxide, 1-ethylbutyl         | 118 | C6H14O2  | 024254-56-6  | 12   |
| 4    |    |   | Butanoic acid, 3-hydroxy-3-methyl-  | 118 | C5H10O3  | 000625-08-1  | 12   |
| 5    |    |   | 7-Methyl-Z-tetradecen-1-ol acetate  | 268 | C17H32O2 | 1000130-99-6 | 12   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG082824\  
Data File : BG062601.D  
Acq On : 28 Aug 2024 18:41  
Operator : MA/JU  
Sample : P3767-01  
Misc :  
ALS Vial : 13 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
P-5-COMPOSITE

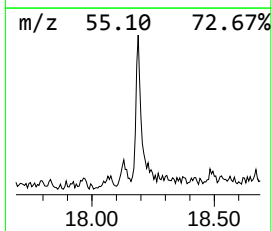
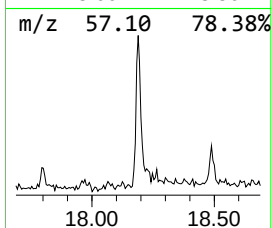
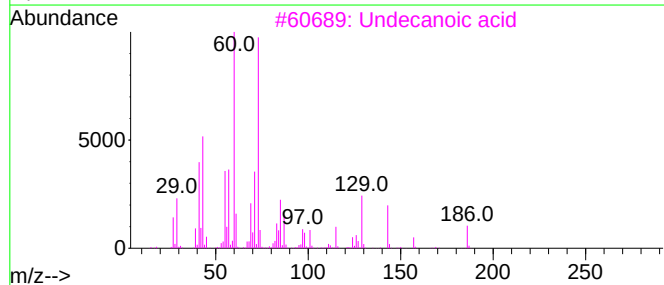
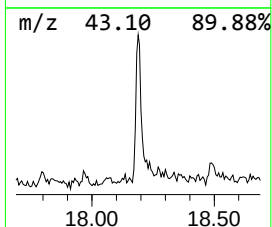
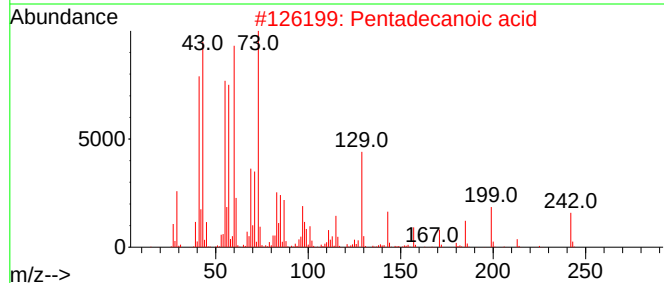
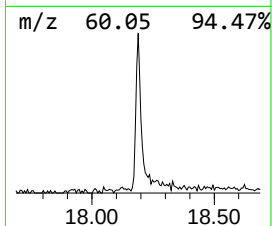
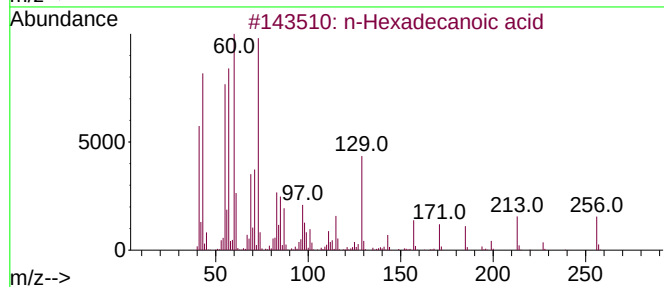
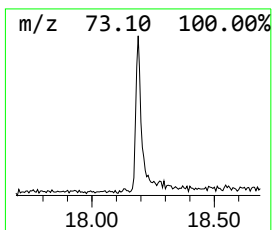
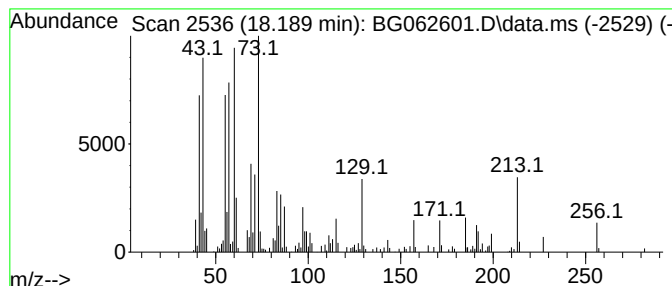
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 5 n-Hexadecanoic acid Concentration Rank 2

| R.T.      | EstConc             | Area   | Relative to ISTD | R.T.        |      |
|-----------|---------------------|--------|------------------|-------------|------|
| 18.189    | 3.96 ng             | 256570 | Phenanthrene-d10 | 17.296      |      |
| 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 | 81   |
| 3         | Undecanoic acid     | 186    | C11H22O2         | 000112-37-8 | 76   |
| 4         | Tetradecanoic acid  | 228    | C14H28O2         | 000544-63-8 | 72   |
| 5         | Tridecanoic acid    | 214    | C13H26O2         | 000638-53-9 | 70   |





Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG082824\  
Data File : BG062601.D  
Acq On : 28 Aug 2024 18:41  
Operator : MA/JU  
Sample : P3767-01  
Misc :  
ALS Vial : 13 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
P-5-COMPOSITE

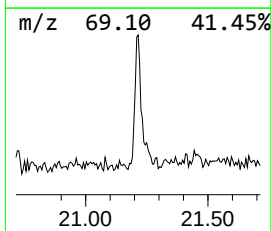
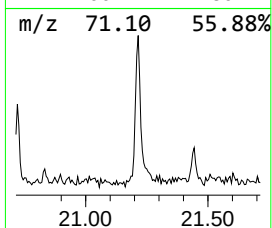
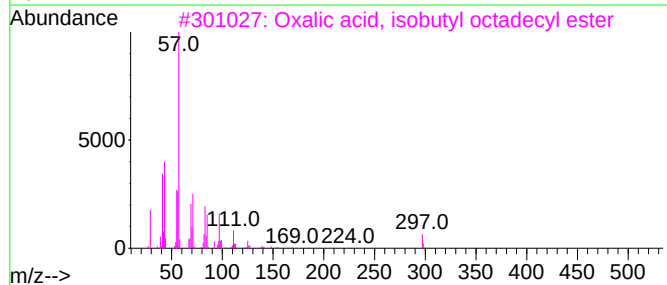
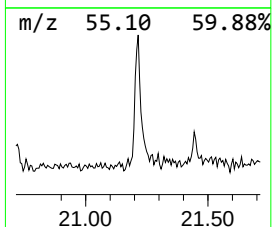
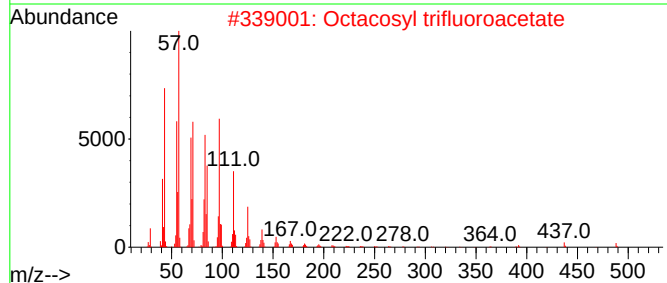
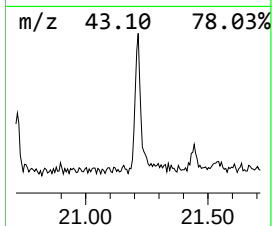
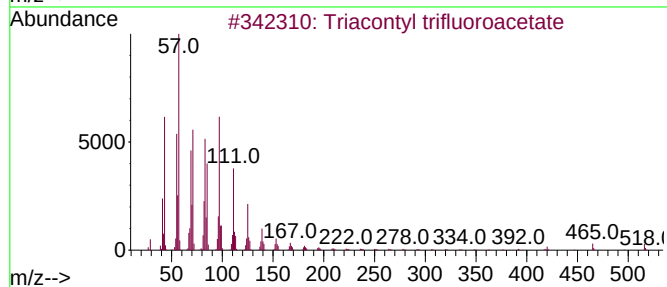
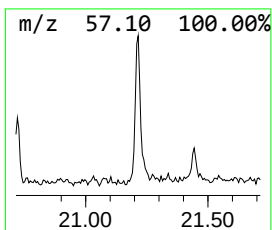
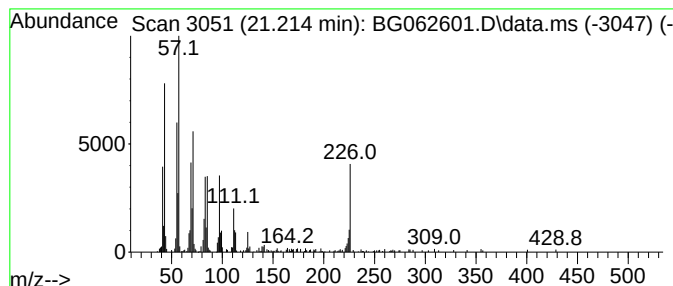
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 6 Triacetyl trifluoroacetate Concentration Rank 5

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 21.214 | 2.79 ng | 246137 | Chrysene-d12     | 21.544 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|------------|--------------|------|
| 1    |    |   | Triacetyl trifluoroacetate          | 534 | C32H61F3O2 | 1000351-75-7 | 58   |
| 2    |    |   | Octacosyl trifluoroacetate          | 506 | C30H57F3O2 | 1000351-74-9 | 58   |
| 3    |    |   | Oxalic acid, isobutyl octadecyl ... | 398 | C24H46O4   | 1000309-38-3 | 58   |
| 4    |    |   | Tetratriacontyl heptafluorobutyrate | 691 | C38H69F7O2 | 1000351-84-1 | 58   |
| 5    |    |   | Triacetyl heptafluorobutyrate       | 634 | C34H61F7O2 | 1000351-83-2 | 58   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG082824\  
Data File : BG062601.D  
Acq On : 28 Aug 2024 18:41  
Operator : MA/JU  
Sample : P3767-01  
Misc :  
ALS Vial : 13 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
P-5-COMPOSITE

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG082724.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

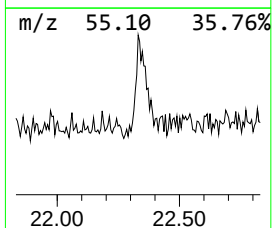
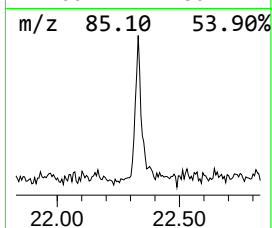
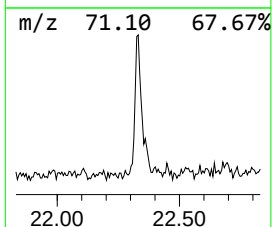
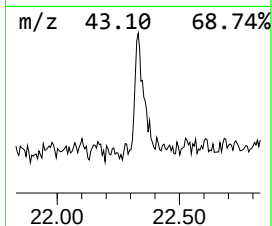
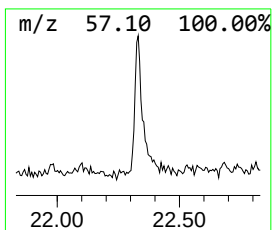
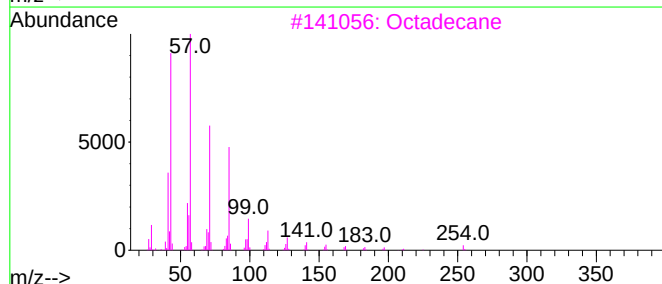
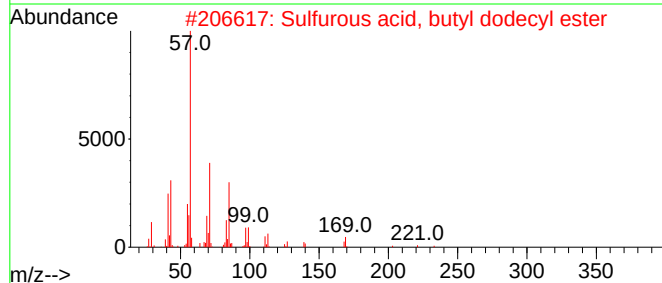
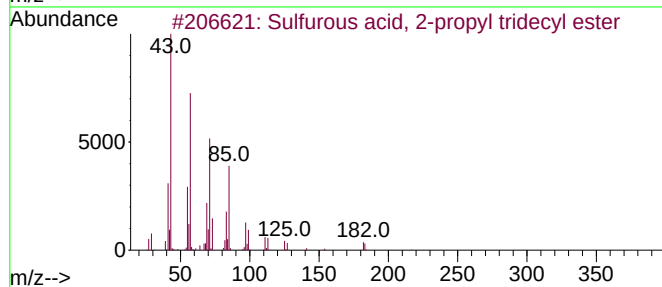
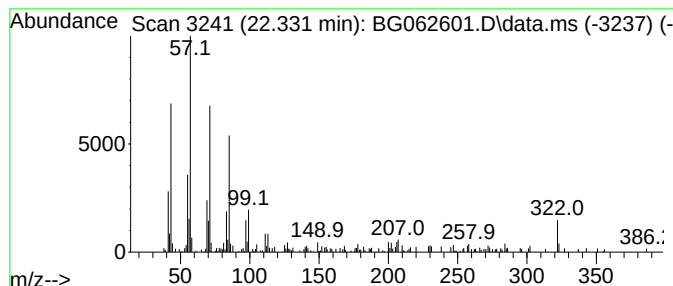
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 7 Sulfurous acid, 2-propyl tr... Concentration Rank 7

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 22.331 | 2.01 ng | 177210 | Chrysene-d12     | 21.544 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|-----------|--------------|------|
| 1    |    |   | Sulfurous acid, 2-propyl tridecy... | 306 | C16H34O3S | 1000309-12-4 | 64   |
| 2    |    |   | Sulfurous acid, butyl dodecyl ester | 306 | C16H34O3S | 1000309-17-9 | 64   |
| 3    |    |   | Octadecane                          | 254 | C18H38    | 000593-45-3  | 60   |
| 4    |    |   | 5,15-Dimethylnonadecane             | 296 | C21H44    | 1000131-09-1 | 55   |
| 5    |    |   | 1-Iodoundecane                      | 282 | C11H23I   | 004282-44-4  | 53   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG082824\  
Data File : BG062601.D  
Acq On : 28 Aug 2024 18:41  
Operator : MA/JU  
Sample : P3767-01  
Misc :  
ALS Vial : 13 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
P-5-COMPOSITE

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG082724.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 |
| (S)-(+)-1,2-Pro... | 3.659  | 3.3     | ng    | 73026    | 1                     | 7.930  | 449590  | 20.0 |
| 2-Pentanone, 4-... | 5.051  | 4.5     | ng    | 102370   | 1                     | 7.930  | 449590  | 20.0 |
| 1-Phenoxypropan... | 11.455 | 3.7     | ng    | 120129   | 2                     | 10.721 | 652221  | 20.0 |
| unknown14.769      | 14.769 | 2.1     | ng    | 103363   | 3                     | 14.552 | 961597  | 20.0 |
| n-Hexadecanoic ... | 18.189 | 4.0     | ng    | 256570   | 4                     | 17.296 | 1296110 | 20.0 |
| Triacetyl trif...  | 21.214 | 2.8     | ng    | 246137   | 5                     | 21.544 | 1766100 | 20.0 |
| Sulfurous acid,... | 22.331 | 2.0     | ng    | 177210   | 5                     | 21.544 | 1766100 | 20.0 |