

Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG062124\  
 Data File : BG061621.D  
 Acq On : 21 Jun 2024 15:29  
 Operator : MA/JU  
 Sample : P2754-08  
 Misc :  
 ALS Vial : 11 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 A4BP7

Integration Parameters: LSCINT.P  
 Integrator: RTE  
 Smoothing : OFF Filtering: 5  
 Sampling : 1 Min Area: 0.1 % 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\SFAM-EPA-BG062024.MA.M  
 Title : SVOA CALIBRATION

Signal : TIC: BG061621.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|--------|----------|------------|----------|-----------|-------|-------------|------------|--------------|------------|
| 1      | 3.738    | 72         | 76       | 81        | rBV   | 36581       | 57908      | 0.17%        | 0.105%     |
| 2      | 5.148    | 310        | 316      | 321       | rBV   | 34451       | 56616      | 0.17%        | 0.102%     |
| 3      | 7.210    | 660        | 667      | 675       | rBV   | 325869      | 530650     | 1.59%        | 0.960%     |
| 4      | 7.398    | 692        | 699      | 708       | rVB   | 217513      | 355292     | 1.06%        | 0.642%     |
| 5      | 7.598    | 725        | 733      | 740       | rBV2  | 277398      | 475554     | 1.42%        | 0.860%     |
| 6      | 8.074    | 807        | 814      | 820       | rBV   | 238567      | 394683     | 1.18%        | 0.714%     |
| 7      | 8.761    | 924        | 931      | 940       | rVB2  | 360009      | 616201     | 1.84%        | 1.114%     |
| 8      | 8.896    | 949        | 954      | 958       | rBV5  | 20619       | 35477      | 0.11%        | 0.064%     |
| 9      | 9.237    | 1005       | 1012     | 1018      | rBV   | 274512      | 468651     | 1.40%        | 0.847%     |
| 10     | 9.795    | 1101       | 1107     | 1112      | rVB2  | 23941       | 38368      | 0.11%        | 0.069%     |
| 11     | 9.960    | 1129       | 1135     | 1145      | rVB2  | 211211      | 380551     | 1.14%        | 0.688%     |
| 12     | 10.495   | 1219       | 1226     | 1236      | rBV   | 359238      | 634002     | 1.90%        | 1.146%     |
| 13     | 10.888   | 1284       | 1293     | 1305      | rVB   | 340219      | 628936     | 1.88%        | 1.137%     |
| 14     | 11.012   | 1308       | 1314     | 1323      | rVV   | 246613      | 463225     | 1.39%        | 0.838%     |
| 15     | 11.617   | 1411       | 1417     | 1427      | rBV3  | 50828       | 103873     | 0.31%        | 0.188%     |
| 16     | 14.108   | 1834       | 1841     | 1849      | rBV   | 676345      | 952013     | 2.85%        | 1.722%     |
| 17     | 14.396   | 1883       | 1890     | 1897      | rVB   | 744420      | 1156662    | 3.46%        | 2.092%     |
| 18     | 14.701   | 1936       | 1942     | 1948      | rVB   | 581050      | 869241     | 2.60%        | 1.572%     |
| 19     | 14.866   | 1962       | 1970     | 1975      | rBV   | 361371      | 587674     | 1.76%        | 1.063%     |
| 20     | 15.101   | 2005       | 2010     | 2016      | rVB8  | 16860       | 33554      | 0.10%        | 0.061%     |
| 21     | 15.689   | 2103       | 2110     | 2117      | rBV   | 970421      | 1484020    | 4.44%        | 2.684%     |
| 22     | 15.788   | 2122       | 2127     | 2133      | rVB   | 256035      | 371929     | 1.11%        | 0.673%     |
| 23     | 17.445   | 2402       | 2409     | 2413      | rVV   | 719552      | 1142253    | 3.42%        | 2.066%     |
| 24     | 17.481   | 2413       | 2415     | 2420      | rVV   | 120946      | 157561     | 0.47%        | 0.285%     |
| 25     | 17.539   | 2420       | 2425     | 2434      | rVB2  | 1071210     | 1639303    | 4.91%        | 2.964%     |
| 26     | 18.039   | 2503       | 2510     | 2516      | rVB8  | 31909       | 73413      | 0.22%        | 0.133%     |
| 27     | 18.332   | 2554       | 2560     | 2572      | rBV3  | 334052      | 538839     | 1.61%        | 0.974%     |
| 28     | 18.509   | 2585       | 2590     | 2595      | rBV6  | 48437       | 83275      | 0.25%        | 0.151%     |
| 29     | 19.220   | 2707       | 2711     | 2716      | rBV8  | 28389       | 51576      | 0.15%        | 0.093%     |
| 30     | 19.490   | 2752       | 2757     | 2762      | rVB   | 222730      | 316298     | 0.95%        | 0.572%     |
| 31     | 19.602   | 2772       | 2776     | 2786      | rBV   | 193418      | 273687     | 0.82%        | 0.495%     |
| 32     | 19.819   | 2807       | 2813     | 2824      | rBV2  | 1138728     | 1921517    | 5.75%        | 3.475%     |
| 33     | 20.072   | 2854       | 2856     | 2862      | rVB7  | 26551       | 36608      | 0.11%        | 0.066%     |
| 34     | 20.336   | 2898       | 2901     | 2904      | rBV4  | 39069       | 52931      | 0.16%        | 0.096%     |
| 35     | 20.841   | 2984       | 2987     | 2991      | rBV3  | 58133       | 91994      | 0.28%        | 0.166%     |
| 36     | 21.112   | 3031       | 3033     | 3038      | rVB   | 74259       | 91105      | 0.27%        | 0.165%     |

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Instrument :  
 BNA\_G  
 ClientSampleId :  
 A4BP7

Integration Parameters: LSCINT.P

Integrator: RTE  
 Smoothing : OFF Filtering: 5  
 Sampling : 1 Min Area: 0.1 % 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\SFAM-EPA-BG062024.MA.M  
 Title : SVOA CALIBRATION

|    |        |      |      |      |      |          |          |         |         |
|----|--------|------|------|------|------|----------|----------|---------|---------|
| 37 | 21.329 | 3066 | 3070 | 3073 | rBV2 | 166176   | 220667   | 0.66%   | 0.399%  |
| 38 | 21.364 | 3073 | 3076 | 3083 | rVB2 | 329101   | 454626   | 1.36%   | 0.822%  |
| 39 | 21.634 | 3113 | 3122 | 3127 | rBV  | 18983288 | 33404144 | 100.00% | 60.404% |
| 40 | 21.705 | 3127 | 3134 | 3140 | rVV2 | 685391   | 1248230  | 3.74%   | 2.257%  |
| 41 | 21.934 | 3170 | 3173 | 3177 | rVB4 | 77174    | 104460   | 0.31%   | 0.189%  |
| 42 | 24.085 | 3536 | 3539 | 3544 | rVB3 | 57526    | 94895    | 0.28%   | 0.172%  |
| 43 | 24.713 | 3636 | 3646 | 3658 | rBV2 | 446547   | 1328596  | 3.98%   | 2.402%  |
| 44 | 24.931 | 3674 | 3683 | 3695 | rVB2 | 459339   | 1280152  | 3.83%   | 2.315%  |

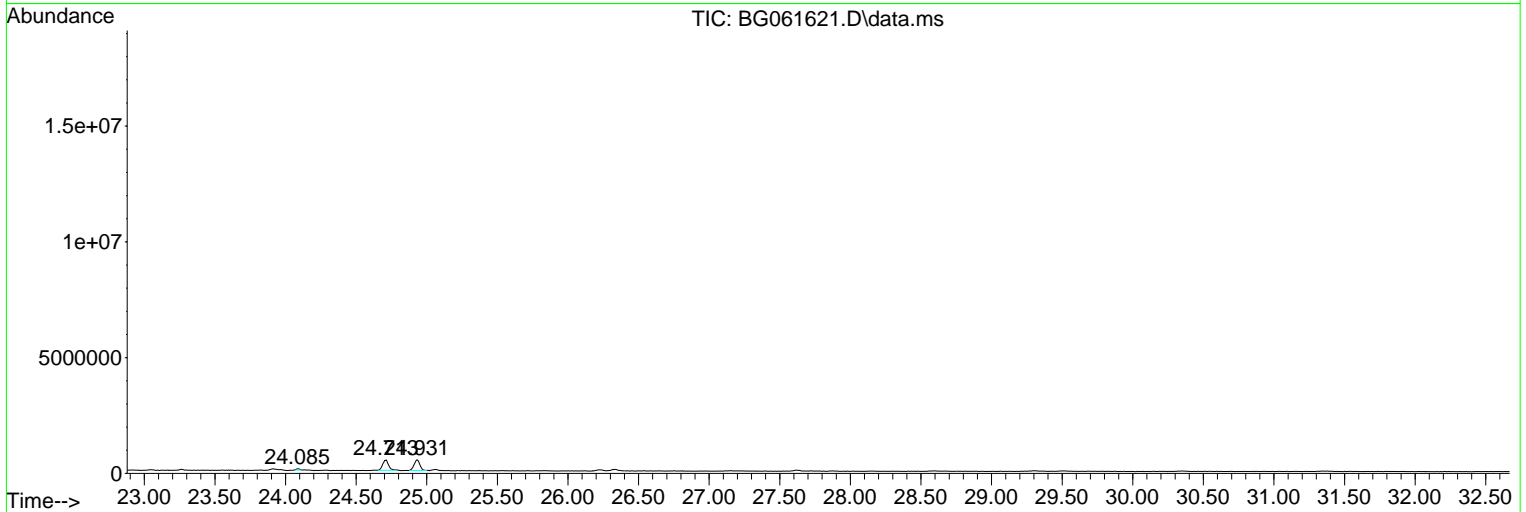
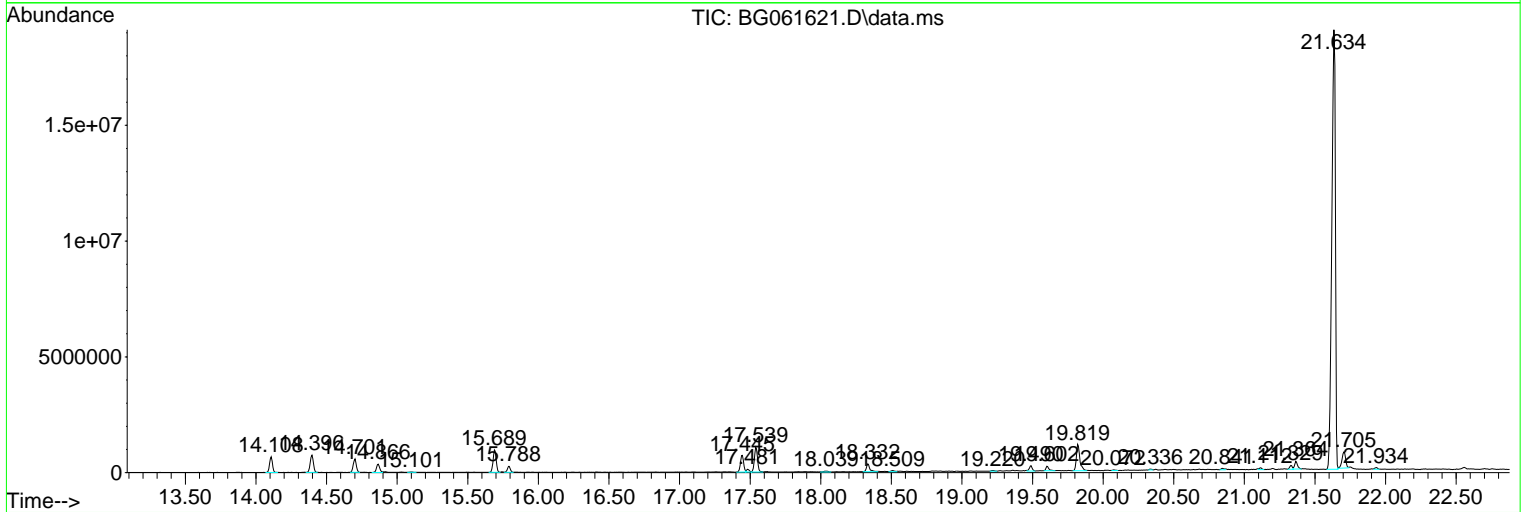
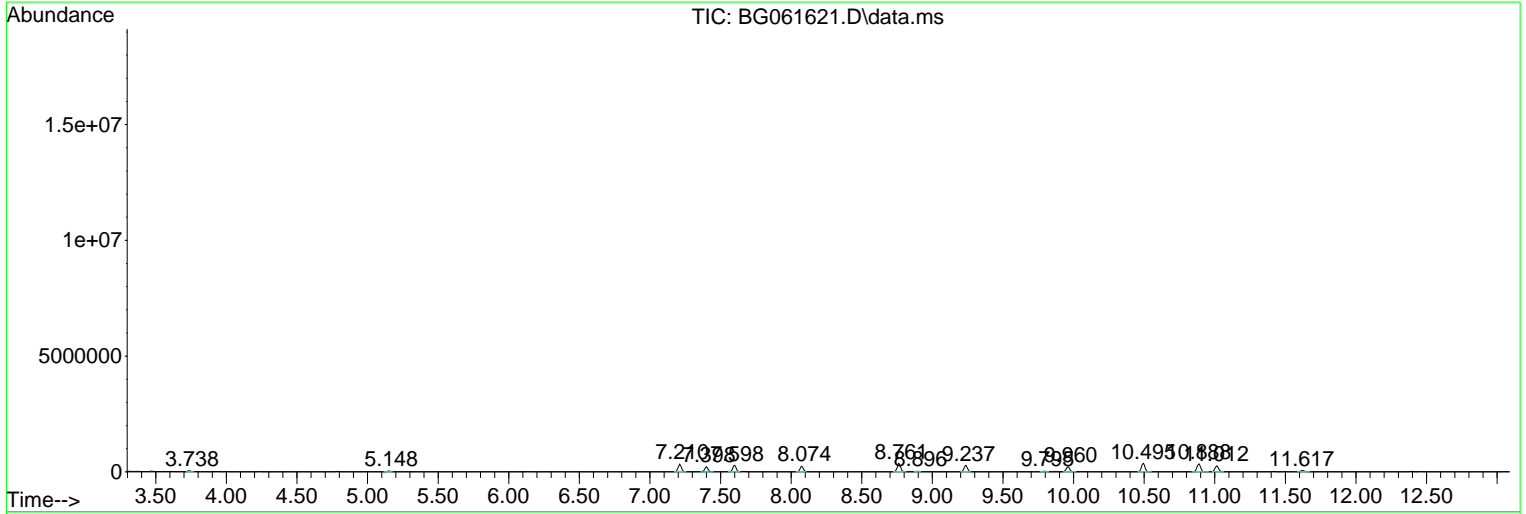
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 ClientSampleId :  
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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\SFAM-EPA-BG062024.MA.M  
 Quant Title : SVOA CALIBRATION

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



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 Sample : P2754-08  
 Misc :  
 ALS Vial : 11 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 A4BP7

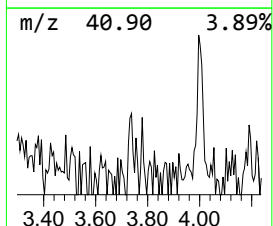
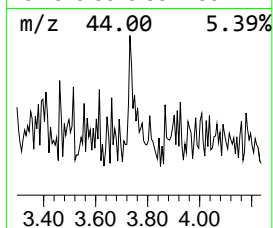
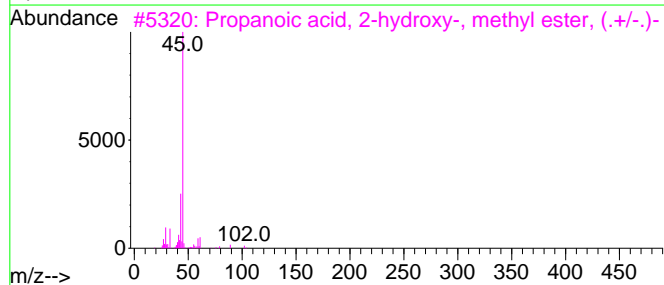
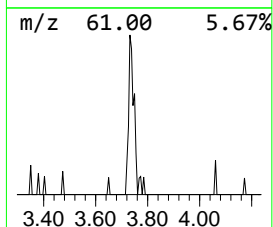
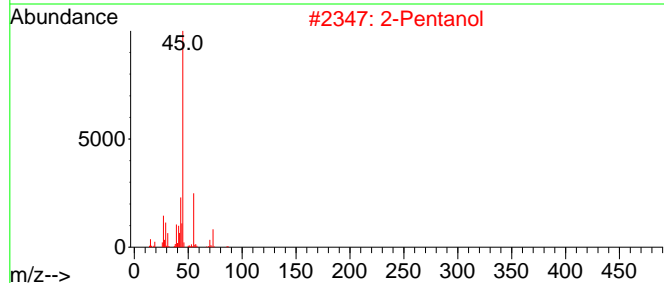
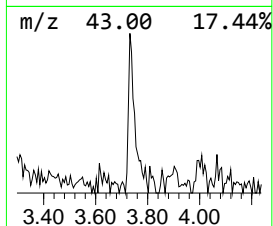
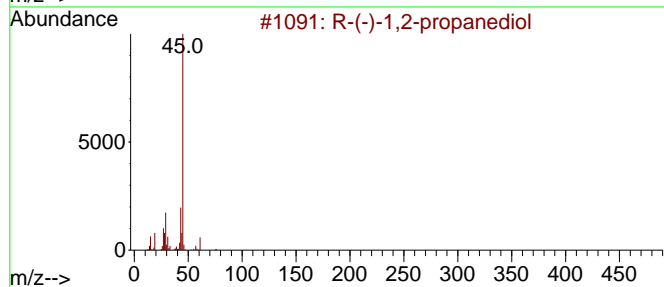
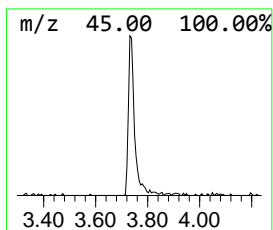
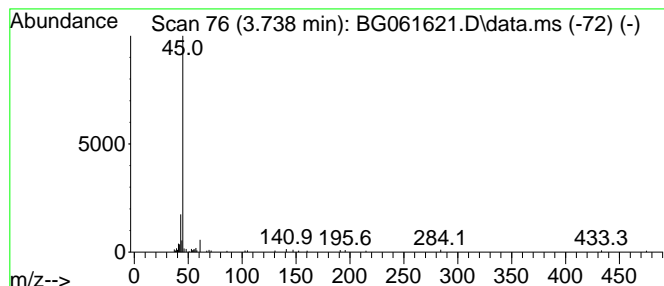
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\SFAM-EPA-BG062024.MA.M  
 Quant Title : SVOA CALIBRATION

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

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 Peak Number 1 unknown-01 Concentration Rank 6

| R.T.  | EstConc    | Area  | Relative to ISTD       | R.T.  |
|-------|------------|-------|------------------------|-------|
| 3.738 | 2.93 ng/ul | 57908 | 1,4-Dichlorobenzene-d4 | 8.074 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|---------|-------------|------|
| 1    |    |   | R-(-)-1,2-propanediol               | 76  | C3H8O2  | 004254-14-2 | 40   |
| 2    |    |   | 2-Pentanol                          | 88  | C5H12O  | 006032-29-7 | 9    |
| 3    |    |   | Propanoic acid, 2-hydroxy-, meth... | 104 | C4H8O3  | 000547-64-8 | 9    |
| 4    |    |   | (S)-(+)-1,2-Propanediol             | 76  | C3H8O2  | 004254-15-3 | 9    |
| 5    |    |   | Methoxyacetic acid, pentyl ester    | 160 | C8H16O3 | 168920-35-2 | 9    |



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Instrument :  
 BNA\_G  
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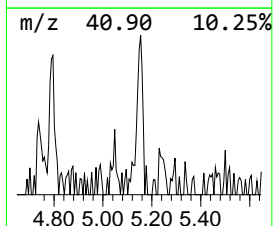
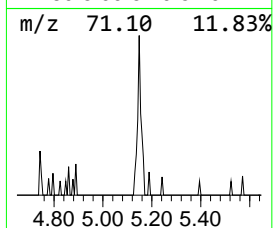
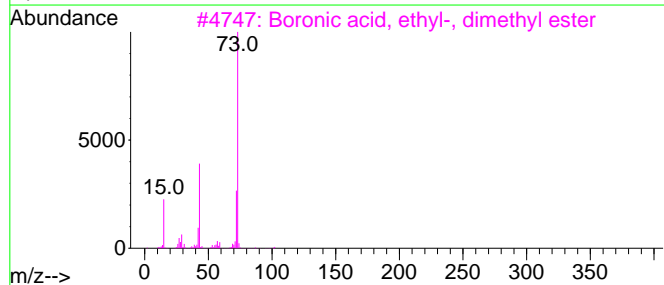
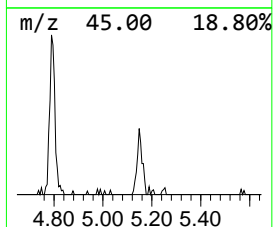
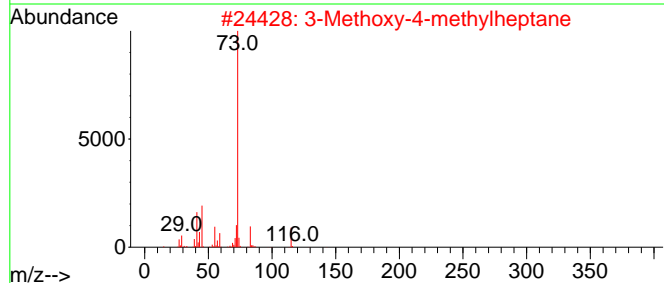
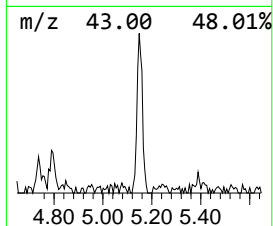
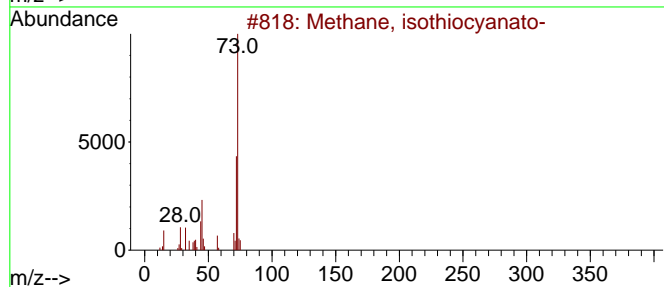
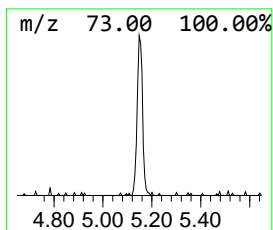
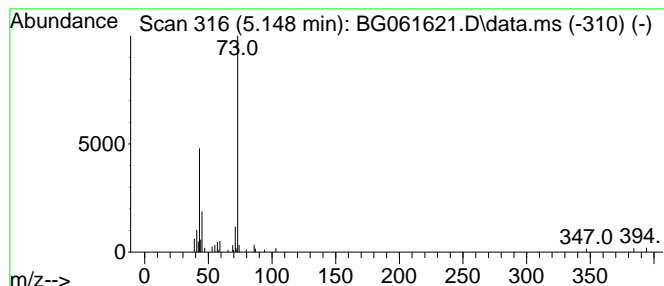
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\SFAM-EPA-BG062024.MA.M  
 Quant Title : SVOA CALIBRATION

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

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 Peak Number 2 unknown-02 Concentration Rank 7

| R.T.  | EstConc    | Area  | Relative to ISTD       | R.T.  |
|-------|------------|-------|------------------------|-------|
| 5.148 | 2.87 ng/ul | 56616 | 1,4-Dichlorobenzene-d4 | 8.074 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|----------|--------------|------|
| 1    |    |   | Methane, isothiocyanato-            | 73  | C2H3NS   | 000556-61-6  | 43   |
| 2    |    |   | 3-Methoxy-4-methylheptane           | 144 | C9H20O   | 1000375-01-3 | 28   |
| 3    |    |   | Boronic acid, ethyl-, dimethyl e... | 102 | C4H11B02 | 007318-82-3  | 25   |
| 4    |    |   | Cyclopropanetetradecanoic acid, ... | 394 | C26H50O2 | 052355-42-7  | 9    |
| 5    |    |   | Pentanol, 5-amino-                  | 103 | C5H13NO  | 002508-29-4  | 9    |



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 Misc :  
 ALS Vial : 11 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
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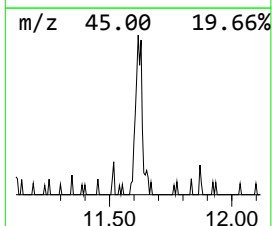
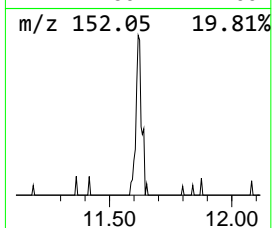
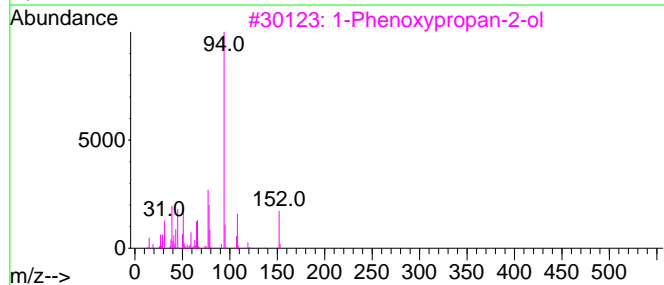
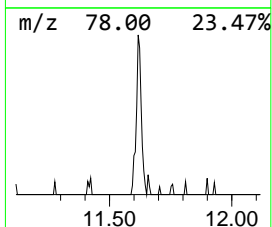
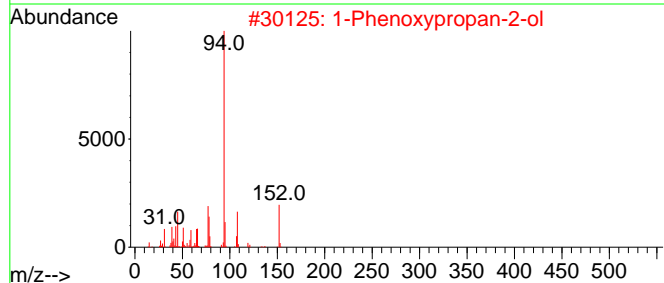
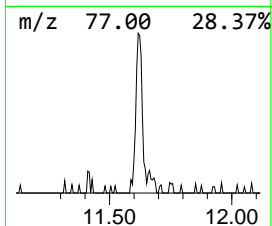
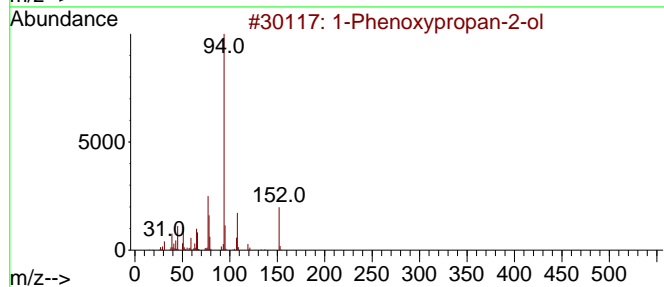
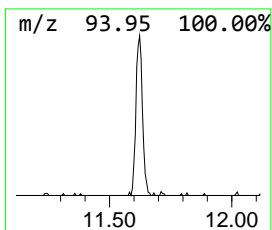
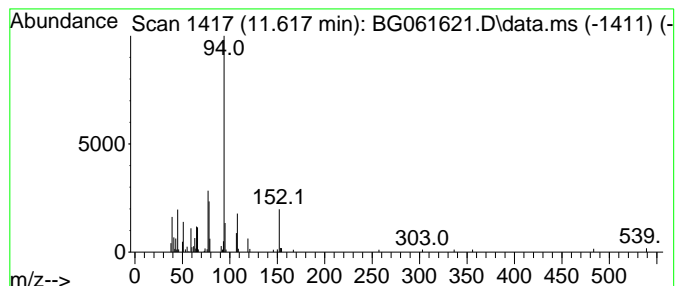
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\SFAM-EPA-BG062024.MA.M  
 Quant Title : SVOA CALIBRATION

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

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 Peak Number 3 1-Phenoxypropan-2-ol Concentration Rank 5

| R.T.   | EstConc    | Area   | Relative to ISTD | R.T.   |
|--------|------------|--------|------------------|--------|
| 11.617 | 3.30 ng/ul | 103873 | Naphthalene-d8   | 10.888 |

| Hit# | of | Tentative ID           | MW  | MolForm | CAS#        | Qual |
|------|----|------------------------|-----|---------|-------------|------|
| 1    | 5  | 1-Phenoxypropan-2-ol   | 152 | C9H12O2 | 000770-35-4 | 97   |
| 2    |    | 1-Phenoxypropan-2-ol   | 152 | C9H12O2 | 000770-35-4 | 94   |
| 3    |    | 1-Phenoxypropan-2-ol   | 152 | C9H12O2 | 000770-35-4 | 93   |
| 4    |    | 1-Propanol, 3-phenoxy- | 152 | C9H12O2 | 006180-61-6 | 87   |
| 5    |    | 1-Phenoxypropan-2-ol   | 152 | C9H12O2 | 000770-35-4 | 87   |



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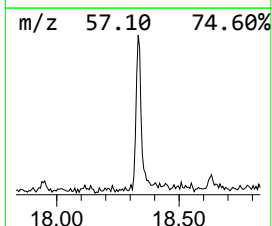
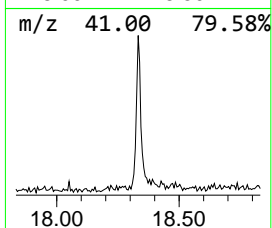
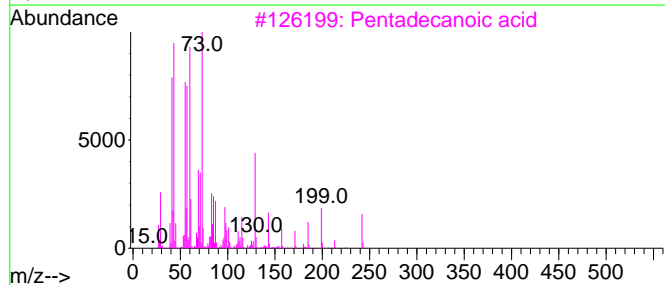
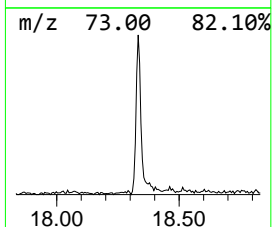
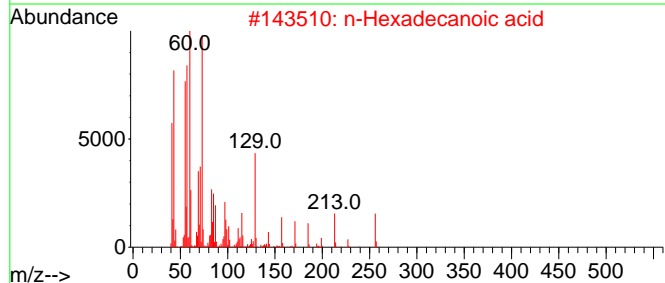
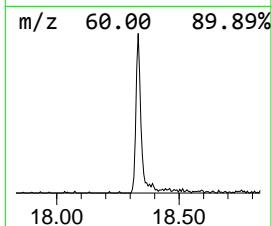
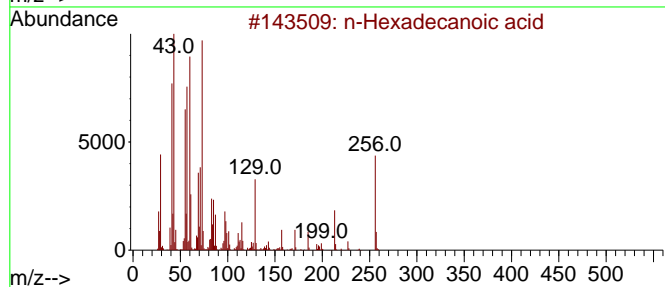
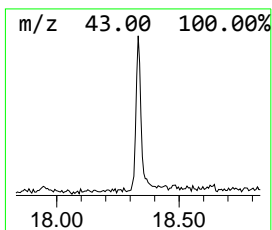
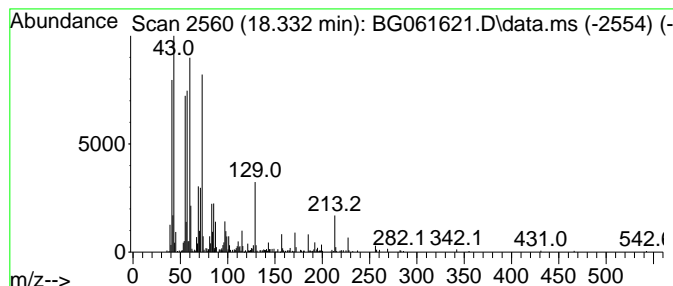
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 Quant Title : SVOA CALIBRATION

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

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 Peak Number 4 n-Hexadecanoic acid Concentration Rank 1

| R.T.   | EstConc    | Area   | Relative to ISTD | R.T.   |
|--------|------------|--------|------------------|--------|
| 18.333 | 9.43 ng/ul | 538839 | Phenanthrene-d10 | 17.445 |

| Hit# | of 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|------|---------------------|-----|----------|-------------|------|
| 1    |      | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 91   |
| 2    |      | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 90   |
| 3    |      | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 87   |
| 4    |      | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 83   |
| 5    |      | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 83   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG062124\  
 Data File : BG061621.D  
 Acq On : 21 Jun 2024 15:29  
 Operator : MA/JU  
 Sample : P2754-08  
 Misc :  
 ALS Vial : 11 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 A4BP7

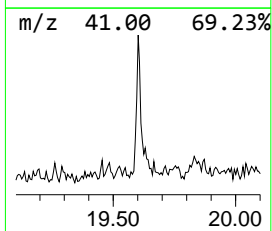
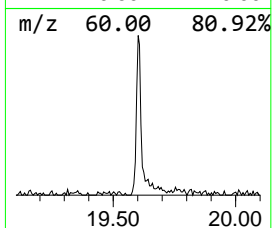
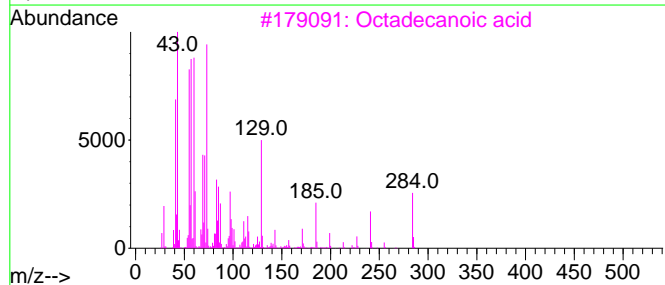
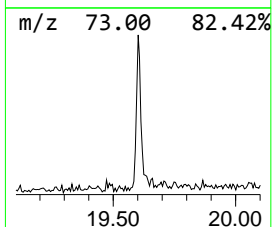
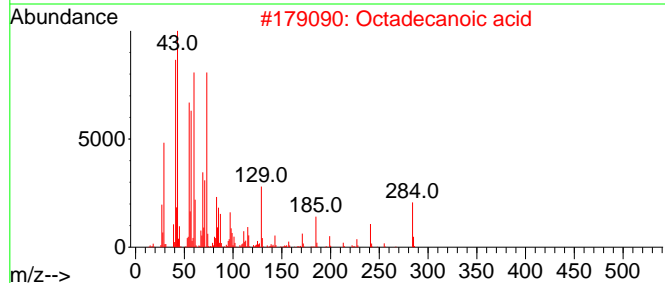
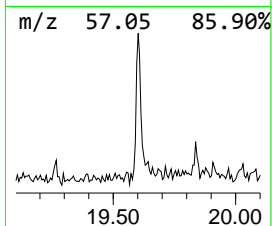
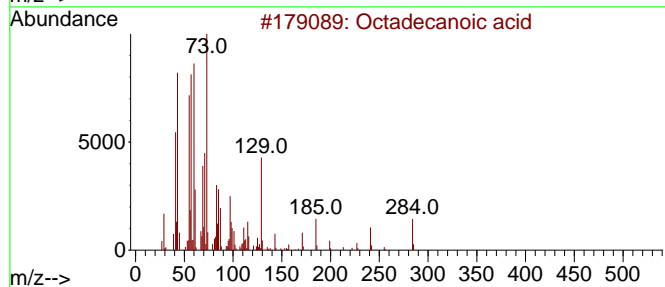
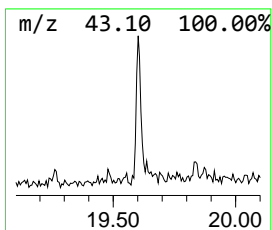
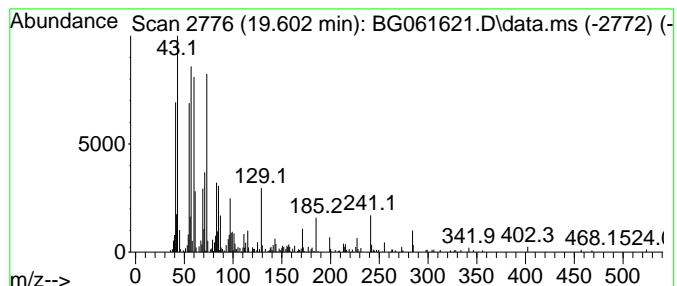
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 Quant Title : SVOA CALIBRATION

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

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 Peak Number 5 Octadecanoic acid Concentration Rank 3

| R.T.   | EstConc    | Area   | Relative to ISTD | R.T.   |
|--------|------------|--------|------------------|--------|
| 19.602 | 4.39 ng/ul | 273687 | Chrysene-d12     | 21.705 |

| Hit# | of | 5 | Tentative ID      | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------|-----|----------|-------------|------|
| 1    |    |   | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 97   |
| 2    |    |   | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 97   |
| 3    |    |   | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 95   |
| 4    |    |   | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 90   |
| 5    |    |   | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 87   |





Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG062124\  
 Data File : BG061621.D  
 Acq On : 21 Jun 2024 15:29  
 Operator : MA/JU  
 Sample : P2754-08  
 Misc :  
 ALS Vial : 11 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 A4BP7

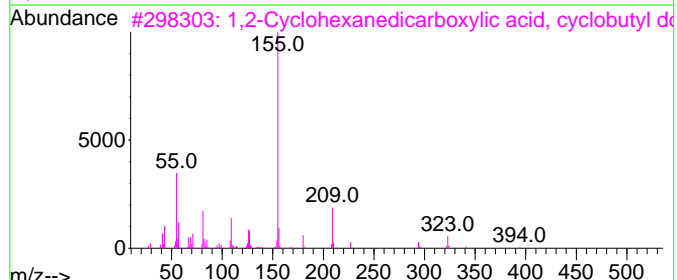
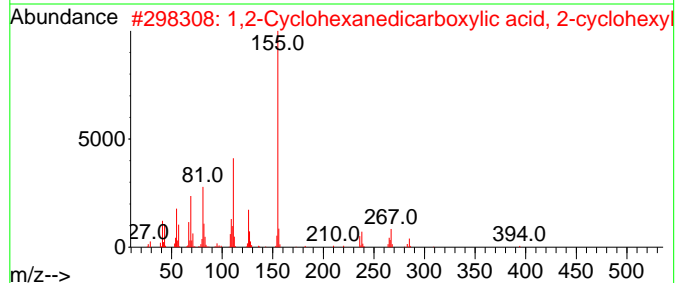
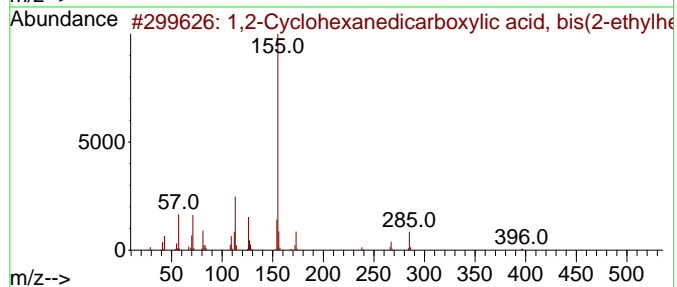
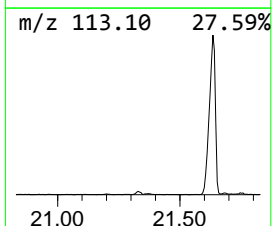
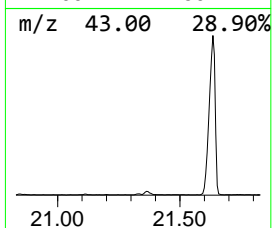
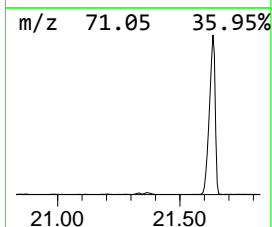
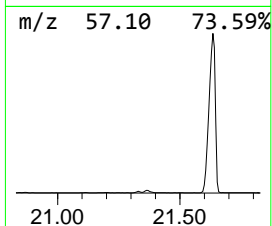
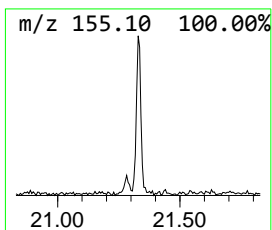
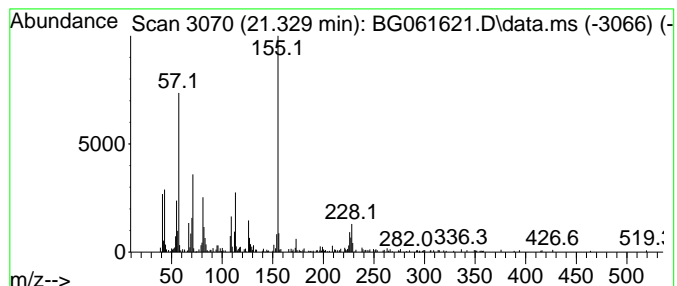
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 Quant Title : SVOA CALIBRATION

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

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 Peak Number 6 1,2-Cyclohexanedicarboxylic... Concentration Rank 4

| R.T.   | EstConc    | Area   | Relative to ISTD | R.T.   |
|--------|------------|--------|------------------|--------|
| 21.329 | 3.54 ng/ul | 220667 | Chrysene-d12     | 21.705 |

| Hit# | of 5 | Tentative ID                        | MW  | MolForm    | CAS#         | Qual |
|------|------|-------------------------------------|-----|------------|--------------|------|
| 1    |      | 1,2-Cyclohexanedicarboxylic acid... | 396 | C24H44O4   | 000084-71-9  | 64   |
| 2    |      | 1,2-Cyclohexanedicarboxylic acid... | 394 | C24H42O4   | 1010339-72-9 | 64   |
| 3    |      | 1,2-Cyclohexanedicarboxylic acid... | 394 | C24H42O4   | 1000339-75-6 | 50   |
| 4    |      | 1,2-Cyclohexanedicarboxylic acid... | 380 | C21H29ClO4 | 1000339-79-2 | 47   |
| 5    |      | 1,2-Cyclohexanedicarboxylic acid... | 298 | C17H30O4   | 1000339-42-5 | 47   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG062124\  
 Data File : BG061621.D  
 Acq On : 21 Jun 2024 15:29  
 Operator : MA/JU  
 Sample : P2754-08  
 Misc :  
 ALS Vial : 11 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 A4BP7

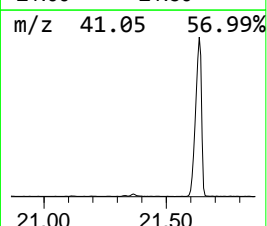
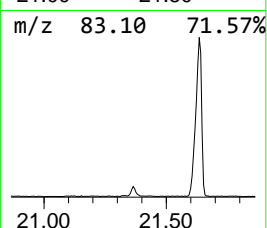
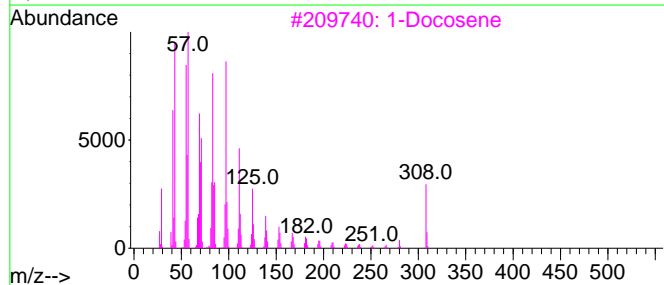
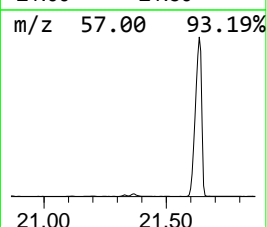
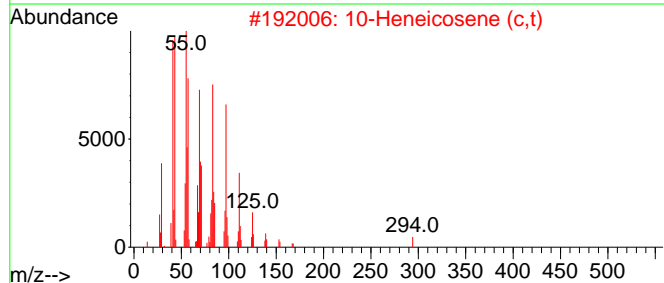
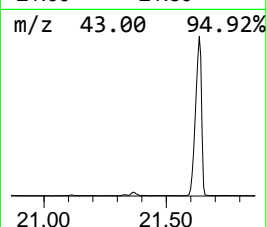
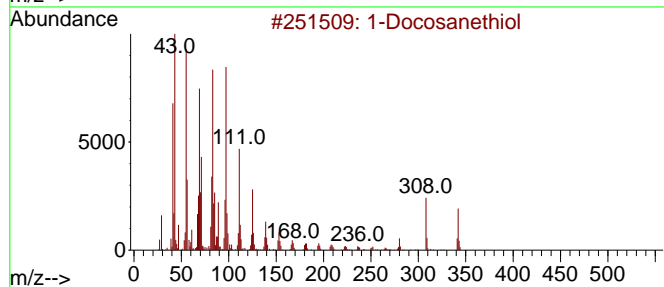
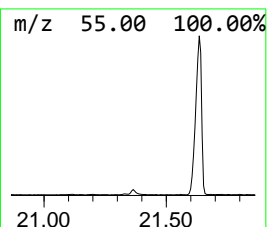
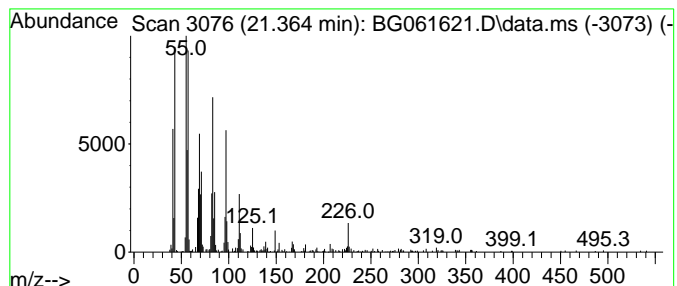
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 Quant Title : SVOA CALIBRATION

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

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 Peak Number 7 1-Docosanethiol Concentration Rank 2

| R.T.   | EstConc    | Area   | Relative to ISTD | R.T.   |
|--------|------------|--------|------------------|--------|
| 21.364 | 7.28 ng/ul | 454626 | Chrysene-d12     | 21.705 |

| Hit# | of | 5 | Tentative ID                   | MW  | MolForm    | CAS#        | Qual |
|------|----|---|--------------------------------|-----|------------|-------------|------|
| 1    |    |   | 1-Docosanethiol                | 342 | C22H46S    | 007773-83-3 | 91   |
| 2    |    |   | 10-Heneicosene (c,t)           | 294 | C21H42     | 095008-11-0 | 90   |
| 3    |    |   | 1-Docosene                     | 308 | C22H44     | 001599-67-3 | 86   |
| 4    |    |   | 1-Docosene                     | 308 | C22H44     | 001599-67-3 | 81   |
| 5    |    |   | Heptadecyl heptafluorobutyrate | 452 | C21H35F7O2 | 959085-66-6 | 76   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG062124\  
 Data File : BG061621.D  
 Acq On : 21 Jun 2024 15:29  
 Operator : MA/JU  
 Sample : P2754-08  
 Misc :  
 ALS Vial : 11 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 A4BP7

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\SFAM-EPA-BG062024.MA.M  
 Quant Title : SVOA 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 |
| unknown-01         | 3.738  | 2.9     | ng/ul | 57908    | 1                     | 8.074  | 394683  | 20.0 |
| unknown-02         | 5.148  | 2.9     | ng/ul | 56616    | 1                     | 8.074  | 394683  | 20.0 |
| 1-Phenoxypropan... | 11.617 | 3.3     | ng/ul | 103873   | 2                     | 10.888 | 628936  | 20.0 |
| n-Hexadecanoic ... | 18.333 | 9.4     | ng/ul | 538839   | 4                     | 17.445 | 1142250 | 20.0 |
| Octadecanoic acid  | 19.602 | 4.4     | ng/ul | 273687   | 5                     | 21.705 | 1248230 | 20.0 |
| 1,2-Cyclohexane... | 21.329 | 3.5     | ng/ul | 220667   | 5                     | 21.705 | 1248230 | 20.0 |
| 1-Docosanethiol    | 21.364 | 7.3     | ng/ul | 454626   | 5                     | 21.705 | 1248230 | 20.0 |