

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF090421\  
 Data File : BF125374.D  
 Acq On : 4 Sep 2021 17:49  
 Operator : JU/CG  
 Sample : M3648-12  
 Misc :  
 ALS Vial : 16 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 20211059-SI-COMP-4-MODIFIED-EL

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\_F\METHODS\8270-BF081821.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125374.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         | 2.187       | 10            | 17          | 28           | rVB      | 2548912        | 3460076       | 81.42%          | 11.946%       |
| 2         | 5.516       | 579           | 583         | 587          | rBV      | 2495668        | 2397697       | 56.42%          | 8.278%        |
| 3         | 6.522       | 750           | 754         | 767          | rBV      | 1997494        | 1823573       | 42.91%          | 6.296%        |
| 4         | 6.898       | 814           | 818         | 821          | rBV      | 1035531        | 877266        | 20.64%          | 3.029%        |
| 5         | 7.463       | 906           | 914         | 917          | rBV      | 2573630        | 2560351       | 60.25%          | 8.840%        |
| 6         | 8.080       | 1015          | 1019        | 1030         | rBV      | 198864         | 320297        | 7.54%           | 1.106%        |
| 7         | 8.180       | 1032          | 1036        | 1039         | rBV      | 1267063        | 1074084       | 25.27%          | 3.708%        |
| 8         | 9.257       | 1214          | 1219        | 1222         | rBV      | 4814150        | 4249770       | 100.00%         | 14.672%       |
| 9         | 9.645       | 1282          | 1285        | 1289         | rBV      | 141727         | 135530        | 3.19%           | 0.468%        |
| 10        | 9.933       | 1326          | 1334        | 1343         | rBV      | 1392570        | 1219839       | 28.70%          | 4.211%        |
| 11        | 10.727      | 1464          | 1469        | 1472         | rBV      | 2900976        | 2679584       | 63.05%          | 9.251%        |
| 12        | 11.421      | 1583          | 1587        | 1594         | rBV      | 1242992        | 1093265       | 25.73%          | 3.774%        |
| 13        | 11.580      | 1611          | 1614        | 1618         | rBV      | 984890         | 778147        | 18.31%          | 2.687%        |
| 14        | 11.804      | 1645          | 1652        | 1655         | rVB4     | 84958          | 75057         | 1.77%           | 0.259%        |
| 15        | 11.939      | 1672          | 1675        | 1679         | rBV2     | 142532         | 145438        | 3.42%           | 0.502%        |
| 16        | 12.727      | 1806          | 1809        | 1818         | rVB2     | 42005          | 53941         | 1.27%           | 0.186%        |
| 17        | 13.010      | 1852          | 1857        | 1860         | rBV      | 4389952        | 3797780       | 89.36%          | 13.112%       |
| 18        | 13.927      | 2009          | 2013        | 2026         | rBV4     | 76044          | 166820        | 3.93%           | 0.576%        |
| 19        | 14.062      | 2033          | 2036        | 2043         | rVB      | 931906         | 831060        | 19.56%          | 2.869%        |
| 20        | 15.556      | 2284          | 2290        | 2300         | rVB      | 716842         | 978482        | 23.02%          | 3.378%        |
| 21        | 16.015      | 2363          | 2368        | 2374         | rVB2     | 42575          | 63324         | 1.49%           | 0.219%        |
| 22        | 16.533      | 2452          | 2456        | 2461         | rVB2     | 39496          | 57742         | 1.36%           | 0.199%        |
| 23        | 17.133      | 2554          | 2558        | 2567         | rVB5     | 29287          | 63249         | 1.49%           | 0.218%        |
| 24        | 17.862      | 2676          | 2682        | 2691         | rVB5     | 23293          | 62476         | 1.47%           | 0.216%        |

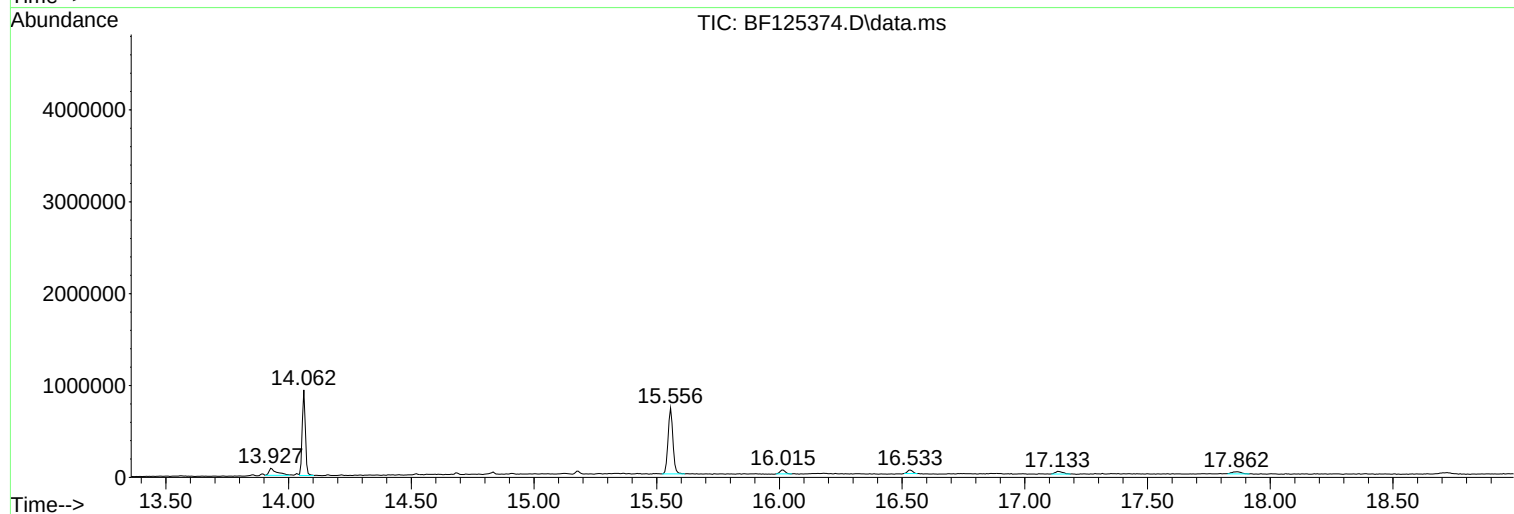
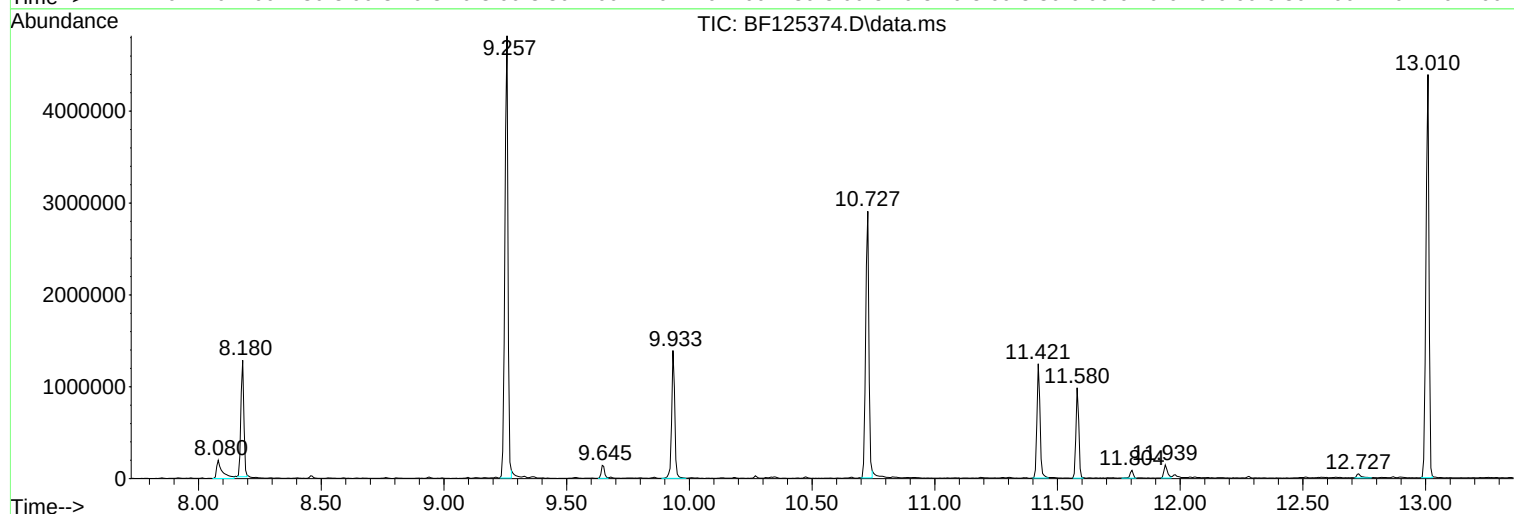
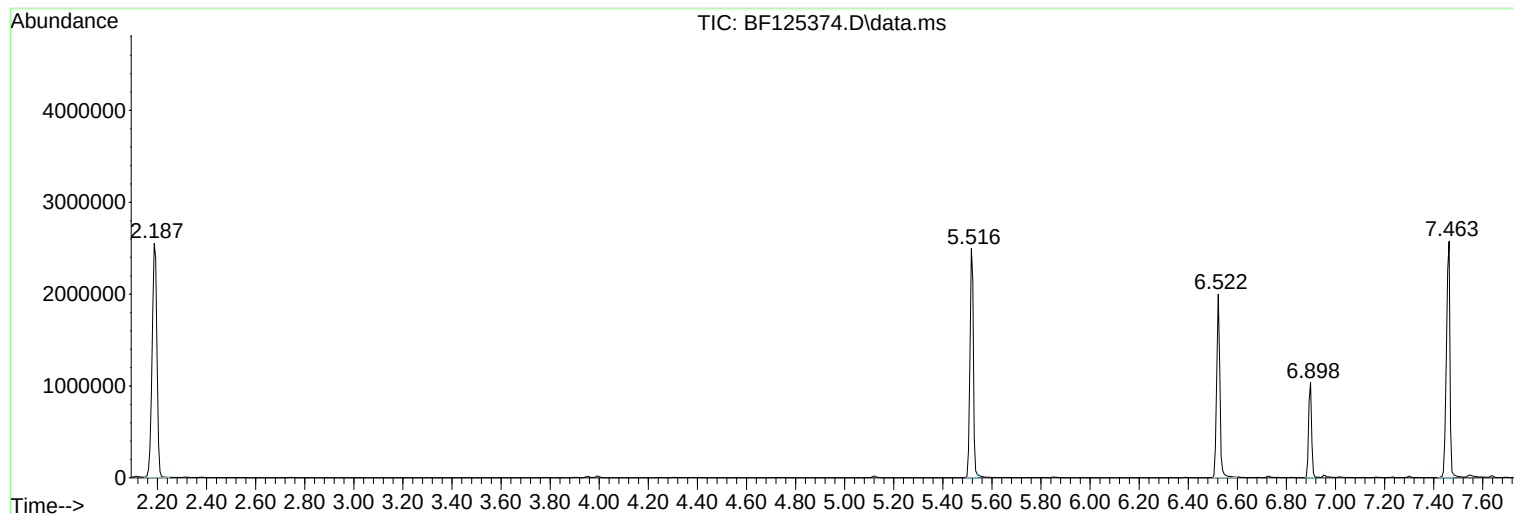
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF081821.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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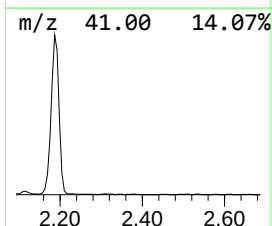
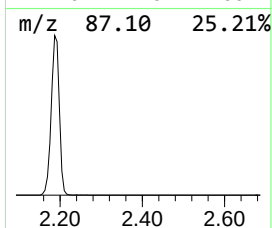
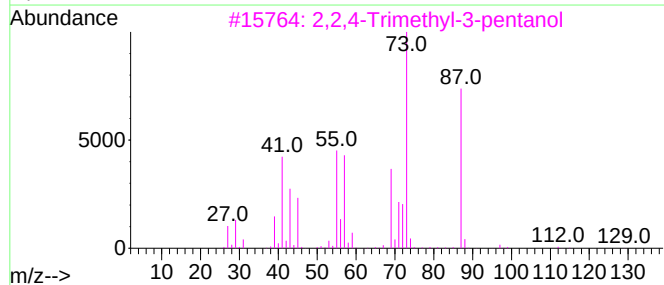
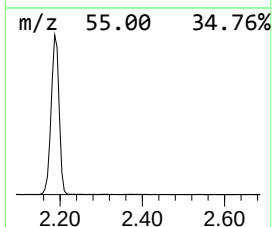
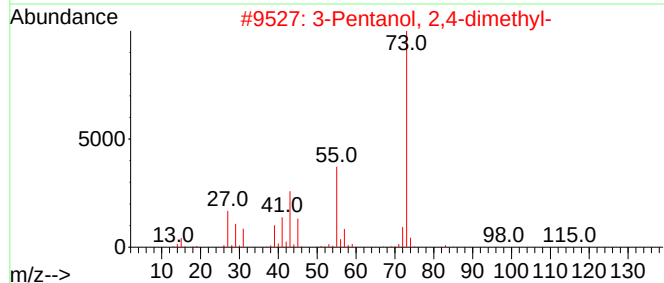
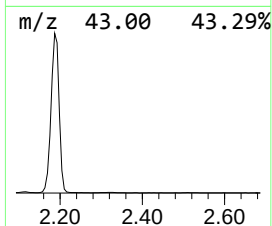
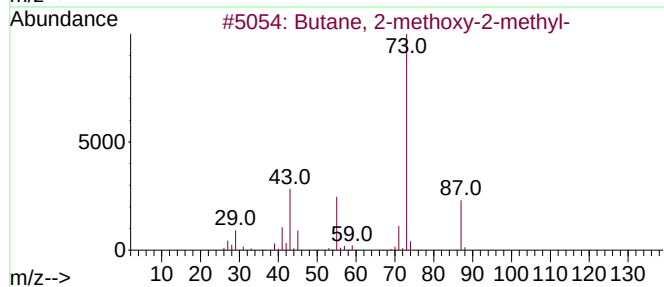
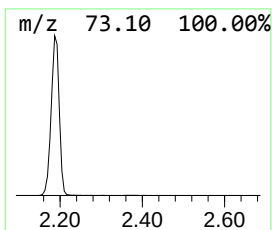
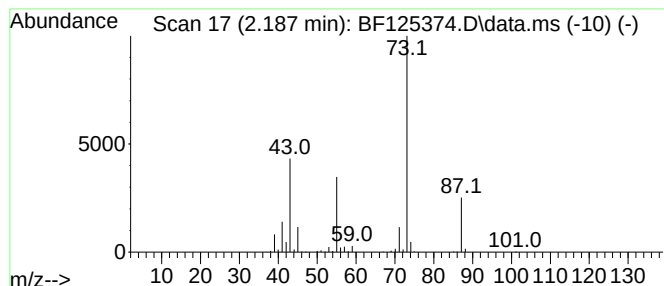
Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF081821.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

| R.T.  | EstConc  | Area    | Relative to ISTD       | R.T.  |
|-------|----------|---------|------------------------|-------|
| 2.187 | 78.88 ng | 3460080 | 1,4-Dichlorobenzene-d4 | 6.898 |

| Hit# | of | 5 | Tentative ID                     | MW  | MolForm  | CAS#        | Qual |
|------|----|---|----------------------------------|-----|----------|-------------|------|
| 1    |    |   | Butane, 2-methoxy-2-methyl-      | 102 | C6H14O   | 000994-05-8 | 83   |
| 2    |    |   | 3-Pentanol, 2,4-dimethyl-        | 116 | C7H16O   | 000600-36-2 | 43   |
| 3    |    |   | 2,2,4-Trimethyl-3-pentanol       | 130 | C8H18O   | 005162-48-1 | 40   |
| 4    |    |   | 1,3-Dioxolane, 2-methyl-         | 88  | C4H8O2   | 000497-26-7 | 23   |
| 5    |    |   | Octanal, 7-methoxy-3,7-dimethyl- | 186 | C11H22O2 | 003613-30-7 | 17   |



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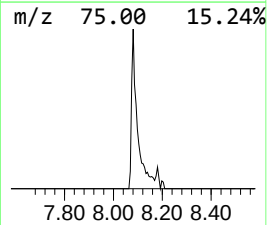
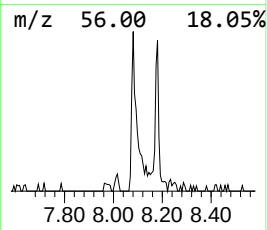
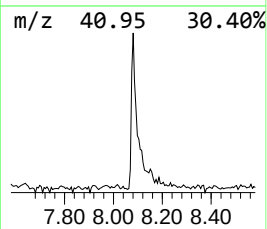
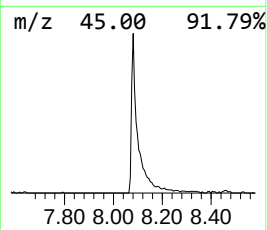
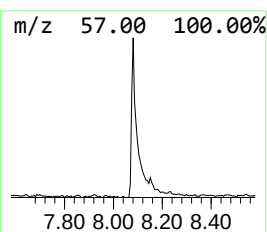
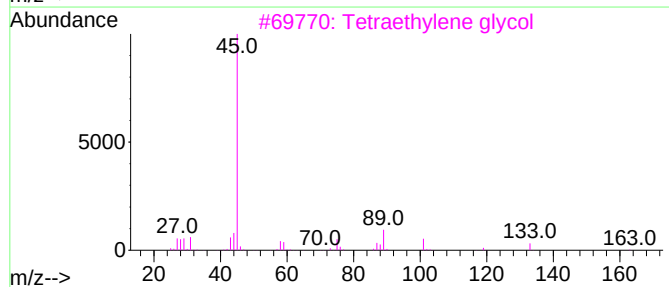
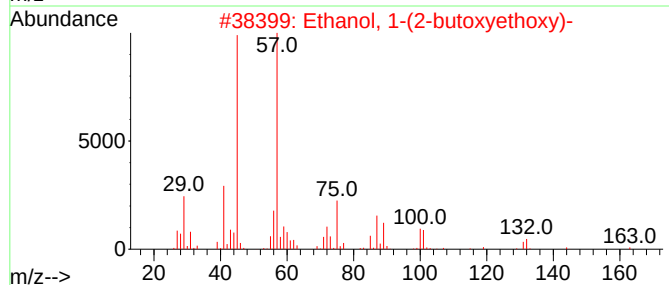
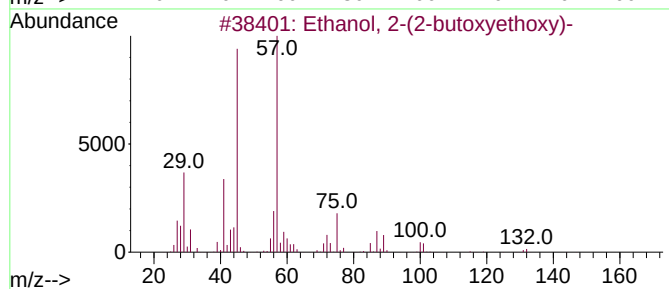
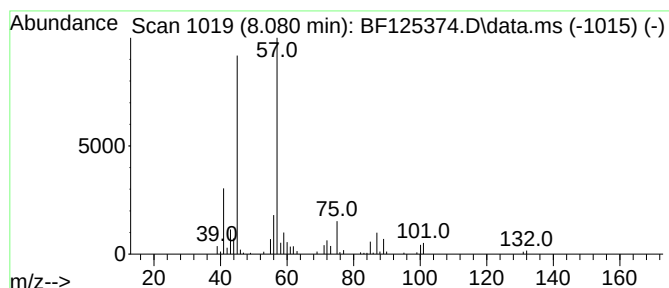
Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF081821.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 8.080 | 5.96 ng | 320297 | Naphthalene-d8   | 8.180 |

| Hit# | of | 5 | Tentative ID                       | MW  | MolForm | CAS#        | Qual |
|------|----|---|------------------------------------|-----|---------|-------------|------|
| 1    |    |   | Ethanol, 2-(2-butoxyethoxy)-       | 162 | C8H18O3 | 000112-34-5 | 90   |
| 2    |    |   | Ethanol, 1-(2-butoxyethoxy)-       | 162 | C8H18O3 | 054446-78-5 | 78   |
| 3    |    |   | Tetraethylene glycol               | 194 | C8H18O5 | 000112-60-7 | 53   |
| 4    |    |   | 3,3-Dimethylbutane-2-ol            | 102 | C6H14O  | 000464-07-3 | 53   |
| 5    |    |   | Ethylene glycol monoisobutyl ether | 118 | C6H14O2 | 004439-24-1 | 45   |



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Misc :  
ALS Vial : 16 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
20211059-SI-COMP-4-MODIFIED-EL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF081821.M  
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TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

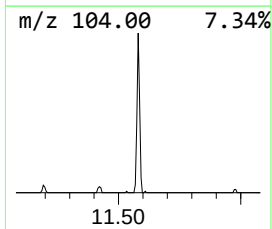
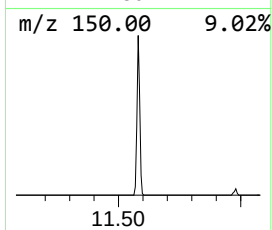
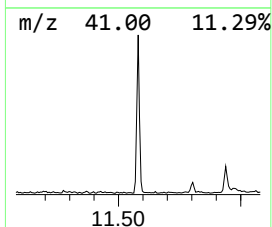
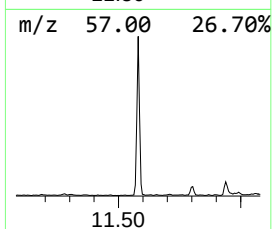
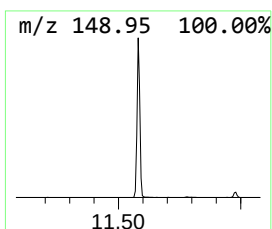
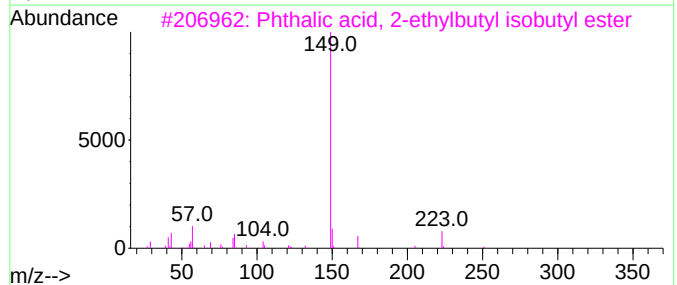
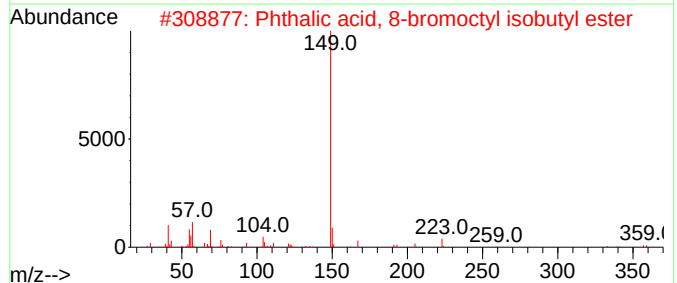
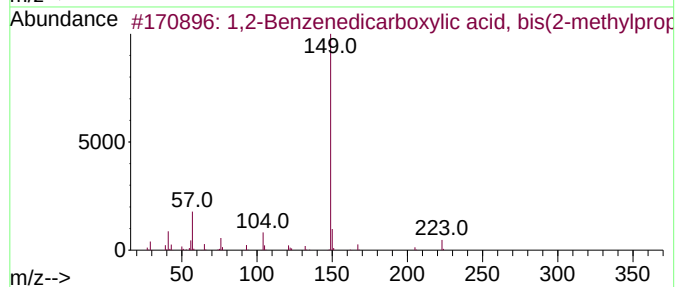
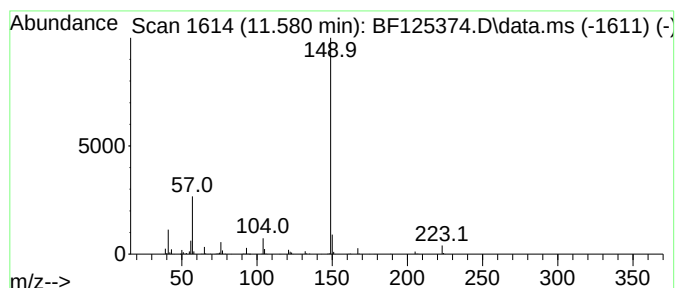
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Peak Number 3 1,2-Benzenedicarboxylic aci... Concentration Rank 2

| R.T.   | EstConc  | Area   | Relative to ISTD | R.T.   |
|--------|----------|--------|------------------|--------|
| 11.580 | 14.24 ng | 778147 | Phenanthrene-d10 | 11.422 |

| Hit# | of | 5 | Tentative ID                         | MW  | MolForm    | CAS#         | Qual |
|------|----|---|--------------------------------------|-----|------------|--------------|------|
| 1    |    |   | 1,2-Benzenedicarboxylic acid, bi...  | 278 | C16H22O4   | 000084-69-5  | 90   |
| 2    |    |   | Phthalic acid, 8-bromooctyl isobu... | 412 | C20H29BrO4 | 1000382-55-3 | 83   |
| 3    |    |   | Phthalic acid, 2-ethylbutyl isob...  | 306 | C18H26O4   | 1000356-88-9 | 78   |
| 4    |    |   | Phthalic acid, isobutyl 4-methyl...  | 334 | C20H30O4   | 1000377-93-8 | 78   |
| 5    |    |   | Phthalic acid, cyclohexylmethyl ...  | 318 | C19H26O4   | 1000309-08-6 | 78   |



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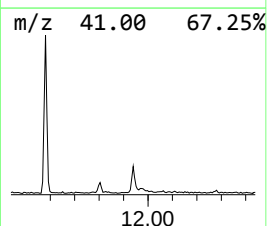
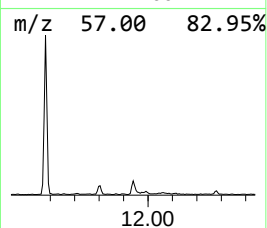
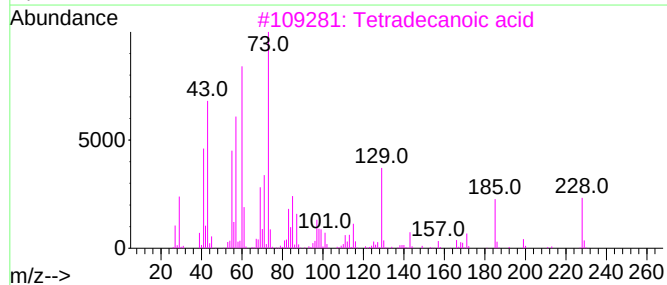
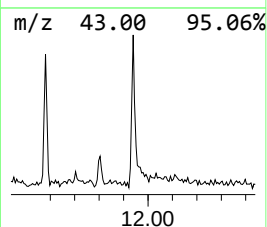
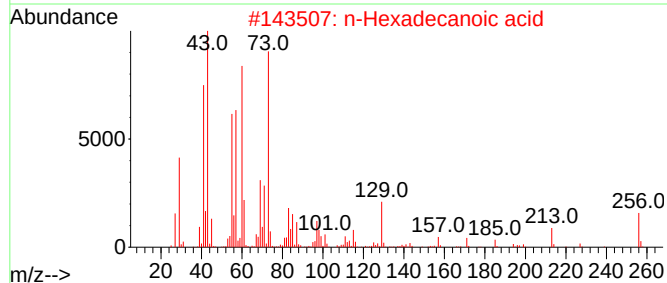
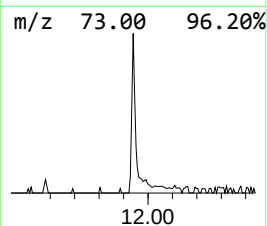
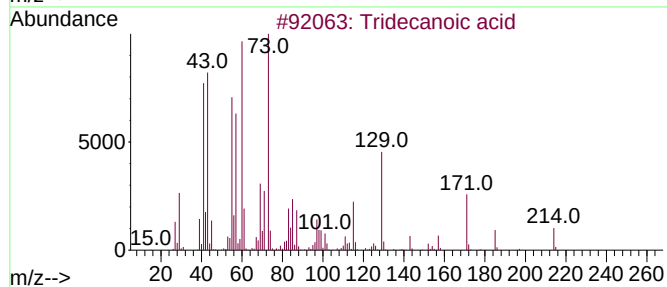
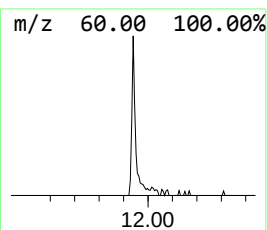
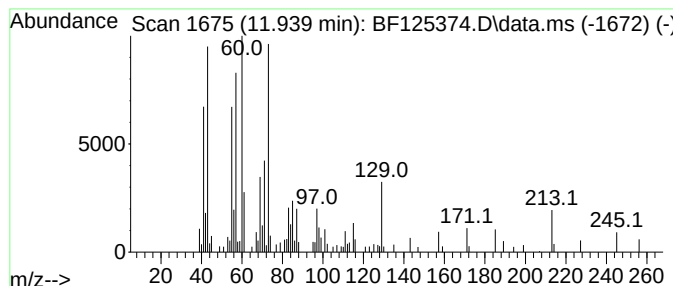
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\*\*\*\*\*  
Peak Number 4 Tridecanoic acid Concentration Rank 5

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 11.939 | 2.66 ng | 145438 | Phenanthrene-d10 | 11.422 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 89   |
| 2    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 83   |
| 3    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 80   |
| 4    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 80   |
| 5    |    |   | n-Decanoic acid     | 172 | C10H20O2 | 000334-48-5 | 62   |



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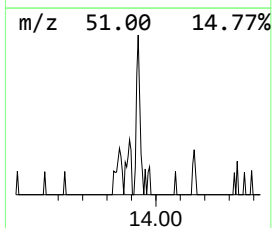
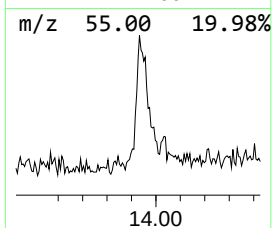
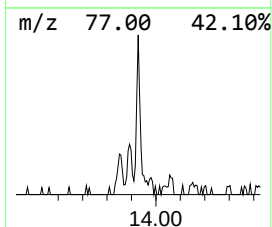
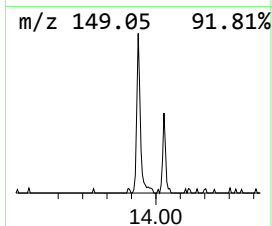
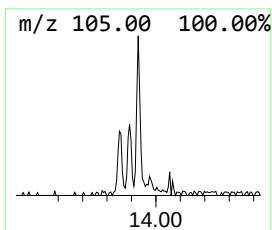
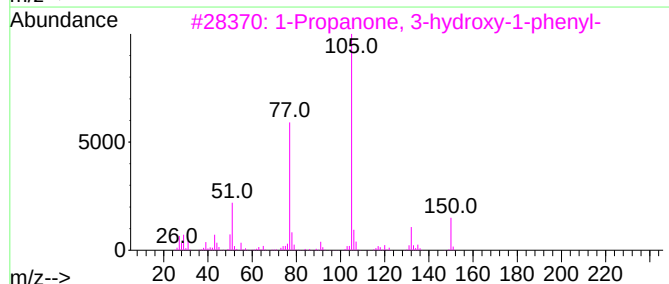
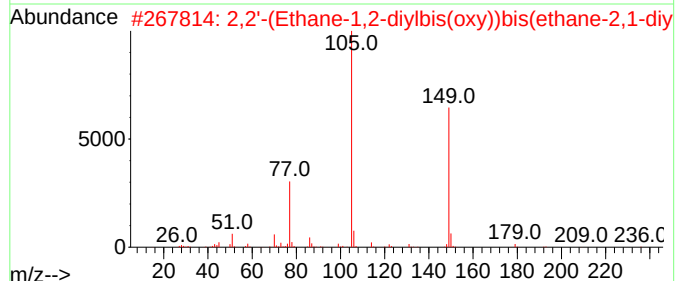
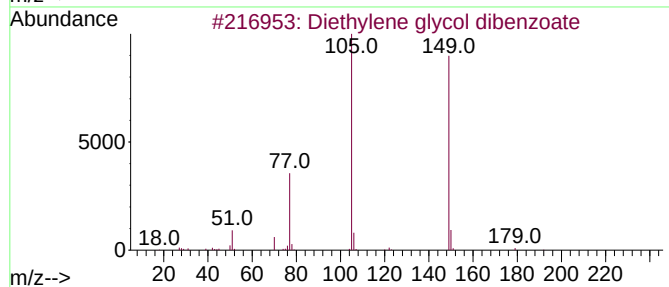
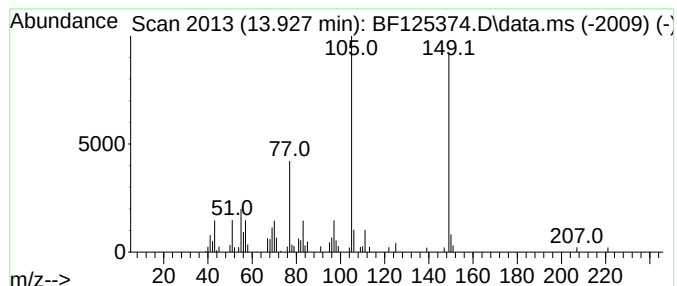
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 Diethylene glycol dibenzoate Concentration Rank 4

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 13.927 | 4.01 ng | 166820 | Chrysene-d12     | 14.063 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|----------|--------------|------|
| 1    |    |   | Diethylene glycol dibenzoate        | 314 | C18H18O5 | 000120-55-8  | 64   |
| 2    |    |   | 2,2'-(Ethane-1,2-diylbis(oxy))bi... | 358 | C20H22O6 | 1000366-99-4 | 64   |
| 3    |    |   | 1-Propanone, 3-hydroxy-1-phenyl-    | 150 | C9H10O2  | 005650-41-9  | 30   |
| 4    |    |   | N-(Methoxymethyl)benzamide          | 165 | C9H11NO2 | 013156-28-0  | 27   |
| 5    |    |   | 1-Phenylpent-4-en-1-one             | 160 | C11H12O  | 003240-29-7  | 22   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF090421\  
Data File : BF125374.D  
Acq On : 4 Sep 2021 17:49  
Operator : JU/CG  
Sample : M3648-12  
Misc :  
ALS Vial : 16 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
20211059-SI-COMP-4-MODIFIED-EL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF081821.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |         |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|---------|------|
|                    |        |         |       |          | #                     | RT     | Resp    | Conc |
| Butane, 2-metho... | 2.187  | 78.9    | ng    | 3460080  | 1                     | 6.898  | 877266  | 20.0 |
| Ethanol, 2-(2-b... | 8.080  | 6.0     | ng    | 320297   | 2                     | 8.180  | 1074080 | 20.0 |
| 1,2-Benzenedica... | 11.580 | 14.2    | ng    | 778147   | 4                     | 11.422 | 1093270 | 20.0 |
| Tridecanoic acid   | 11.939 | 2.7     | ng    | 145438   | 4                     | 11.422 | 1093270 | 20.0 |
| Diethylene glyc... | 13.927 | 4.0     | ng    | 166820   | 5                     | 14.063 | 831060  | 20.0 |