

Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM081924\  
 Data File : BM047255.D  
 Acq On : 19 Aug 2024 16:48  
 Operator : RC/JU  
 Sample : P3580-02  
 Misc :  
 ALS Vial : 12 Sample Multiplier: 1

Instrument :  
 BNA\_M  
 ClientSampleId :  
 926-K1-SD-0.5-1-081224

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\_M\Methods\8270-BM081024.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM047255.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         | 3.263       | 61            | 64          | 77           | rVB      | 47891          | 83259         | 1.80%           | 0.279%        |
| 2         | 4.569       | 281           | 286         | 292          | rVB      | 47085          | 71085         | 1.54%           | 0.238%        |
| 3         | 5.016       | 356           | 362         | 373          | rBV      | 1163070        | 1774656       | 38.39%          | 5.945%        |
| 4         | 6.581       | 621           | 628         | 640          | rBV      | 1146182        | 1854194       | 40.11%          | 6.212%        |
| 5         | 7.363       | 752           | 761         | 767          | rBV      | 503029         | 760757        | 16.46%          | 2.549%        |
| 6         | 8.510       | 948           | 956         | 966          | rBV      | 730125         | 1175883       | 25.44%          | 3.939%        |
| 7         | 9.092       | 1049          | 1055        | 1061         | rBV2     | 28255          | 46656         | 1.01%           | 0.156%        |
| 8         | 10.122      | 1222          | 1230        | 1239         | rBV      | 623833         | 1033610       | 22.36%          | 3.463%        |
| 9         | 10.880      | 1353          | 1359        | 1368         | rBV2     | 75161          | 152273        | 3.29%           | 0.510%        |
| 10        | 12.627      | 1649          | 1656        | 1668         | rBV      | 1745383        | 2644252       | 57.20%          | 8.858%        |
| 11        | 13.904      | 1865          | 1873        | 1885         | rBV      | 58716          | 172931        | 3.74%           | 0.579%        |
| 12        | 14.021      | 1887          | 1893        | 1901         | rVB      | 1021405        | 1494839       | 32.33%          | 5.008%        |
| 13        | 14.274      | 1928          | 1936        | 1942         | rBV6     | 45938          | 114448        | 2.48%           | 0.383%        |
| 14        | 14.880      | 2032          | 2039        | 2043         | rBV      | 44125          | 74691         | 1.62%           | 0.250%        |
| 15        | 15.533      | 2144          | 2150        | 2162         | rBV      | 2175753        | 3024394       | 65.42%          | 10.132%       |
| 16        | 16.786      | 2358          | 2363        | 2369         | rBV      | 1383197        | 1985419       | 42.95%          | 6.651%        |
| 17        | 17.721      | 2517          | 2522        | 2530         | rBV      | 409260         | 728838        | 15.77%          | 2.442%        |
| 18        | 17.786      | 2530          | 2533        | 2538         | rVB      | 73526          | 118051        | 2.55%           | 0.395%        |
| 19        | 18.868      | 2713          | 2717        | 2720         | rBV      | 80748          | 102276        | 2.21%           | 0.343%        |
| 20        | 19.027      | 2739          | 2744        | 2756         | rBV      | 714142         | 1271823       | 27.51%          | 4.261%        |
| 21        | 19.233      | 2776          | 2779        | 2783         | rVB      | 55873          | 67465         | 1.46%           | 0.226%        |
| 22        | 19.456      | 2812          | 2817        | 2825         | rBV      | 3751112        | 4623018       | 100.00%         | 15.487%       |
| 23        | 20.768      | 3036          | 3040        | 3051         | rBV      | 360723         | 582142        | 12.59%          | 1.950%        |
| 24        | 21.027      | 3079          | 3084        | 3089         | rBV      | 2119285        | 2901836       | 62.77%          | 9.721%        |
| 25        | 23.733      | 3537          | 3544        | 3559         | rVB      | 1288304        | 2992137       | 64.72%          | 10.024%       |

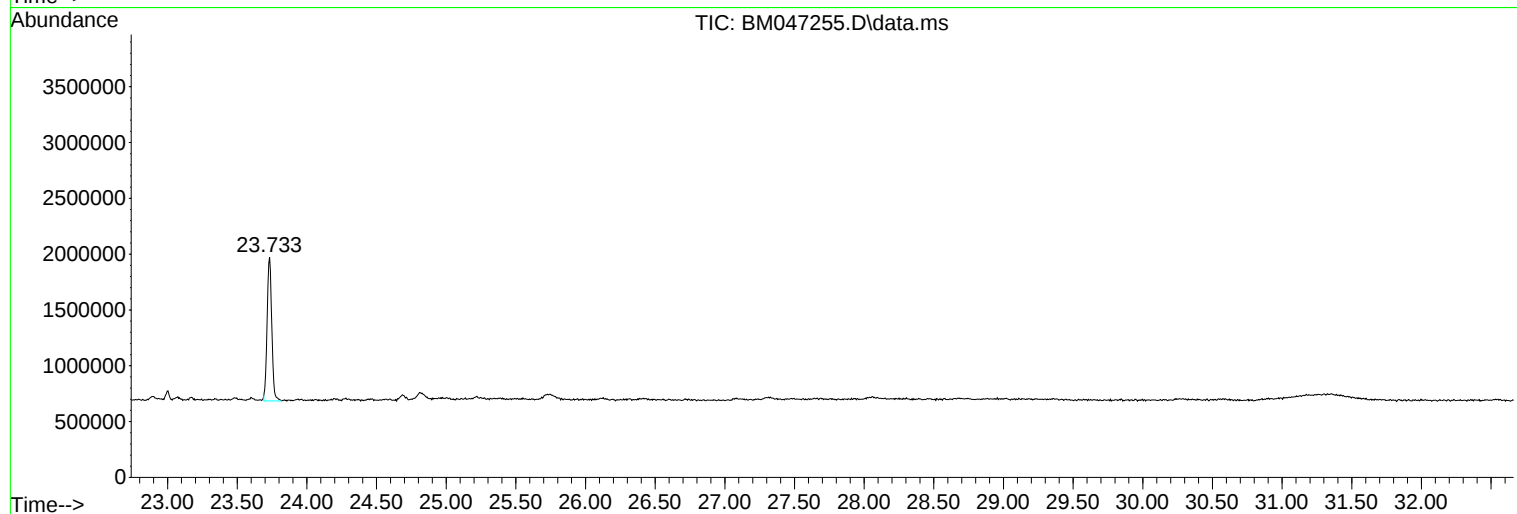
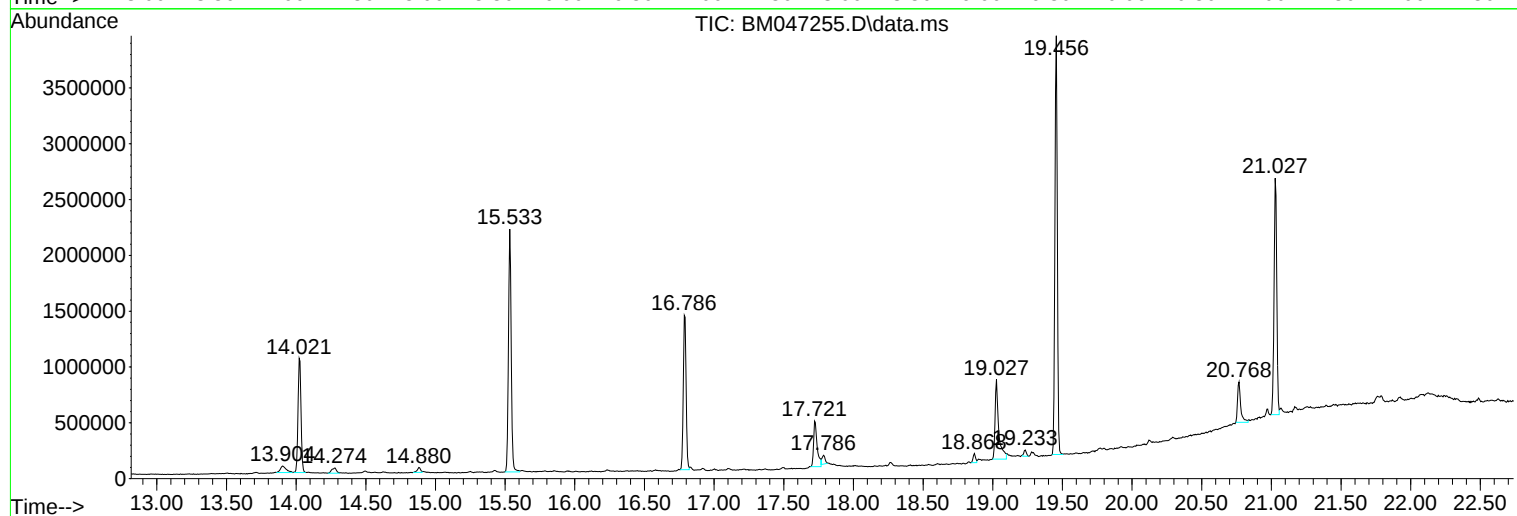
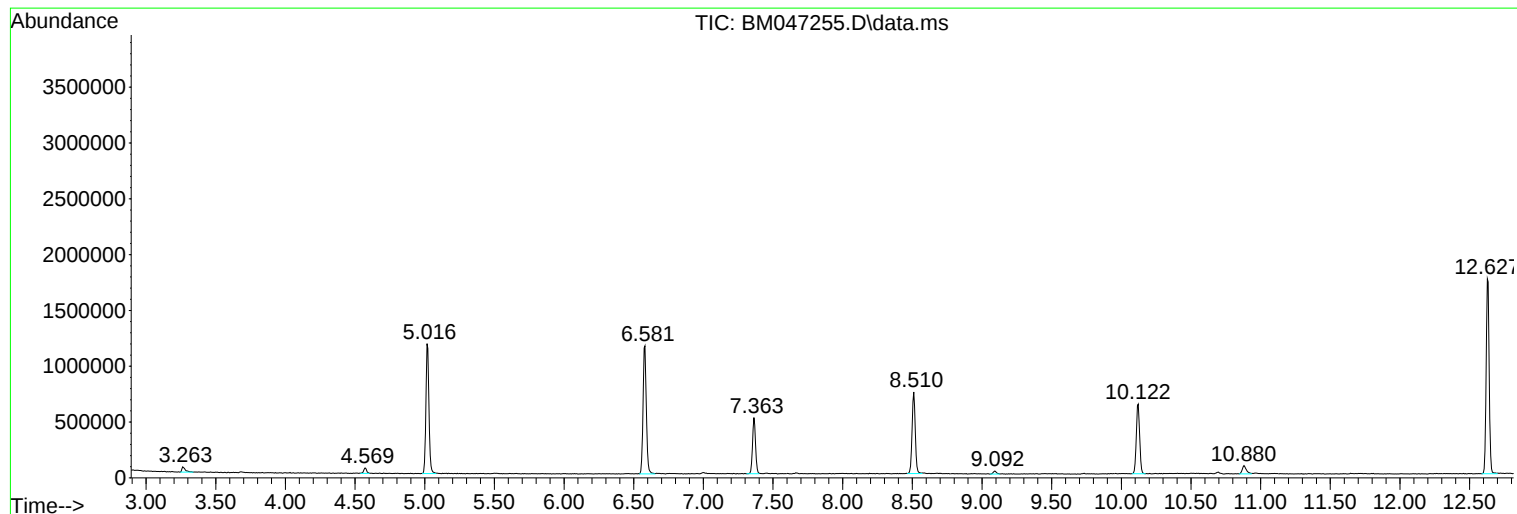
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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM081024.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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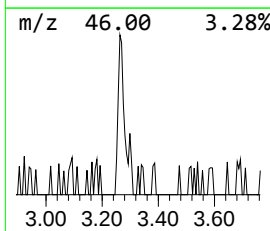
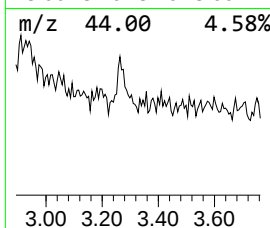
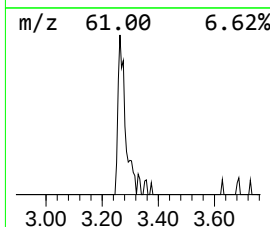
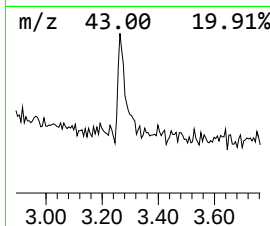
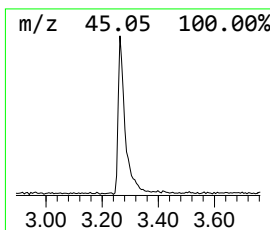
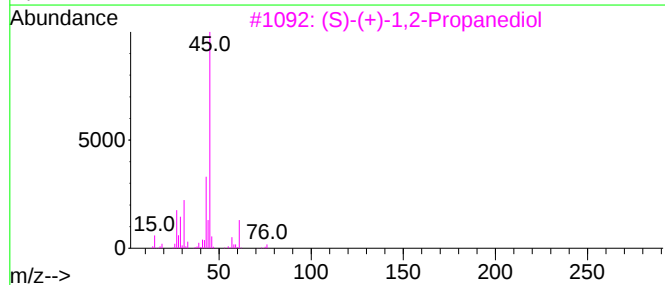
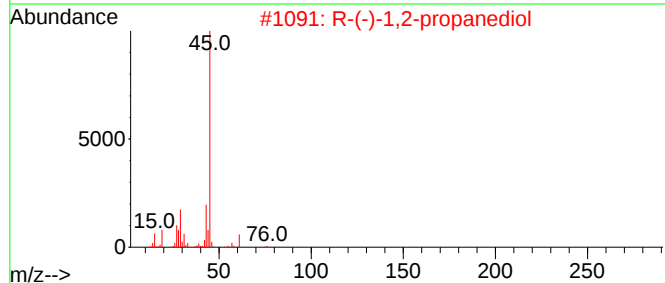
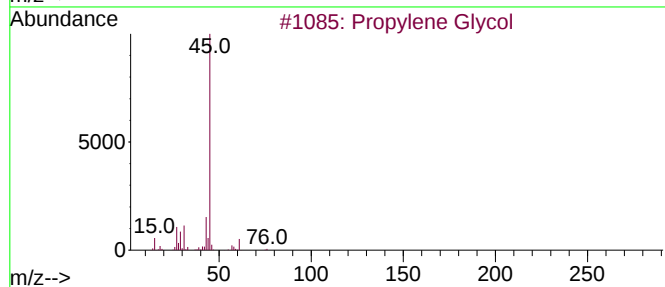
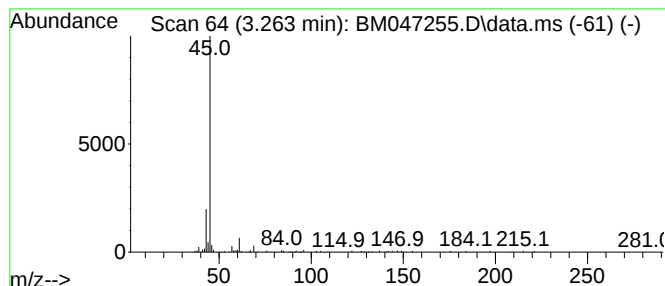
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM081024.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 Propylene Glycol Concentration Rank 6

| R.T.  | EstConc | Area  | Relative to ISTD       | R.T.  |
|-------|---------|-------|------------------------|-------|
| 3.263 | 2.19 ng | 83259 | 1,4-Dichlorobenzene-d4 | 7.363 |

| Hit# | of | 5 | Tentative ID            | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------|-----|---------|-------------|------|
| 1    |    |   | Propylene Glycol        | 76  | C3H8O2  | 000057-55-6 | 64   |
| 2    |    |   | R-(-)-1,2-propanediol   | 76  | C3H8O2  | 004254-14-2 | 39   |
| 3    |    |   | (S)-(+)-1,2-Propanediol | 76  | C3H8O2  | 004254-15-3 | 14   |
| 4    |    |   | Isopropyl Alcohol       | 60  | C3H8O   | 000067-63-0 | 9    |
| 5    |    |   | 2,4-Pentanediol         | 104 | C5H12O2 | 000625-69-4 | 9    |



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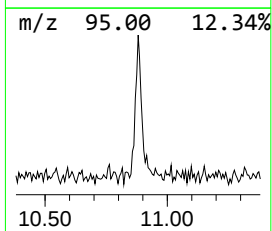
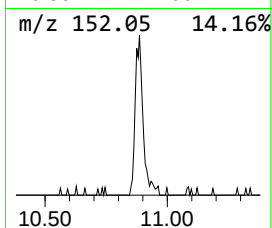
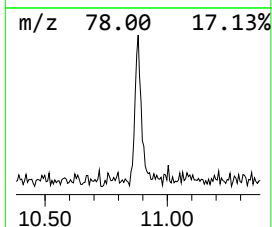
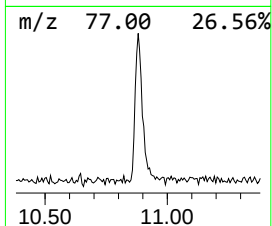
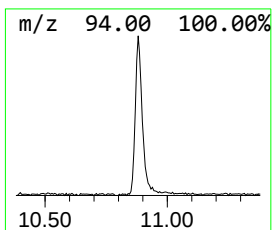
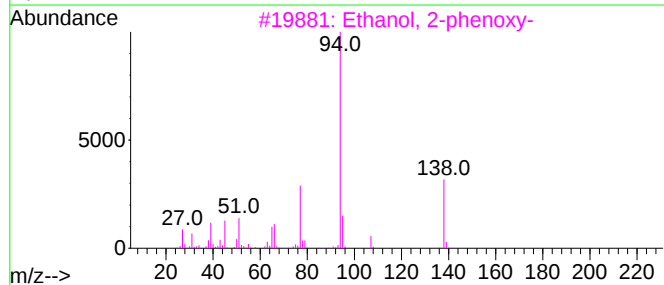
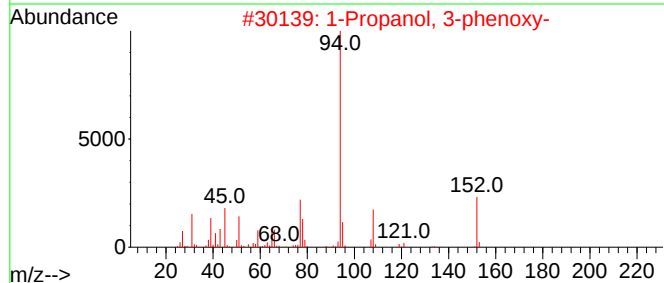
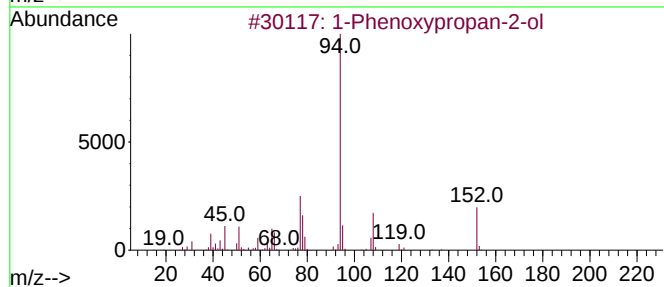
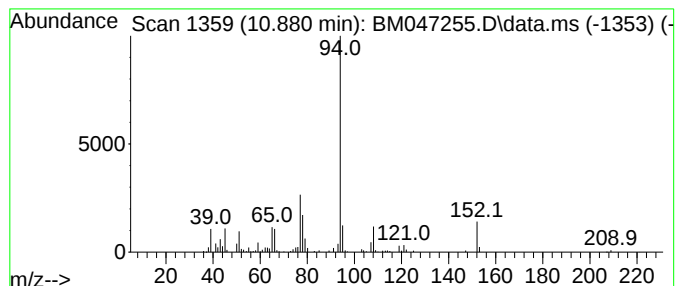
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TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 1-Phenoxypropan-2-ol Concentration Rank 4

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 10.881 | 2.95 ng | 152273 | Naphthalene-d8   | 10.122 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | 1-Phenoxypropan-2-ol                | 152 | C9H12O2  | 000770-35-4 | 94   |
| 2    |    |   | 1-Propanol, 3-phenoxy-              | 152 | C9H12O2  | 006180-61-6 | 83   |
| 3    |    |   | Ethanol, 2-phenoxy-                 | 138 | C8H10O2  | 000122-99-6 | 64   |
| 4    |    |   | 1-Propanol, 2-phenoxy-              | 152 | C9H12O2  | 004169-04-4 | 64   |
| 5    |    |   | Carbonic acid, neopentyl phenyl ... | 208 | C12H16O3 | 013183-19-2 | 59   |



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ALS Vial : 12 Sample Multiplier: 1

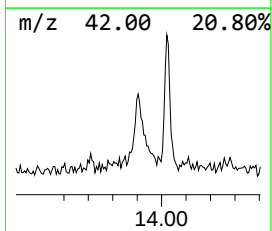
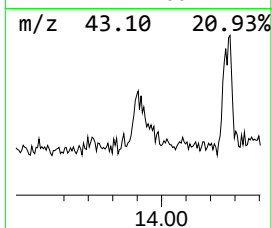
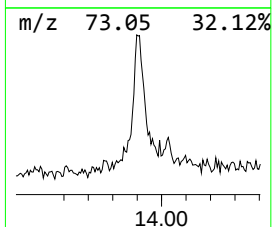
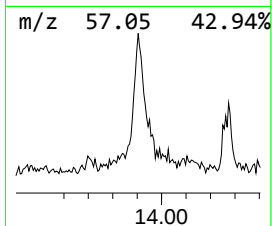
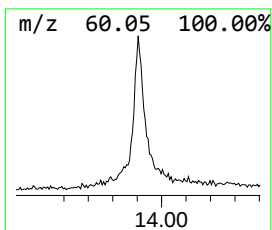
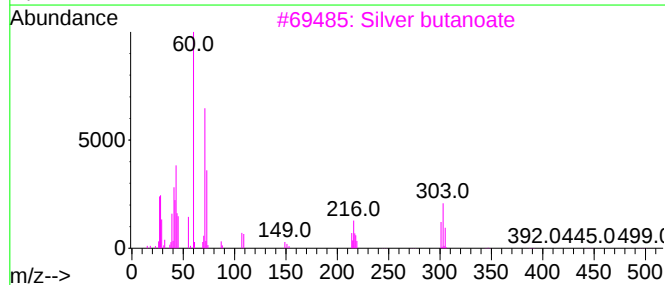
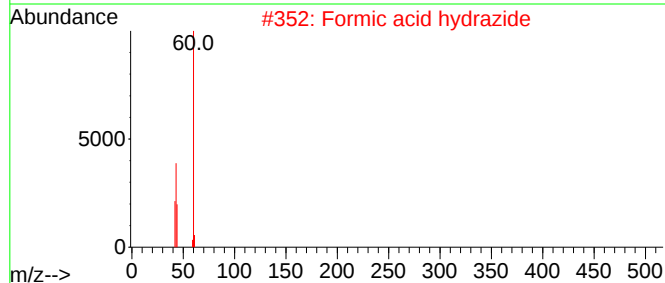
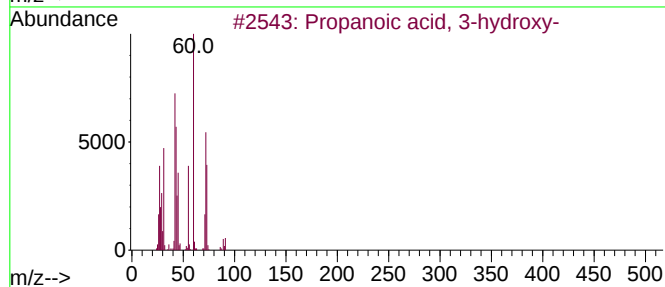
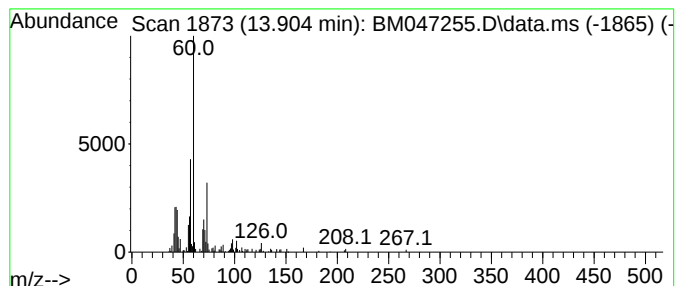
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TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 Propanoic acid, 3-hydroxy- Concentration Rank 5

| R.T.      | EstConc                             | Area   | Relative to ISTD | R.T.        |      |
|-----------|-------------------------------------|--------|------------------|-------------|------|
| 13.904    | 2.31 ng                             | 172931 | Acenaphthene-d10 | 14.027      |      |
| Hit# of 5 | Tentative ID                        | MW     | MolForm          | CAS#        | Qual |
| 1         | Propanoic acid, 3-hydroxy-          | 90     | C3H6O3           | 000503-66-2 | 53   |
| 2         | Formic acid hydrazide               | 60     | CH4N2O           | 000624-84-0 | 53   |
| 3         | Silver butanoate                    | 194    | C4H7AgO2         | 005076-24-4 | 50   |
| 4         | .beta.-D-Glucopyranose, 1,6-anhy... | 162    | C6H10O5          | 000498-07-7 | 50   |
| 5         | Heptanoic acid                      | 130    | C7H14O2          | 000111-14-8 | 47   |



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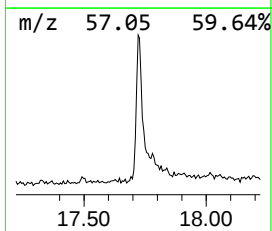
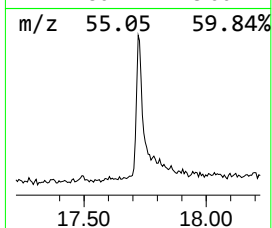
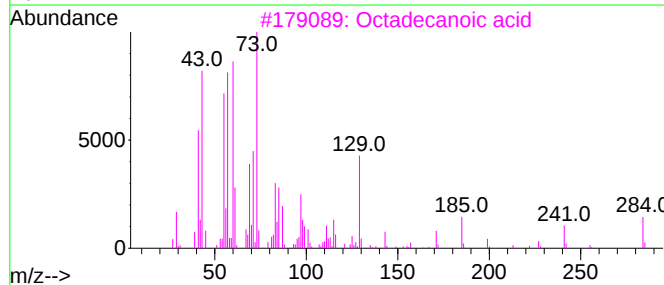
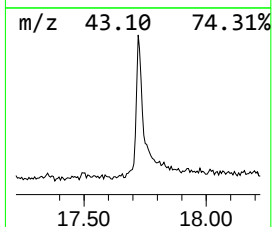
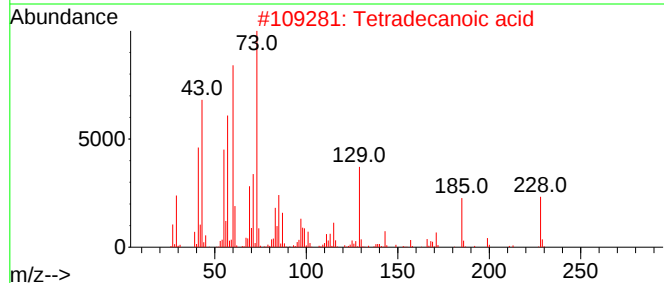
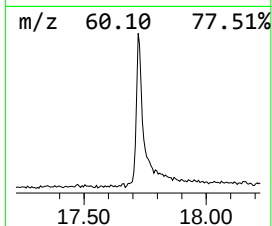
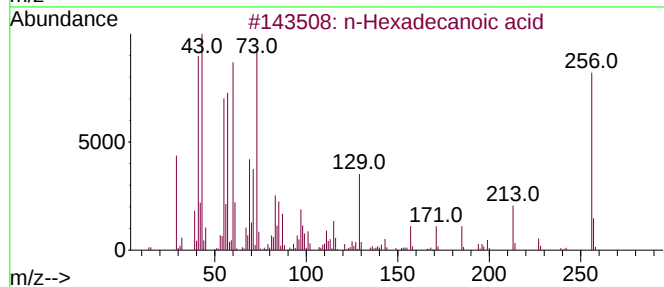
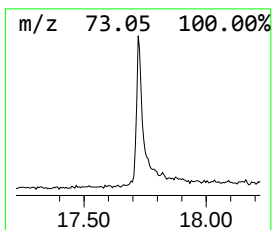
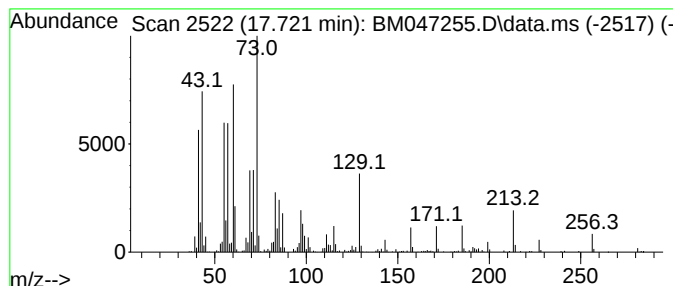
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\*\*\*\*\*  
Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 17.721 | 7.34 ng | 728838 | Phenanthrene-d10 | 16.786 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 99   |
| 2    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 94   |
| 3    |    |   | Octadecanoic acid   | 284 | C18H36O2 | 000057-11-4 | 90   |
| 4    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 87   |
| 5    |    |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 64   |



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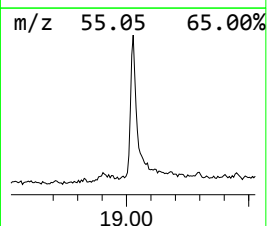
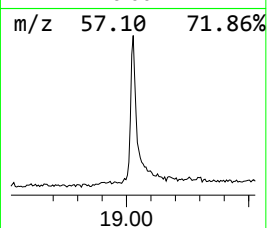
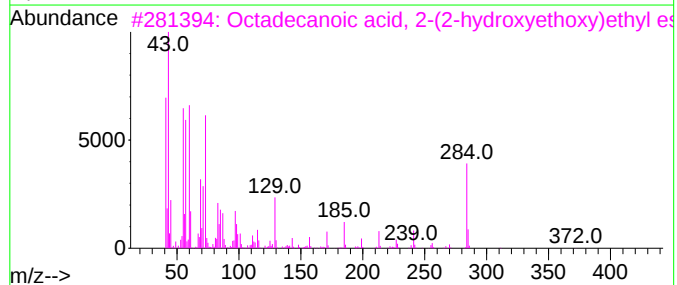
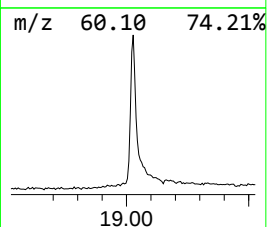
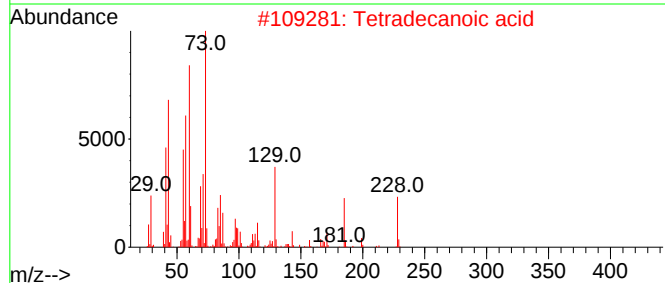
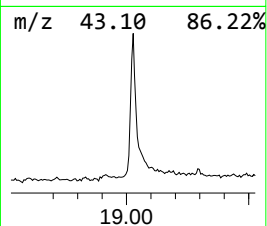
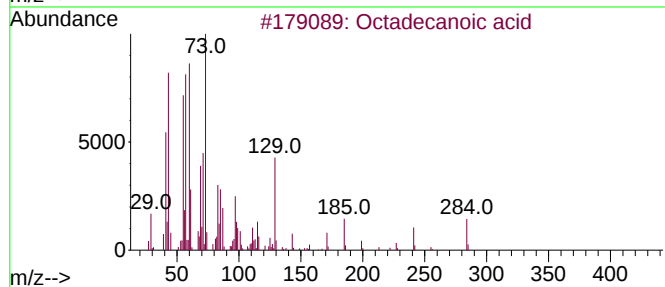
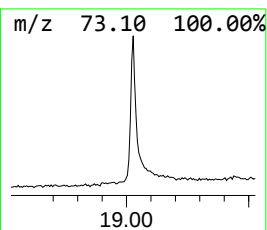
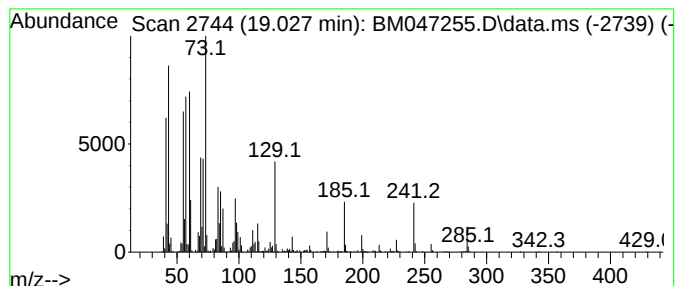
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM081024.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 5 Octadecanoic acid Concentration Rank 1

| R.T.   | EstConc | Area    | Relative to ISTD | R.T.   |
|--------|---------|---------|------------------|--------|
| 19.027 | 8.77 ng | 1271820 | Chrysene-d12     | 21.027 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | Octadecanoic acid                   | 284 | C18H36O2 | 000057-11-4 | 99   |
| 2    |    |   | Tetradecanoic acid                  | 228 | C14H28O2 | 000544-63-8 | 83   |
| 3    |    |   | Octadecanoic acid, 2-(2-hydroxye... | 372 | C22H44O4 | 000106-11-6 | 72   |
| 4    |    |   | n-Decanoic acid                     | 172 | C10H20O2 | 000334-48-5 | 70   |
| 5    |    |   | Pentadecanoic acid                  | 242 | C15H30O2 | 001002-84-2 | 58   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM081924\  
Data File : BM047255.D  
Acq On : 19 Aug 2024 16:48  
Operator : RC/JU  
Sample : P3580-02  
Misc :  
ALS Vial : 12 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
926-K1-SD-0.5-1-081224

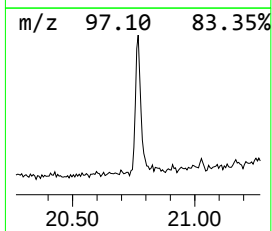
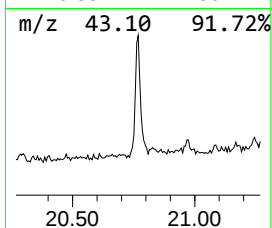
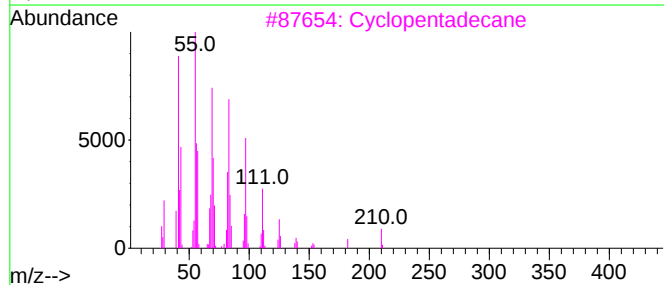
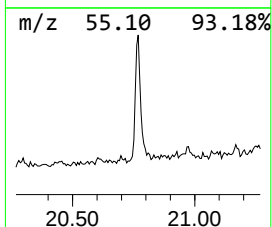
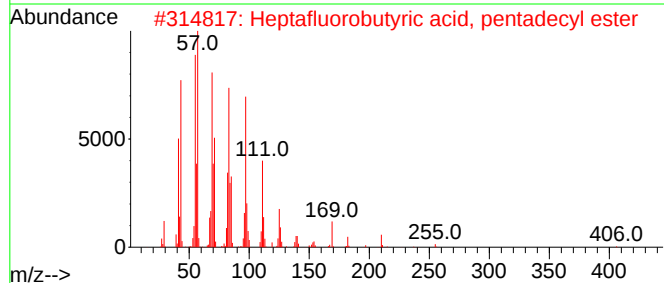
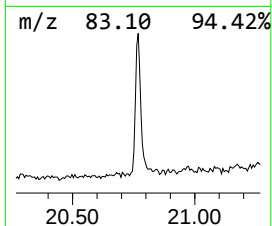
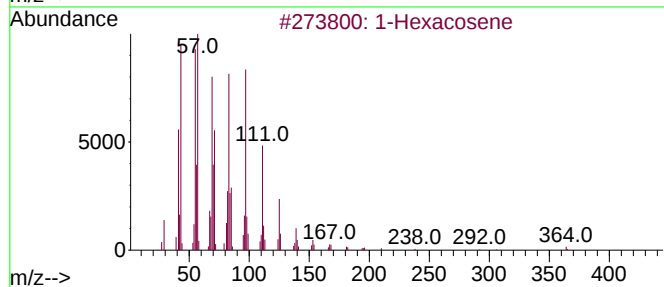
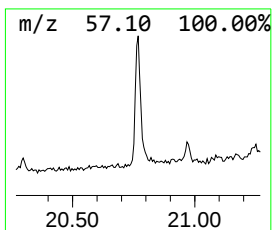
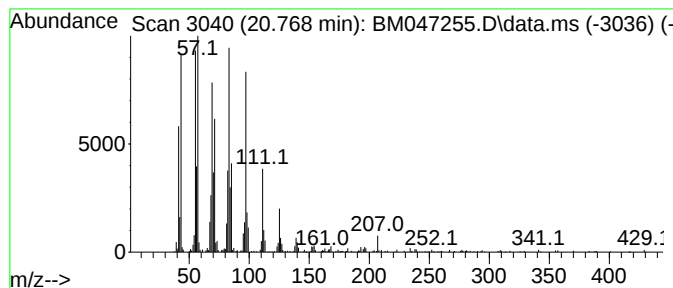
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM081024.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 6 1-Hexacosene Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 20.768 | 4.01 ng | 582142 | Chrysene-d12     | 21.027 |

| Hit# | of                                  | 5 | Tentative ID | MW  | MolForm    | CAS#        | Qual |
|------|-------------------------------------|---|--------------|-----|------------|-------------|------|
| 1    | 1-Hexacosene                        |   |              | 364 | C26H52     | 018835-33-1 | 94   |
| 2    | Heptafluorobutyric acid, pentade... |   |              | 424 | C19H31F7O2 | 959261-23-5 | 94   |
| 3    | Cyclopentadecane                    |   |              | 210 | C15H30     | 000295-48-7 | 93   |
| 4    | Trifluoroacetic acid, pentadecyl... |   |              | 324 | C17H31F3O2 | 959010-23-2 | 91   |
| 5    | Pentacos-1-ene                      |   |              | 350 | C25H50     | 016980-85-1 | 91   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM081924\  
Data File : BM047255.D  
Acq On : 19 Aug 2024 16:48  
Operator : RC/JU  
Sample : P3580-02  
Misc :  
ALS Vial : 12 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
926-K1-SD-0.5-1-081224

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM081024.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 |
| Propylene Glycol   | 3.263  | 2.2     | ng    | 83259    | 1                     | 7.363  | 760757  | 20.0 |
| 1-Phenoxypropan... | 10.881 | 3.0     | ng    | 152273   | 2                     | 10.122 | 1033610 | 20.0 |
| Propanoic acid,... | 13.904 | 2.3     | ng    | 172931   | 3                     | 14.027 | 1494840 | 20.0 |
| n-Hexadecanoic ... | 17.721 | 7.3     | ng    | 728838   | 4                     | 16.786 | 1985420 | 20.0 |
| Octadecanoic acid  | 19.027 | 8.8     | ng    | 1271820  | 5                     | 21.027 | 2901840 | 20.0 |
| 1-Hexacosene       | 20.768 | 4.0     | ng    | 582142   | 5                     | 21.027 | 2901840 | 20.0 |