

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF100622\  
 Data File : BF130563.D  
 Acq On : 06 Oct 2022 22:05  
 Operator : CG\JU  
 Sample : N5020-01  
 Misc :  
 ALS Vial : 19 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 TR-5-100522

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-BF091422.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130563.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         | 4.793       | 455           | 460         | 470          | rBV      | 418939         | 542655        | 1.46%           | 0.999%        |
| 2         | 5.222       | 529           | 533         | 551          | rBV      | 1848723        | 1754180       | 4.72%           | 3.229%        |
| 3         | 6.263       | 706           | 710         | 713          | rBV      | 1816843        | 1612165       | 4.33%           | 2.968%        |
| 4         | 6.616       | 766           | 770         | 777          | rVB      | 563399         | 439816        | 1.18%           | 0.810%        |
| 5         | 7.187       | 862           | 867         | 870          | rBV      | 1102996        | 1051174       | 2.83%           | 1.935%        |
| 6         | 7.898       | 984           | 988         | 991          | rBV      | 637964         | 510860        | 1.37%           | 0.940%        |
| 7         | 8.975       | 1167          | 1171        | 1174         | rBV      | 2253711        | 1709338       | 4.60%           | 3.146%        |
| 8         | 9.645       | 1282          | 1285        | 1289         | rVB      | 631035         | 482369        | 1.30%           | 0.888%        |
| 9         | 10.433      | 1415          | 1419        | 1429         | rVB      | 1262748        | 1055752       | 2.84%           | 1.943%        |
| 10        | 11.128      | 1533          | 1537        | 1539         | rBV      | 623440         | 503284        | 1.35%           | 0.926%        |
| 11        | 12.716      | 1803          | 1807        | 1810         | rBV      | 1914420        | 1834134       | 4.93%           | 3.376%        |
| 12        | 13.251      | 1884          | 1898        | 1901         | rBV      | 13012326       | 37199529      | 100.00%         | 68.475%       |
| 13        | 13.504      | 1937          | 1941        | 1945         | rBV      | 2182462        | 2086971       | 5.61%           | 3.842%        |
| 14        | 13.769      | 1981          | 1986        | 1989         | rBV      | 609754         | 582463        | 1.57%           | 1.072%        |
| 15        | 14.251      | 2065          | 2068        | 2070         | rVV2     | 271872         | 381637        | 1.03%           | 0.703%        |
| 16        | 14.345      | 2081          | 2084        | 2086         | rBV      | 517770         | 456592        | 1.23%           | 0.840%        |
| 17        | 14.404      | 2090          | 2094        | 2095         | rBV      | 491387         | 532896        | 1.43%           | 0.981%        |
| 18        | 14.521      | 2107          | 2114        | 2116         | rBV      | 626936         | 1197911       | 3.22%           | 2.205%        |
| 19        | 15.151      | 2217          | 2221        | 2224         | rBV      | 341213         | 391738        | 1.05%           | 0.721%        |

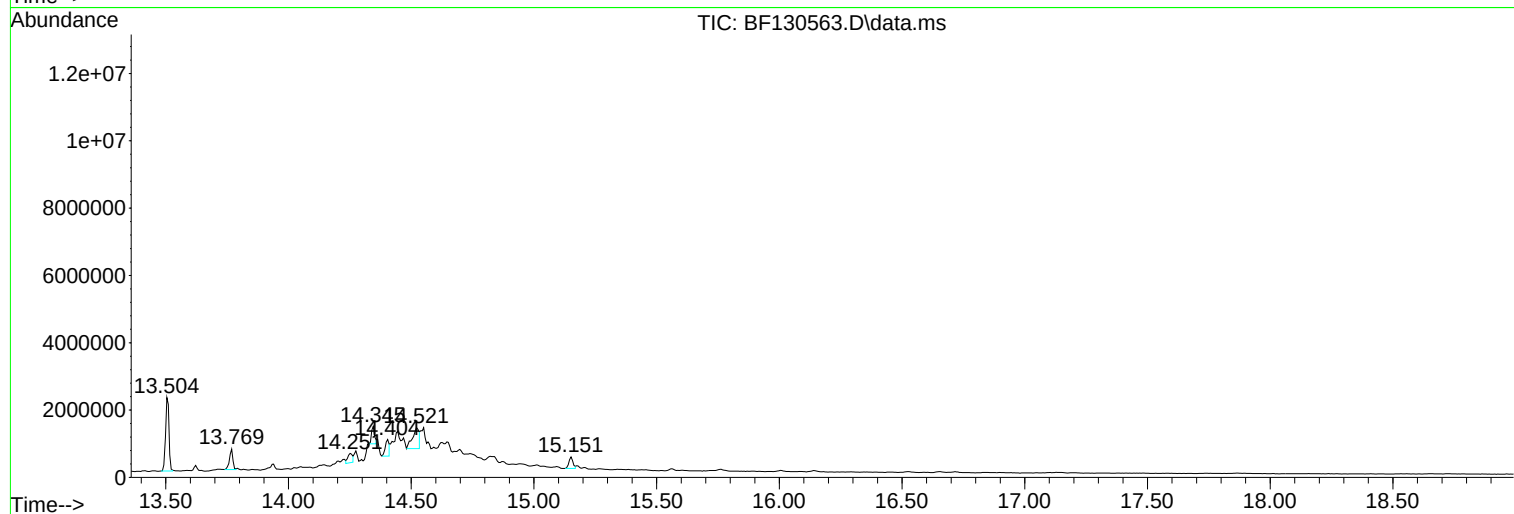
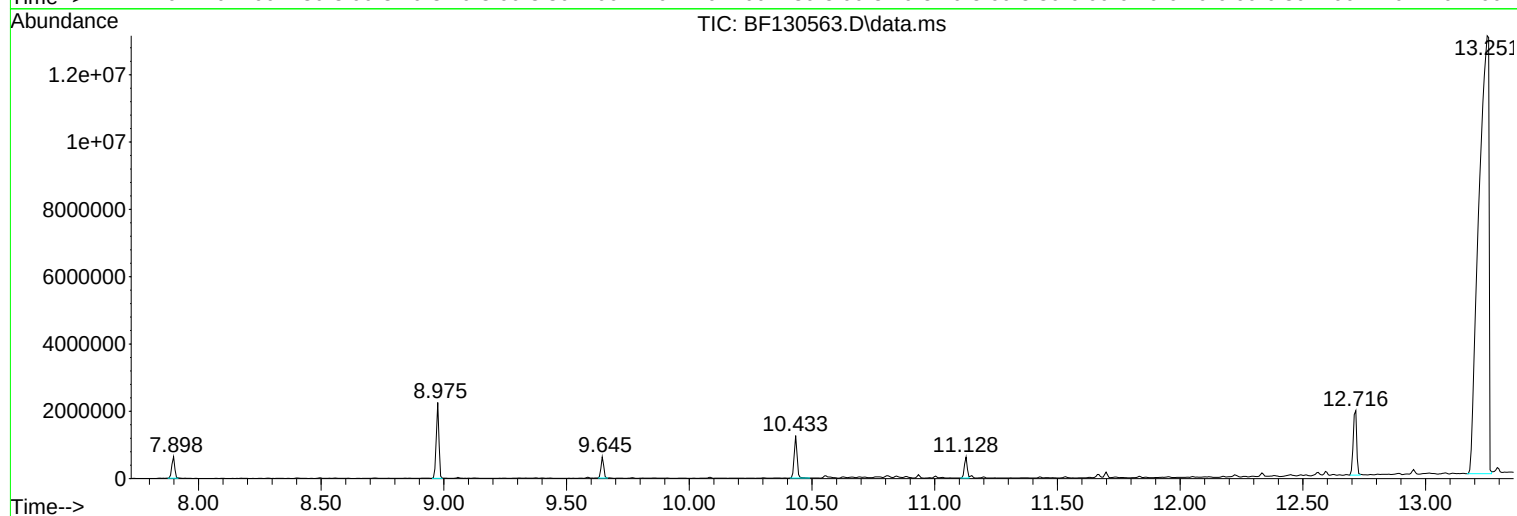
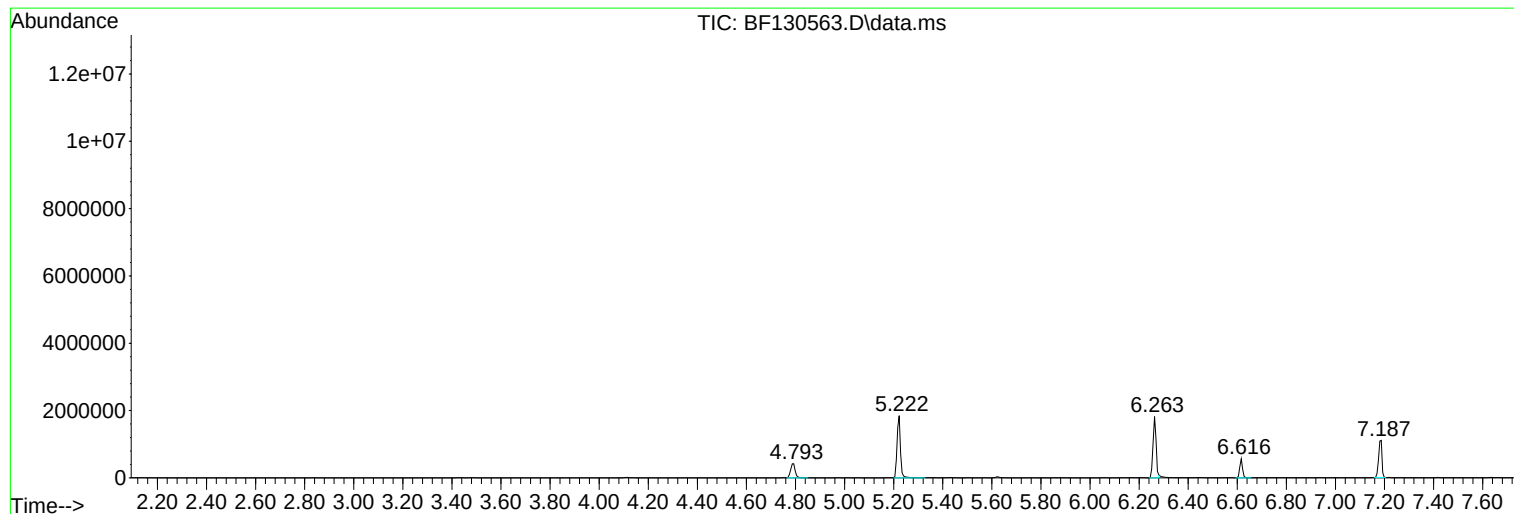
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BNA\_F  
ClientSampleId :  
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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF091422.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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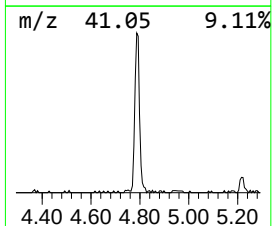
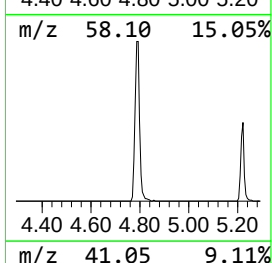
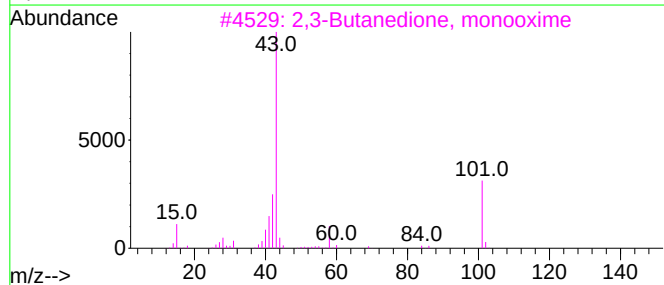
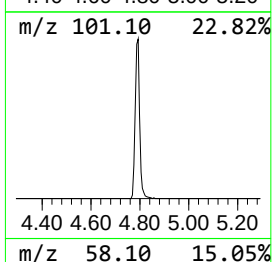
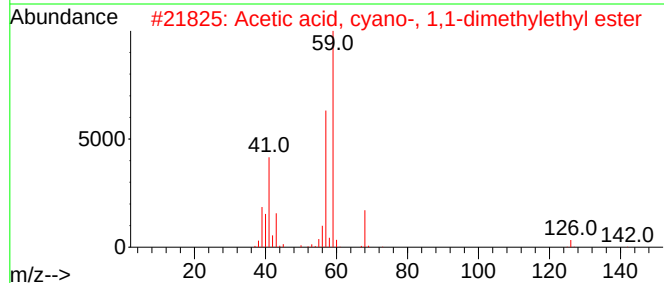
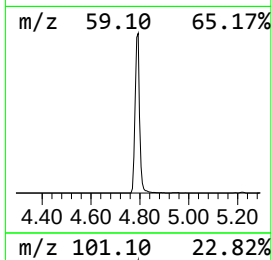
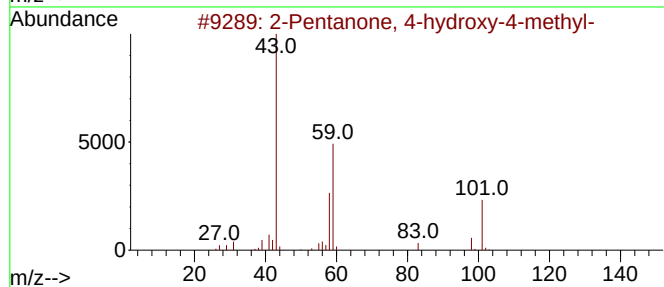
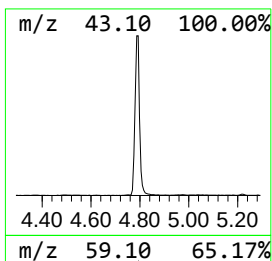
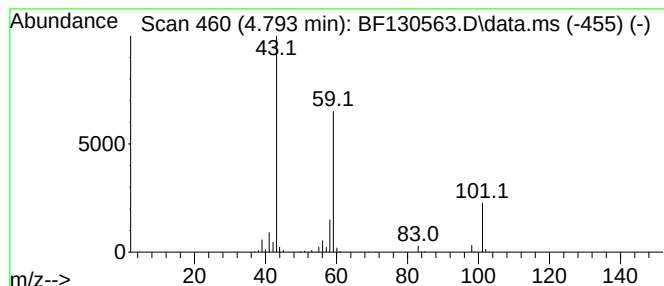
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T.  | EstConc  | Area   | Relative to ISTD       | R.T.  |
|-------|----------|--------|------------------------|-------|
| 4.793 | 24.68 ng | 542655 | 1,4-Dichlorobenzene-d4 | 6.616 |

| Hit# | of                                  | 5   | Tentative ID | MW          | MolForm | CAS# | Qual |
|------|-------------------------------------|-----|--------------|-------------|---------|------|------|
| 1    | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2      | 000123-42-2 | 56      |      |      |
| 2    | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2     | 001116-98-9 | 23      |      |      |
| 3    | 2,3-Butanedione, monooxime          | 101 | C4H7NO2      | 000057-71-6 | 17      |      |      |
| 4    | 1-Propen-2-ol, acetate              | 100 | C5H8O2       | 000108-22-5 | 10      |      |      |
| 5    | Butane, 1-ethoxy-                   | 102 | C6H14O       | 000628-81-9 | 9       |      |      |



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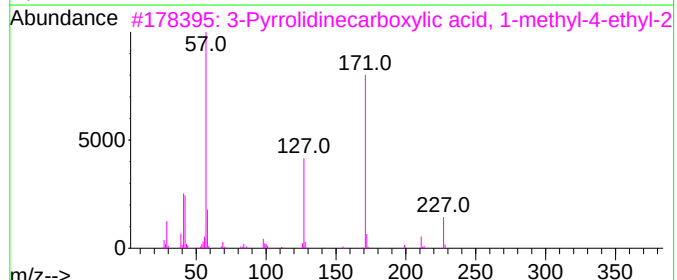
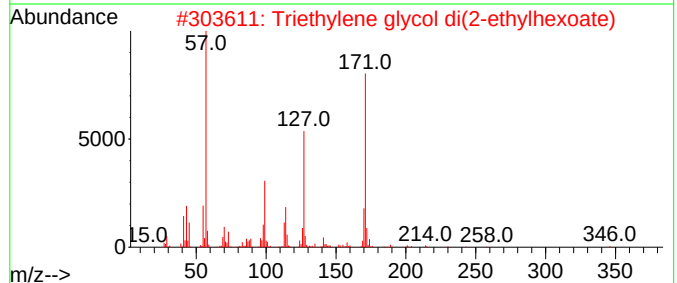
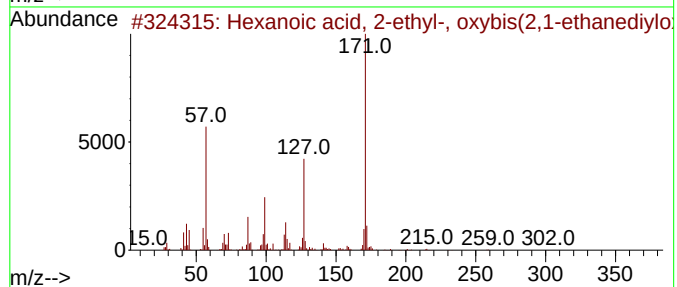
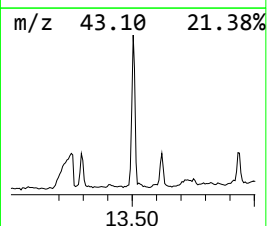
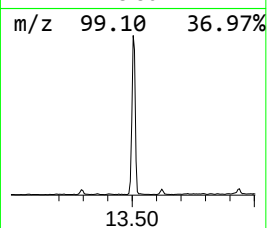
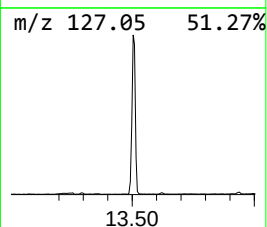
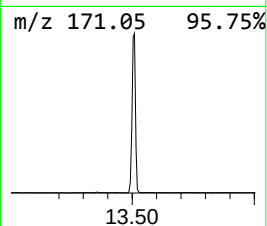
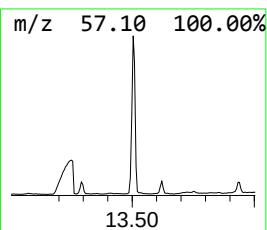
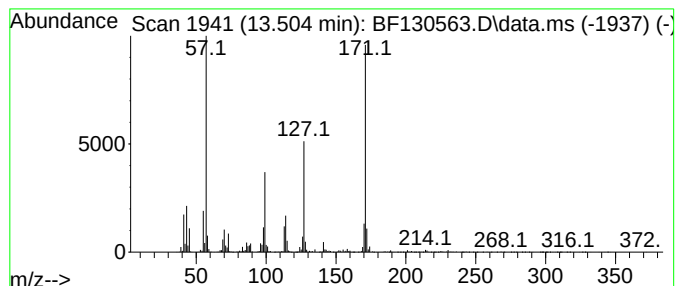
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF091422.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 2 Hexanoic acid, 2-ethyl-, ox... Concentration Rank 1

| R.T.      | EstConc                             | Area    | Relative to ISTD | R.T.         |      |
|-----------|-------------------------------------|---------|------------------|--------------|------|
| 13.504    | 71.66 ng                            | 2086970 | Chrysene-d12     | 13.769       |      |
| Hit# of 5 | Tentative ID                        | MW      | MolForm          | CAS#         | Qual |
| 1         | Hexanoic acid, 2-ethyl-, oxybis(... | 446     | C24H46O7         | 018268-70-7  | 91   |
| 2         | Triethylene glycol di(2-ethylhex... | 402     | C22H42O6         | 000094-28-0  | 81   |
| 3         | 3-Pyrrolidinecarboxylic acid, 1-... | 284     | C15H28N2O3       | 1000196-95-3 | 59   |
| 4         | 3-Chlorothiobenzamide               | 171     | C7H6ClNS         | 002548-79-0  | 43   |
| 5         | 2,6-Difluorophenyl isocyanate       | 171     | C7H3F2NS         | 065295-69-4  | 38   |



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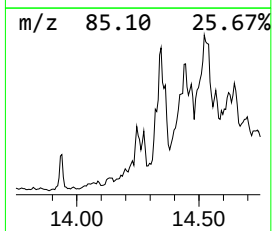
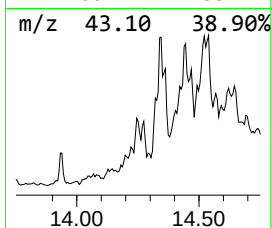
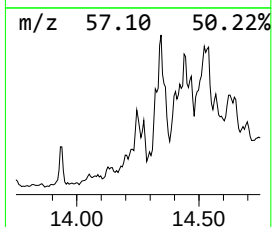
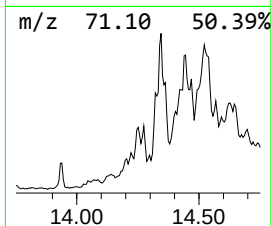
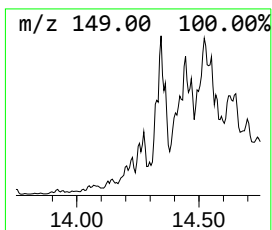
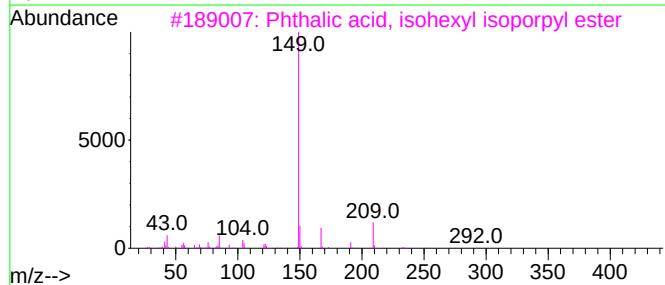
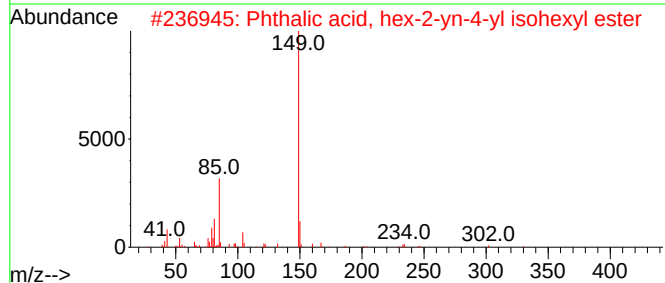
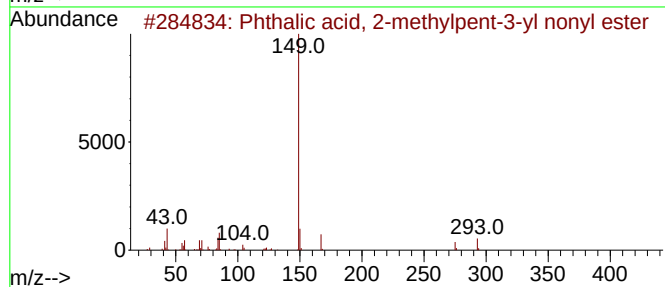
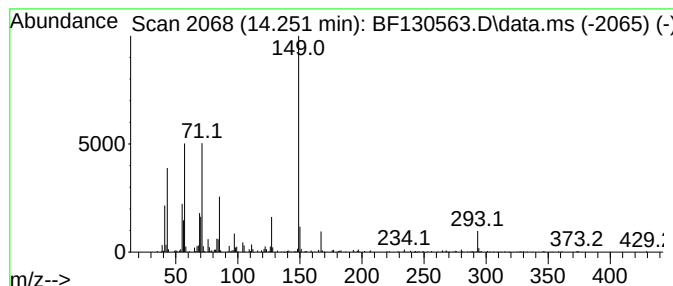
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TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 Phthalic acid, 2-methylpent... Concentration Rank 5

| R.T.   | EstConc  | Area   | Relative to ISTD | R.T.   |
|--------|----------|--------|------------------|--------|
| 14.251 | 13.10 ng | 381637 | Chrysene-d12     | 13.769 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|----------|--------------|------|
| 1    |    |   | Phthalic acid, 2-methylpent-3-yl... | 376 | C23H36O4 | 1000356-91-4 | 50   |
| 2    |    |   | Phthalic acid, hex-2-yn-4-yl iso... | 330 | C20H26O4 | 1000315-20-0 | 49   |
| 3    |    |   | Phthalic acid, isohexyl isoporpy... | 292 | C17H24O4 | 1000315-00-4 | 49   |
| 4    |    |   | Phthalic acid, isohexyl octadecy... | 502 | C32H54O4 | 1000308-96-9 | 47   |
| 5    |    |   | Phthalic acid, heptyl isoporpyl ... | 306 | C18H26O4 | 1000315-00-1 | 45   |



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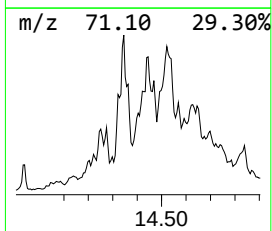
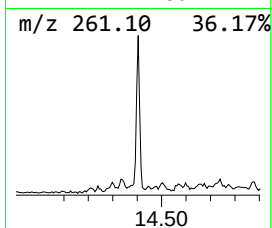
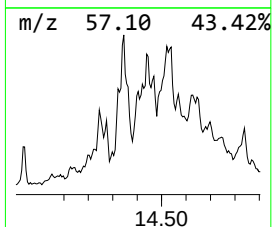
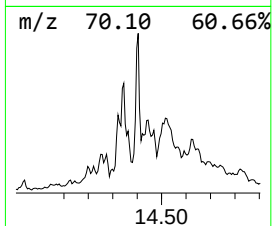
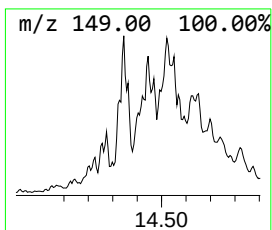
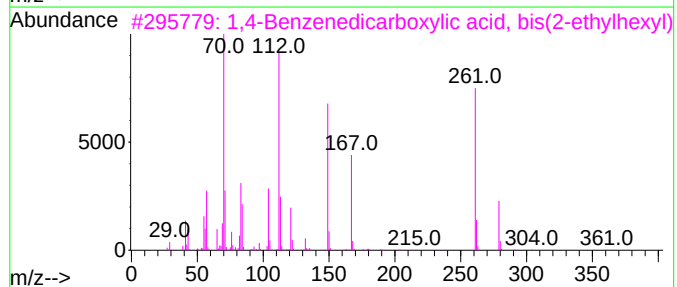
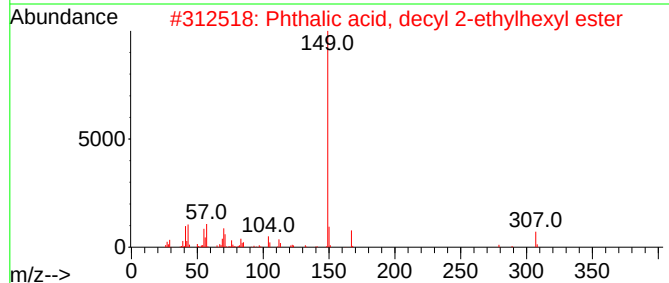
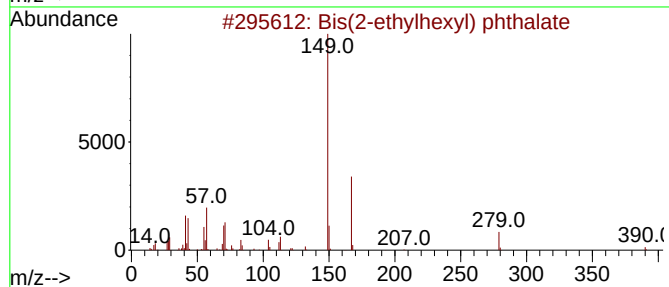
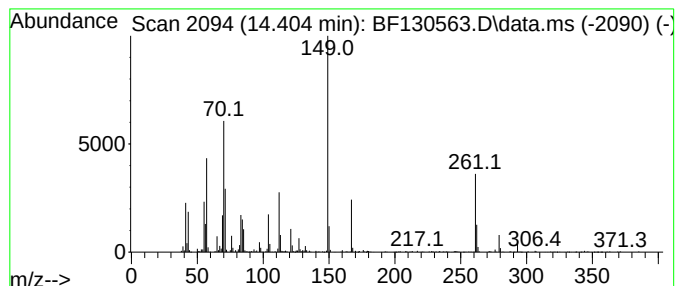
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TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 unknown14.404 Concentration Rank 4

| R.T.   | EstConc  | Area   | Relative to ISTD | R.T.   |
|--------|----------|--------|------------------|--------|
| 14.404 | 18.30 ng | 532896 | Chrysene-d12     | 13.769 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|----------|--------------|------|
| 1    |    |   | Bis(2-ethylhexyl) phthalate         | 390 | C24H38O4 | 000117-81-7  | 47   |
| 2    |    |   | Phthalic acid, decyl 2-ethylhexy... | 418 | C26H42O4 | 1000309-00-0 | 43   |
| 3    |    |   | 1,4-Benzenedicarboxylic acid, bi... | 390 | C24H38O4 | 006422-86-2  | 38   |
| 4    |    |   | Phthalic acid, 3-methylbut-3-eny... | 346 | C21H30O4 | 1000357-10-6 | 38   |
| 5    |    |   | Phthalic acid, hex-3-yl isohexyl... | 334 | C20H30O4 | 1000356-95-6 | 38   |



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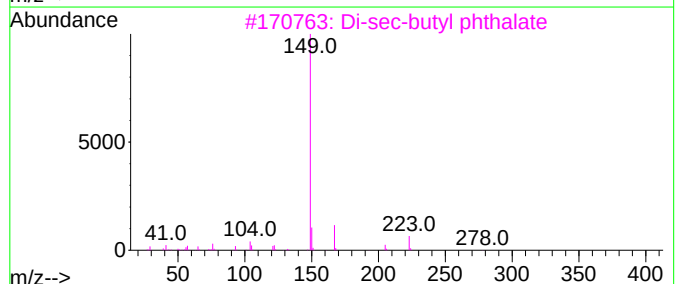
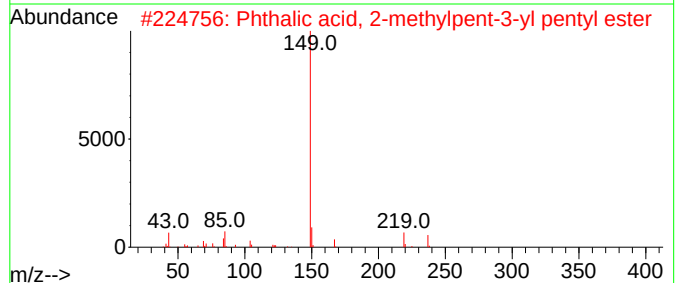
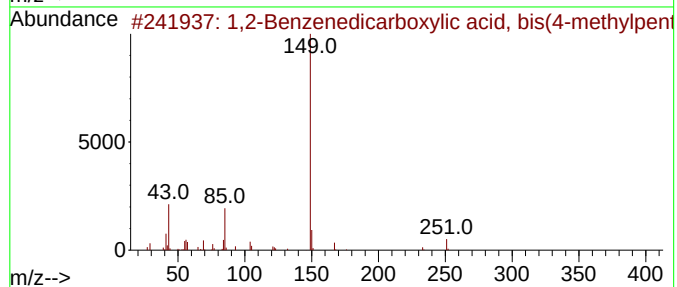
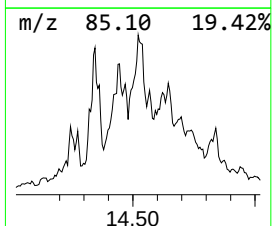
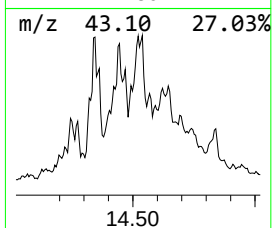
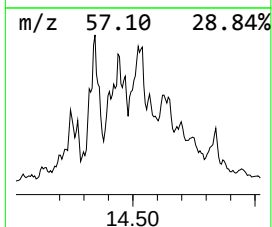
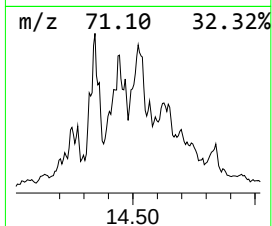
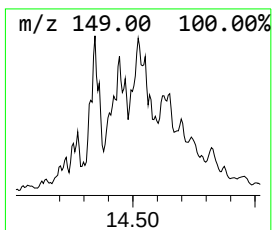
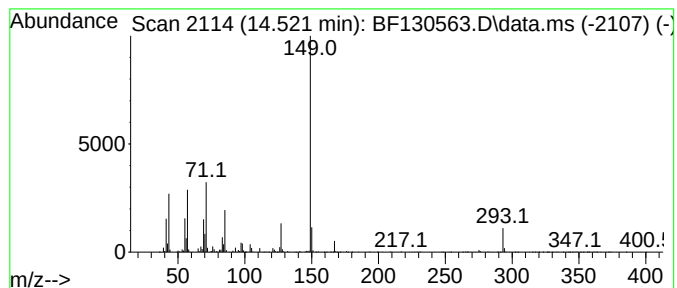
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 1,2-Benzenedicarboxylic aci... Concentration Rank 2

| R.T.   | EstConc  | Area    | Relative to ISTD | R.T.   |
|--------|----------|---------|------------------|--------|
| 14.521 | 61.16 ng | 1197910 | Perylene-d12     | 15.151 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|----------|--------------|------|
| 1    |    |   | 1,2-Benzenedicarboxylic acid, bi... | 334 | C20H30O4 | 000146-50-9  | 58   |
| 2    |    |   | Phthalic acid, 2-methylpent-3-yl... | 320 | C19H28O4 | 1000356-90-9 | 50   |
| 3    |    |   | Di-sec-butyl phthalate              | 278 | C16H22O4 | 1000373-65-4 | 49   |
| 4    |    |   | 1,2-Benzenedicarboxylic acid, di... | 362 | C22H34O4 | 003648-21-3  | 49   |
| 5    |    |   | Phthalic acid, neopentyl propyl ... | 278 | C16H22O4 | 1000308-97-2 | 49   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF100622\  
Data File : BF130563.D  
Acq On : 06 Oct 2022 22:05  
Operator : CG\JU  
Sample : N5020-01  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
TR-5-100522

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF091422.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 |
| 2-Pentanone, 4-... | 4.793  | 24.7    | ng    | 542655   | 1                     | 6.616  | 439816 | 20.0 |
| Hexanoic acid, ... | 13.504 | 71.7    | ng    | 2086970  | 5                     | 13.769 | 582463 | 20.0 |
| Phthalic acid, ... | 14.251 | 13.1    | ng    | 381637   | 5                     | 13.769 | 582463 | 20.0 |
| unknown14.404      | 14.404 | 18.3    | ng    | 532896   | 5                     | 13.769 | 582463 | 20.0 |
| 1,2-Benzenedica... | 14.521 | 61.2    | ng    | 1197910  | 6                     | 15.151 | 391738 | 20.0 |