

Data Path : Z:\HPCHEM1\BNA G\DATA\BG091817\  
 Data File : BG028801.D  
 Acq On : 18 Sep 2017 19:00  
 Operator : SJ/JU  
 Sample : I5259-01  
 Misc :  
 ALS Vial : 11 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 20170603-COMP-D

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:\HPCHEM1\BNA\_G\METHODS\8270-BG091217.M  
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

| 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         | 5.857       | 380           | 386         | 397          | rBV      | 286951         | 480379        | 14.75%          | 3.494%        |
| 2         | 7.438       | 649           | 655         | 671          | rBV      | 183997         | 354558        | 10.89%          | 2.579%        |
| 3         | 7.820       | 712           | 720         | 734          | rBV      | 496119         | 900691        | 27.66%          | 6.551%        |
| 4         | 8.290       | 792           | 800         | 807          | rBV2     | 107454         | 193920        | 5.96%           | 1.410%        |
| 5         | 8.613       | 848           | 855         | 868          | rBV      | 447605         | 793702        | 24.37%          | 5.773%        |
| 6         | 9.459       | 990           | 999         | 1012         | rBV      | 369071         | 703012        | 21.59%          | 5.113%        |
| 7         | 11.110      | 1273          | 1280        | 1293         | rBV      | 152043         | 283409        | 8.70%           | 2.061%        |
| 8         | 13.525      | 1682          | 1691        | 1701         | rBV      | 1198477        | 1829373       | 56.18%          | 13.306%       |
| 9         | 14.342      | 1825          | 1830        | 1839         | rBV2     | 57057          | 94984         | 2.92%           | 0.691%        |
| 10        | 14.906      | 1919          | 1926        | 1935         | rVB2     | 272242         | 441267        | 13.55%          | 3.209%        |
| 11        | 15.705      | 2058          | 2062        | 2069         | rVB2     | 22527          | 34089         | 1.05%           | 0.248%        |
| 12        | 16.398      | 2173          | 2180        | 2193         | rBV      | 1152422        | 1800918       | 55.31%          | 13.099%       |
| 13        | 17.661      | 2388          | 2395        | 2402         | rBV2     | 406799         | 647996        | 19.90%          | 4.713%        |
| 14        | 18.302      | 2496          | 2504        | 2510         | rBV3     | 65833          | 96689         | 2.97%           | 0.703%        |
| 15        | 18.513      | 2534          | 2540        | 2549         | rBV2     | 50196          | 86164         | 2.65%           | 0.627%        |
| 16        | 19.770      | 2750          | 2754        | 2760         | rBV3     | 33242          | 54131         | 1.66%           | 0.394%        |
| 17        | 19.906      | 2771          | 2777        | 2782         | rBV      | 133543         | 165162        | 5.07%           | 1.201%        |
| 18        | 20.246      | 2829          | 2835        | 2843         | rBV      | 2496180        | 3256287       | 100.00%         | 23.684%       |
| 19        | 21.568      | 3055          | 3060        | 3069         | rBV10    | 18780          | 51123         | 1.57%           | 0.372%        |
| 20        | 21.980      | 3123          | 3130        | 3139         | rBV      | 403396         | 760232        | 23.35%          | 5.529%        |
| 21        | 25.446      | 3708          | 3720        | 3736         | rBV2     | 225956         | 720901        | 22.14%          | 5.243%        |

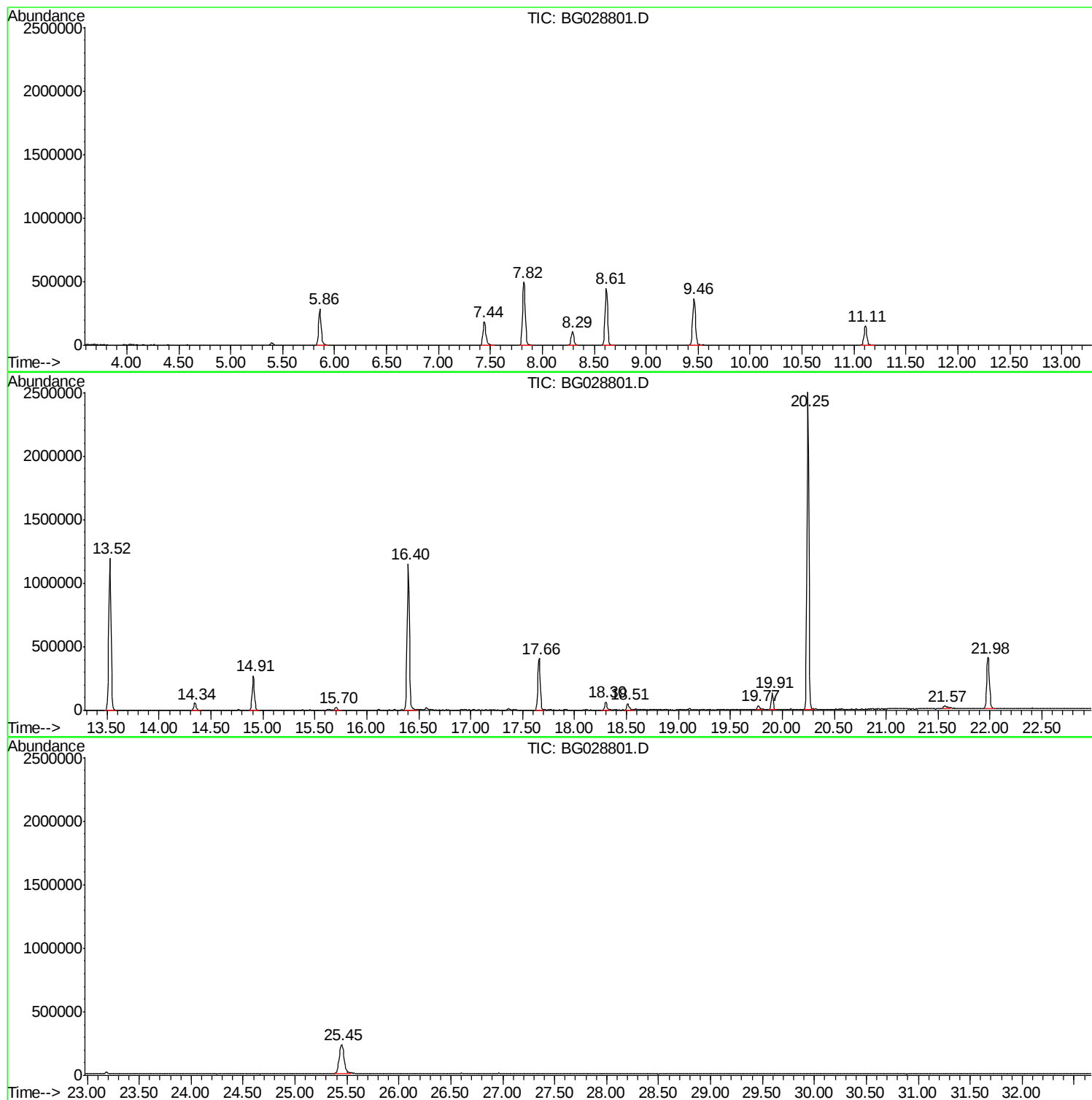
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG091217.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L  
TIC Integration Parameters: LSCINT.P



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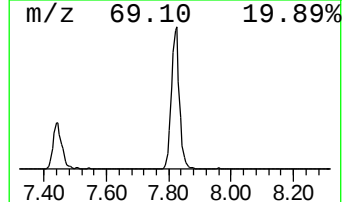
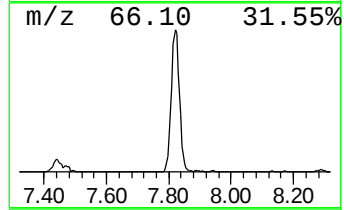
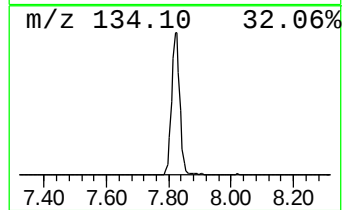
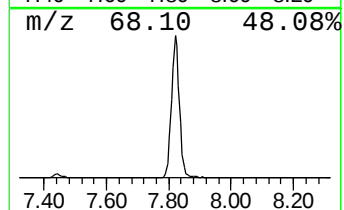
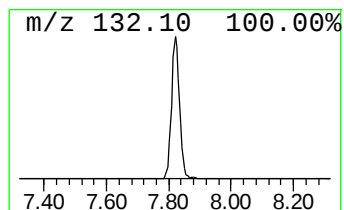
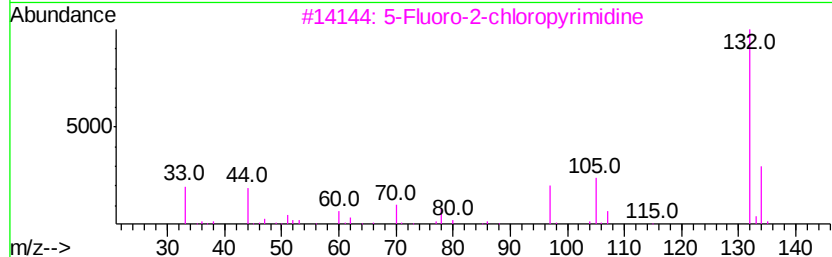
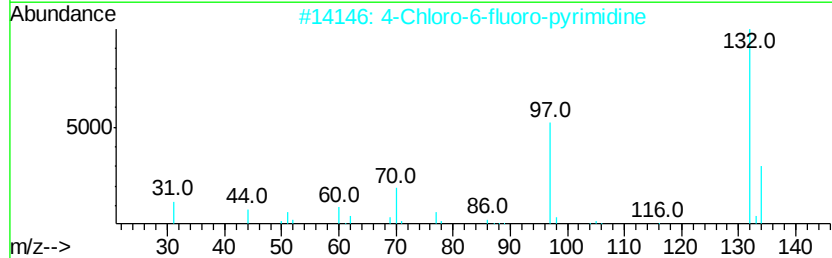
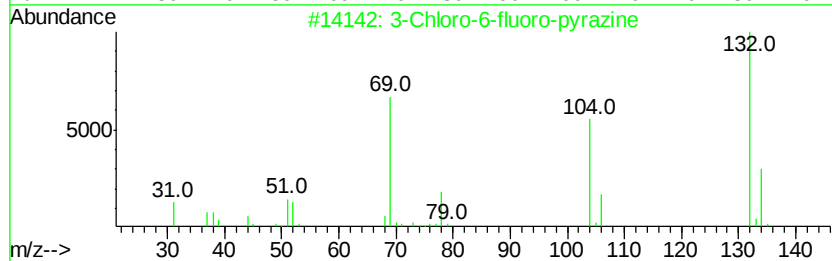
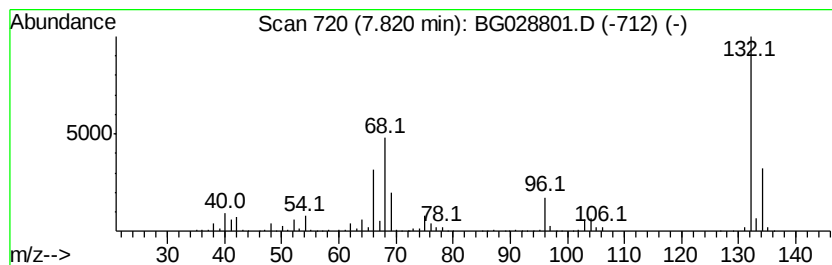
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TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 1 unknown7.82 Concentration Rank 1

| R.T.      | EstConc                             | Area   | Relative to ISTD       | R.T.         |      |
|-----------|-------------------------------------|--------|------------------------|--------------|------|
| 7.82      | 92.89 ng                            | 900691 | 1,4-Dichlorobenzene-d4 | 8.29         |      |
| Hit# of 5 | Tentative ID                        | MW     | MolForm                | CAS#         | Qual |
| 1         | 3-Chloro-6-fluoro-pyrazine          | 132    | C4H2ClFN2              | 1000146-10-7 | 27   |
| 2         | 4-Chloro-6-fluoro-pyrimidine        | 132    | C4H2ClFN2              | 051422-01-6  | 27   |
| 3         | 5-Fluoro-2-chloropyrimidine         | 132    | C4H2ClFN2              | 062802-42-0  | 16   |
| 4         | 1,3,5-Trifluorobenzene              | 132    | C6H3F3                 | 000372-38-3  | 14   |
| 5         | 2H-Cyclopenta[d]pyridazine, 2-me... | 132    | C8H8N2                 | 022291-85-6  | 12   |



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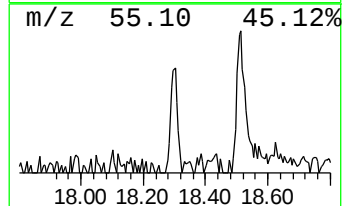
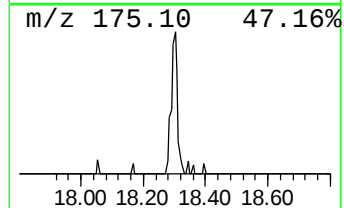
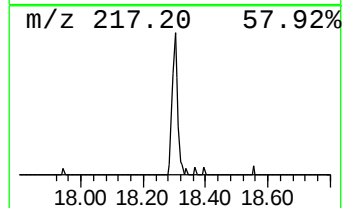
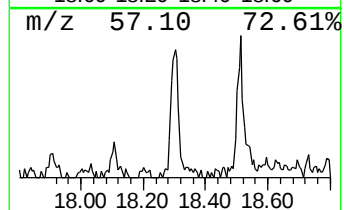
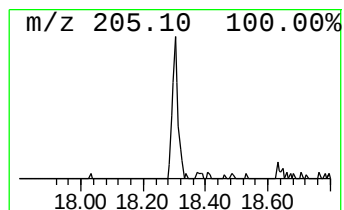
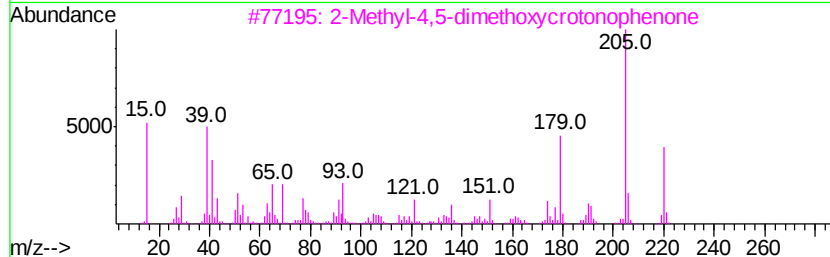
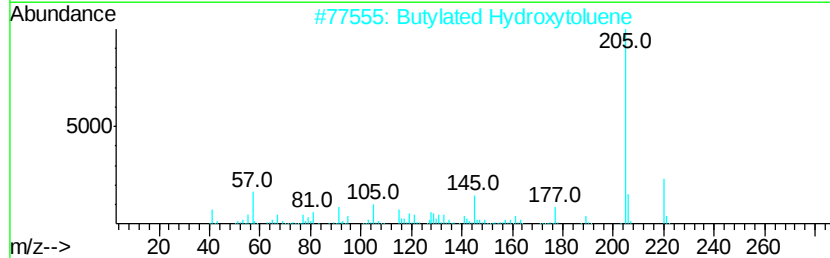
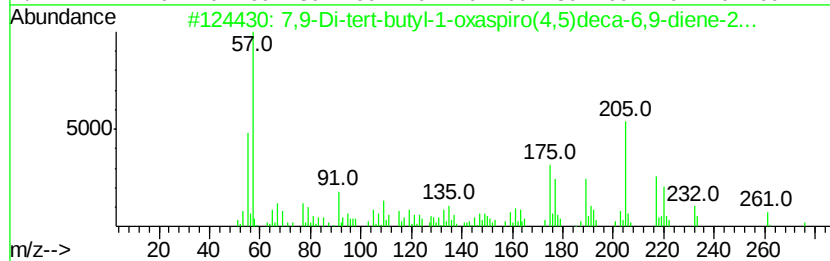
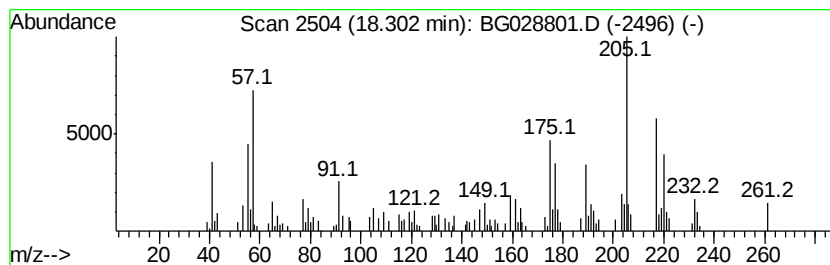
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Peak Number 3 7,9-Di-tert-butyl-1-oxaspiro... Concentration Rank 4

| R.T.    | EstConc                             | Area         | Relative to ISTD | R.T.        |      |      |
|---------|-------------------------------------|--------------|------------------|-------------|------|------|
| 18.30   | 2.98 ng                             | 96689        | Phenanthrene-d10 | 17.66       |      |      |
| Hit# of | 5                                   | Tentative ID | MW               | MolForm     | CAS# | Qual |
| 1       | 7,9-Di-tert-butyl-1-oxaspiro(4,5... | 276          | C17H24O3         | 082304-66-3 | 83   |      |
| 2       | Butylated Hydroxytoluene            | 220          | C15H24O          | 000128-37-0 | 46   |      |
| 3       | 2-Methyl-4,5-dimethoxycrotonophe... | 220          | C13H16O3         | 207233-94-1 | 45   |      |
| 4       | 1-Ethyl-2-methylphenanthrene        | 220          | C17H16           | 061983-53-7 | 41   |      |
| 5       | 1,3-Pentadiene, 1,1-diphenyl-, (Z)- | 220          | C17H16           | 015295-31-5 | 38   |      |



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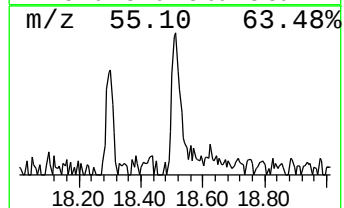
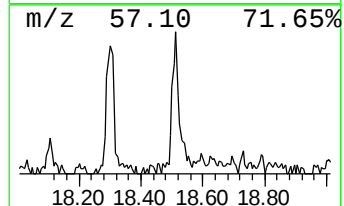
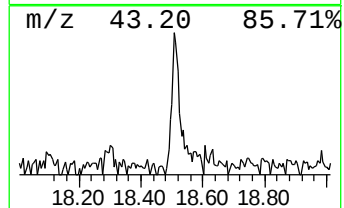
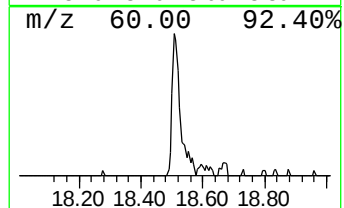
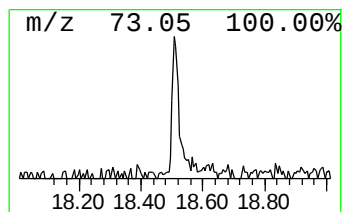
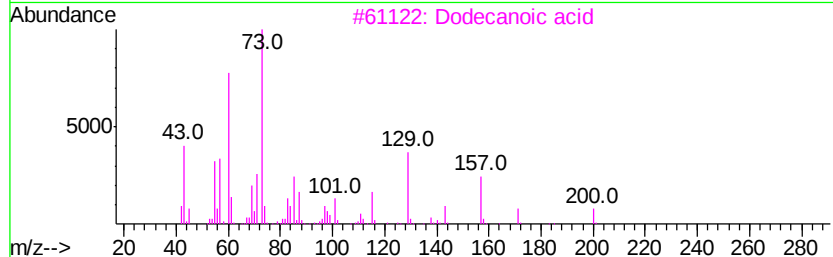
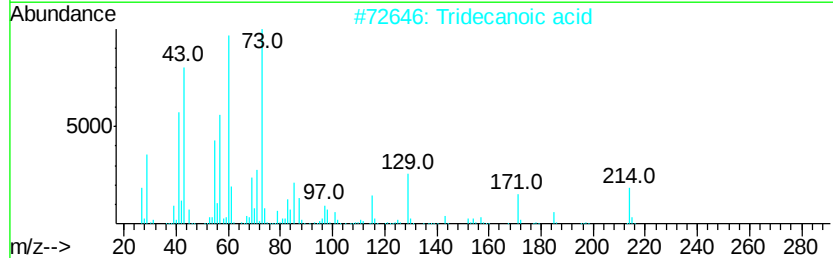
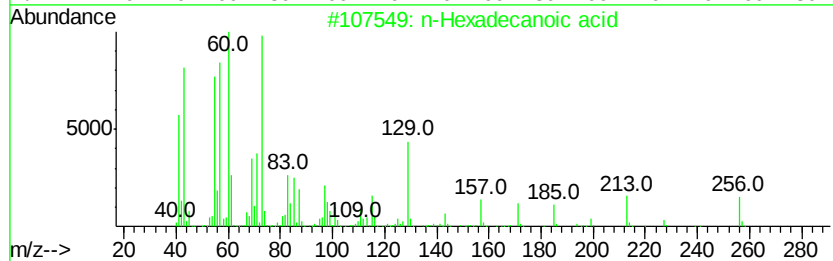
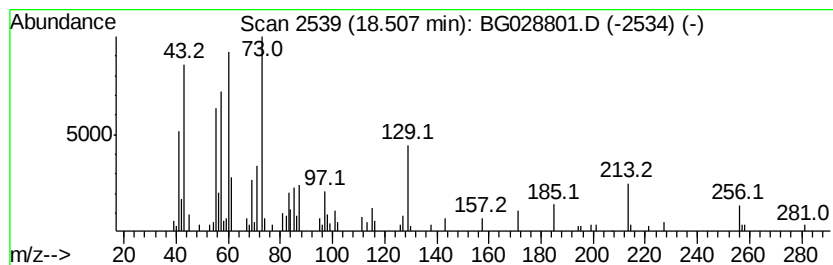
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ClientSampleId :  
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

| R.T.      | EstConc             | Area  | Relative to ISTD |             | R.T.  |
|-----------|---------------------|-------|------------------|-------------|-------|
| 18.51     | 2.66 ng             | 86164 | Phenanthrene-d10 |             | 17.66 |
| Hit# of 5 | Tentative ID        | MW    | MolForm          | CAS#        | Qual  |
| 1         | n-Hexadecanoic acid | 256   | C16H32O2         | 000057-10-3 | 83    |
| 2         | Tridecanoic acid    | 214   | C13H26O2         | 000638-53-9 | 81    |
| 3         | Dodecanoic acid     | 200   | C12H24O2         | 000143-07-7 | 59    |
| 4         | Tetradecanoic acid  | 228   | C14H28O2         | 000544-63-8 | 59    |
| 5         | n-Decanoic acid     | 172   | C10H20O2         | 000334-48-5 | 50    |



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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG091217.M  
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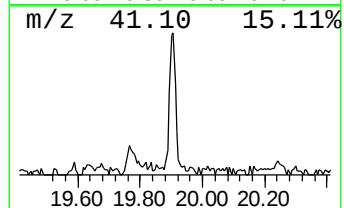
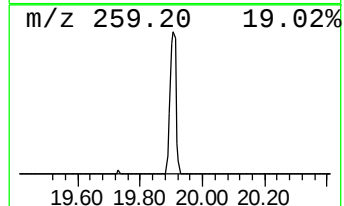
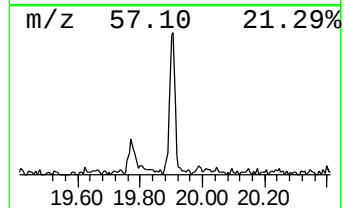
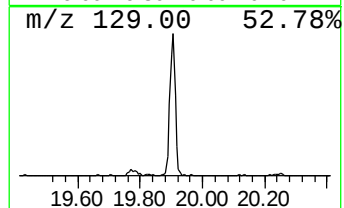
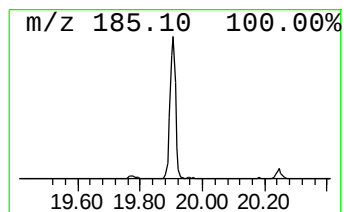
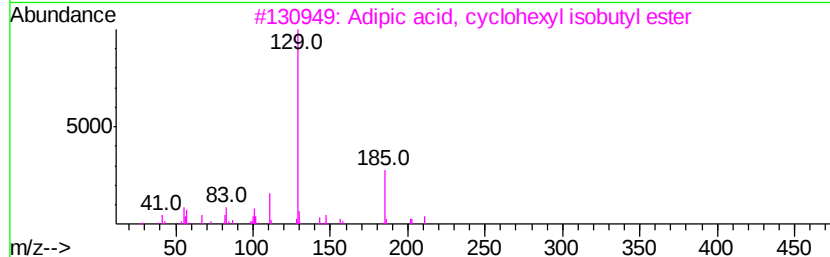
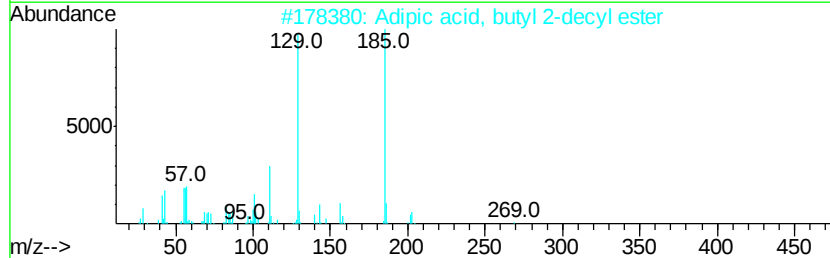
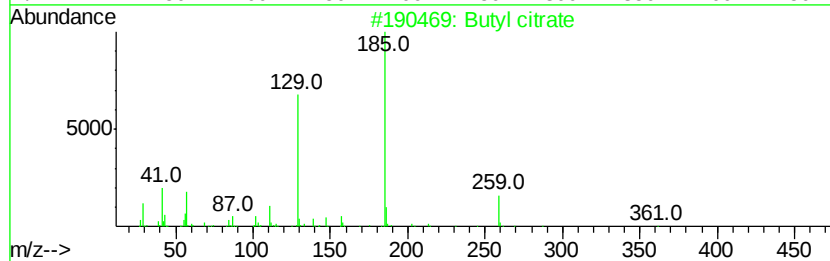
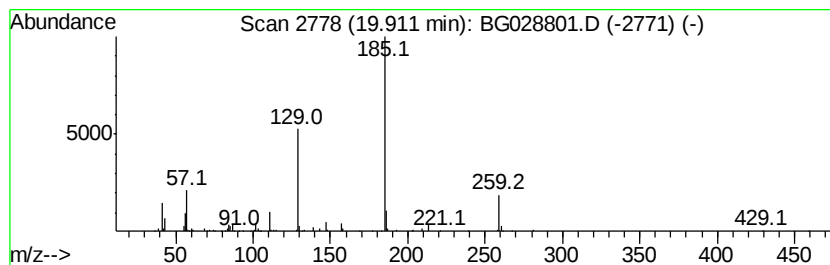
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\*\*\*\*\*  
Peak Number 5 Butyl citrate Concentration Rank 3

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 19.91 | 4.35 ng | 165162 | Chrysene-d12     | 21.98 |

| Hit# of | 5 | Tentative ID                         | MW  | MolForm  | CAS#         | Qual |
|---------|---|--------------------------------------|-----|----------|--------------|------|
| 1       |   | Butyl citrate                        | 360 | C18H32O7 | 000077-94-1  | 91   |
| 2       |   | Adipic acid, butyl 2-decyl ester     | 342 | C20H38O4 | 1000353-59-7 | 64   |
| 3       |   | Adipic acid, cyclohexyl isobutyl...  | 284 | C16H28O4 | 1000324-25-8 | 64   |
| 4       |   | Adipic acid, butyl pent-4-en-2-yl... | 270 | C15H26O4 | 1000354-11-9 | 59   |
| 5       |   | Tributyl acetyl citrate              | 402 | C20H34O8 | 000077-90-7  | 56   |



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| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                      |       |         |       |          | #                     | RT    | Resp   | Conc |
| unknown7.82          | 7.82  | 92.9    | ng    | 900691   | 1                     | 8.29  | 193920 | 20.0 |
| 7,9-Di-tert-butyl... | 18.30 | 3.0     | ng    | 96689    | 4                     | 17.66 | 647996 | 20.0 |
| n-Hexadecanoic acid  | 18.51 | 2.7     | ng    | 86164    | 4                     | 17.66 | 647996 | 20.0 |
| Butyl citrate        | 19.91 | 4.3     | ng    | 165162   | 5                     | 21.98 | 760232 | 20.0 |