

Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF021318\  
 Data File : BF102954.D  
 Acq On : 13 Feb 2018 11:54  
 Operator : SJ/JU  
 Sample : PB106454BL  
 Misc :  
 ALS Vial : 4 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 PB106454BL

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\_F\METHODS\8270-BF020318.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         | 2.193       | 10            | 18          | 26           | rVB      | 46171          | 73848         | 1.71%           | 0.194%        |
| 2         | 5.116       | 508           | 515         | 521          | rBV      | 96176          | 134044        | 3.10%           | 0.352%        |
| 3         | 5.498       | 575           | 580         | 583          | rBV      | 3973150        | 4066994       | 94.07%          | 10.689%       |
| 4         | 6.498       | 745           | 750         | 753          | rBV      | 3489428        | 3951455       | 91.40%          | 10.385%       |
| 5         | 6.639       | 769           | 774         | 778          | rBV      | 3692482        | 4028466       | 93.18%          | 10.587%       |
| 6         | 6.869       | 810           | 813         | 817          | rBV      | 1216517        | 1047787       | 24.24%          | 2.754%        |
| 7         | 7.028       | 836           | 840         | 843          | rBV      | 3435131        | 3113665       | 72.02%          | 8.183%        |
| 8         | 7.434       | 904           | 909         | 912          | rBV      | 2646072        | 2678251       | 61.95%          | 7.039%        |
| 9         | 8.151       | 1027          | 1031        | 1035         | rBV      | 1535415        | 1432839       | 33.14%          | 3.766%        |
| 10        | 9.228       | 1209          | 1214        | 1217         | rBV      | 4372677        | 4323345       | 100.00%         | 11.362%       |
| 11        | 9.910       | 1325          | 1330        | 1336         | rVB      | 1735466        | 1581168       | 36.57%          | 4.156%        |
| 12        | 10.698      | 1458          | 1464        | 1467         | rBV      | 2628741        | 2646177       | 61.21%          | 6.955%        |
| 13        | 11.398      | 1578          | 1583        | 1586         | rBV      | 1782295        | 1574194       | 36.41%          | 4.137%        |
| 14        | 12.792      | 1816          | 1820        | 1823         | rBV      | 246593         | 199940        | 4.62%           | 0.525%        |
| 15        | 12.980      | 1847          | 1852        | 1856         | rBV      | 3769077        | 4278634       | 98.97%          | 11.245%       |
| 16        | 13.498      | 1936          | 1940        | 1944         | rBV      | 167164         | 163068        | 3.77%           | 0.429%        |
| 17        | 14.033      | 2027          | 2031        | 2039         | rVB      | 1541560        | 1423594       | 32.93%          | 3.741%        |
| 18        | 14.792      | 2157          | 2160        | 2167         | rVB      | 40191          | 45758         | 1.06%           | 0.120%        |
| 19        | 15.509      | 2276          | 2282        | 2290         | rBV      | 939433         | 1194998       | 27.64%          | 3.141%        |
| 20        | 15.957      | 2353          | 2358        | 2362         | rBV2     | 31979          | 45858         | 1.06%           | 0.121%        |
| 21        | 16.462      | 2441          | 2444        | 2449         | rVB3     | 27588          | 45565         | 1.05%           | 0.120%        |

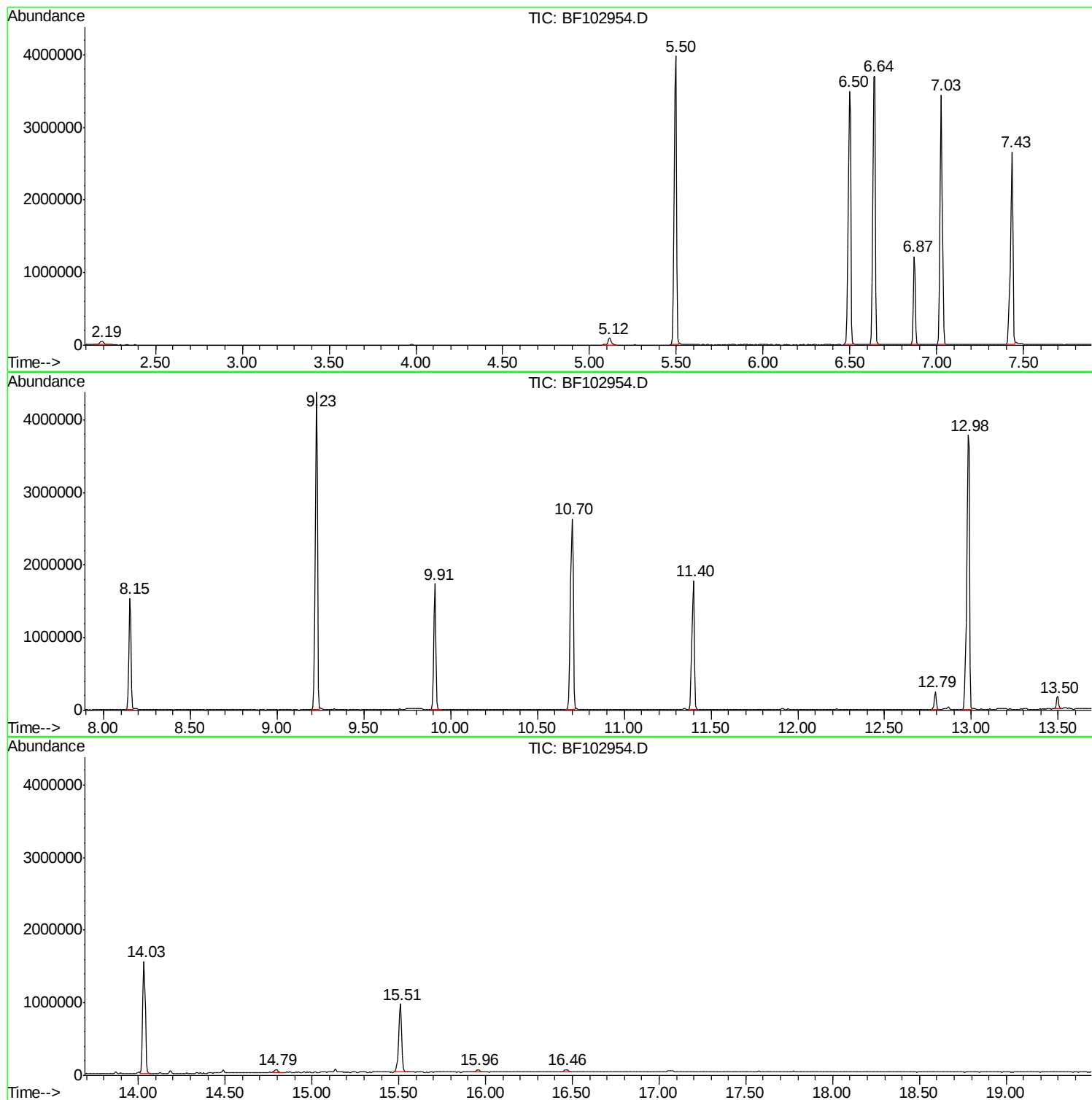
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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF020318.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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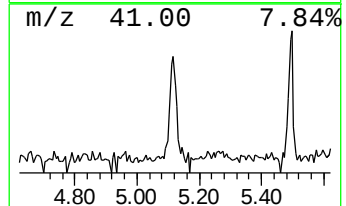
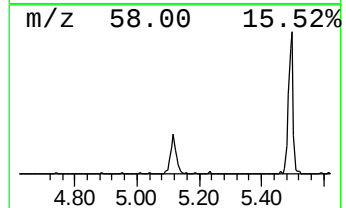
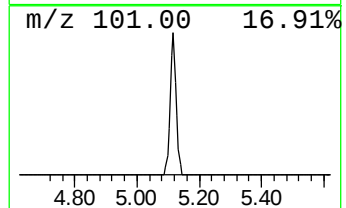
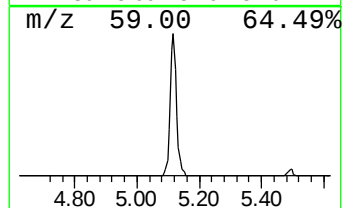
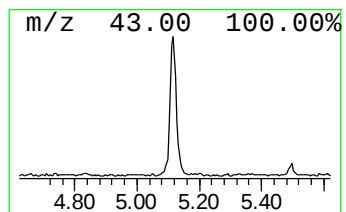
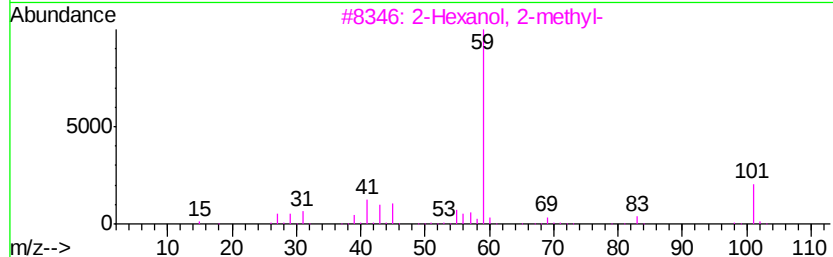
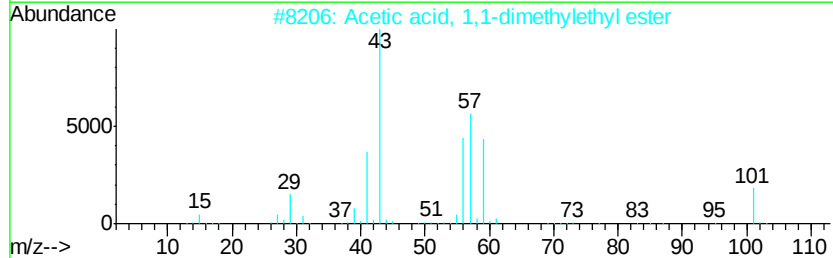
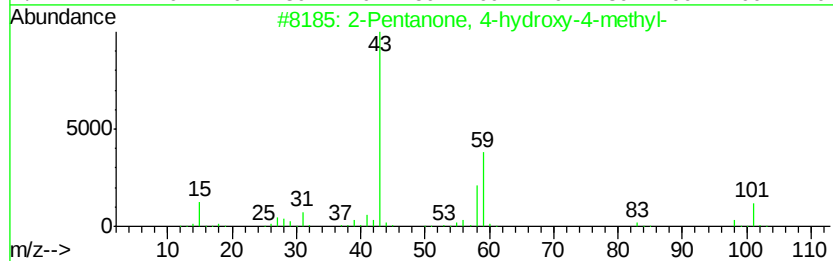
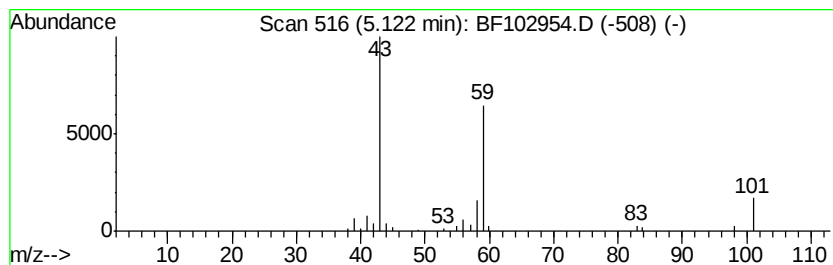
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

| R.T. | EstConc | Area   | Relative to ISTD       | R.T. |
|------|---------|--------|------------------------|------|
| 5.12 | 2.56 ng | 134044 | 1,4-Dichlorobenzene-d4 | 6.87 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2  | 000123-42-2 | 59   |
| 2    |    |   | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2  | 000540-88-5 | 42   |
| 3    |    |   | 2-Hexanol, 2-methyl-                | 116 | C7H16O   | 000625-23-0 | 25   |
| 4    |    |   | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 17   |
| 5    |    |   | 2,3-Butanedione, monooxime          | 101 | C4H7NO2  | 000057-71-6 | 16   |



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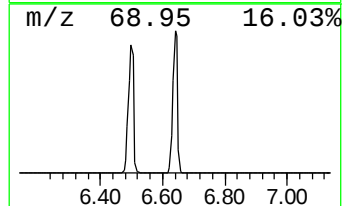
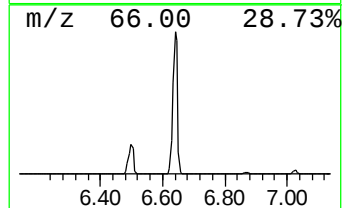
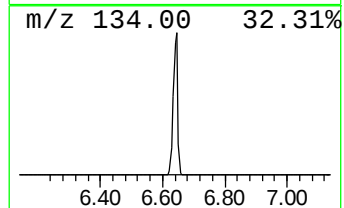
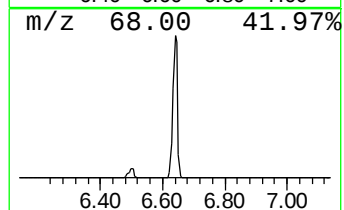
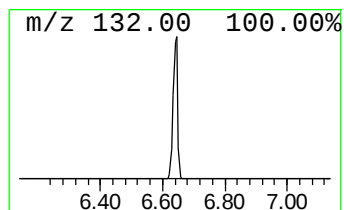
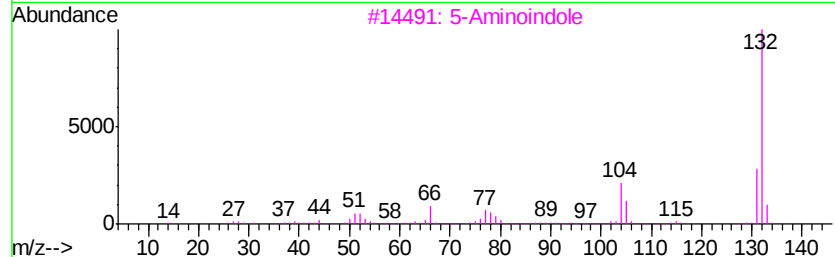
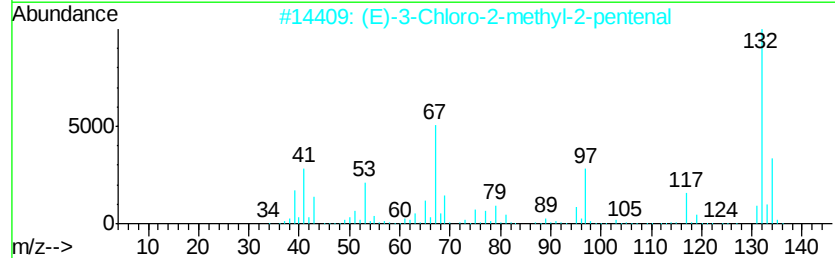
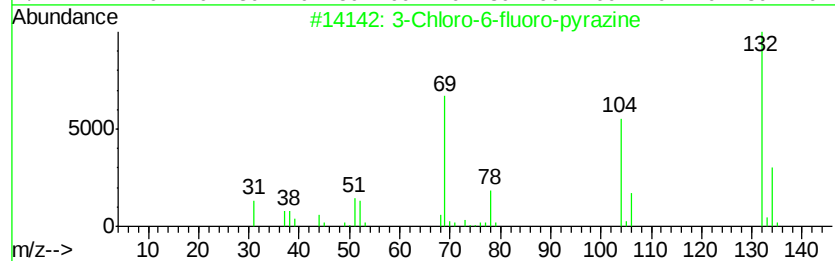
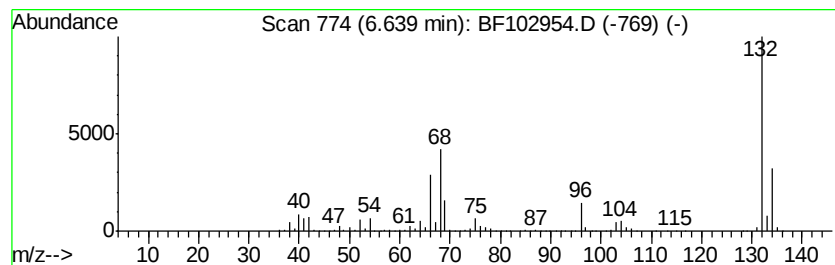
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TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 2 unknown6.64 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.64 | 76.89 ng | 4028470 | 1,4-Dichlorobenzene-d4 | 6.87 |

| Hit# | of | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|-------------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 3-Chloro-6-fluoro-pyrazine          | 132 | C4H2ClFN2 | 1000146-10-7 | 27   |
| 2    |    | (E)-3-Chloro-2-methyl-2-pentenal    | 132 | C6H9ClO   | 031357-76-3  | 17   |
| 3    |    | 5-Aminoindole                       | 132 | C8H8N2    | 005192-03-0  | 12   |
| 4    |    | Tranylcypromine-propionyl           | 189 | C12H15NO  | 1000123-86-3 | 10   |
| 5    |    | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12    | 028749-81-7  | 9    |



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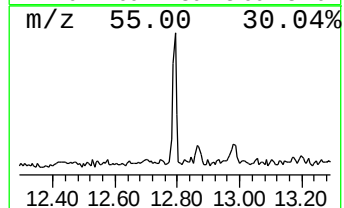
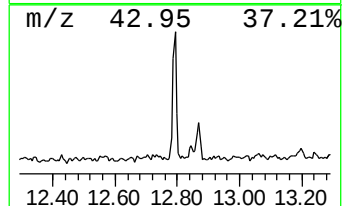
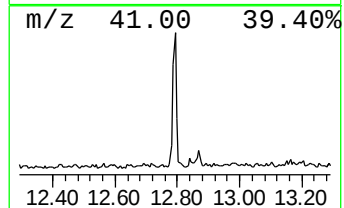
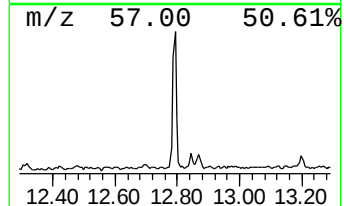
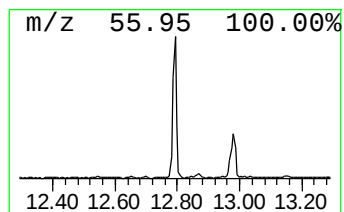
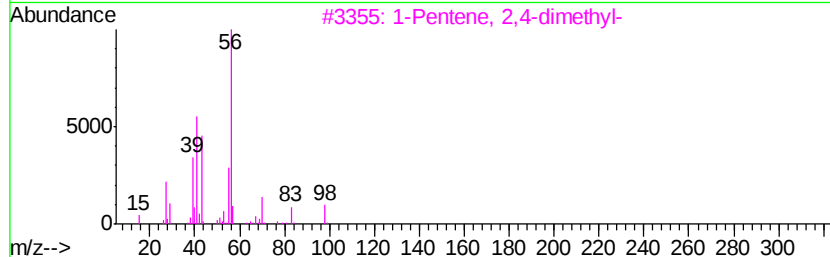
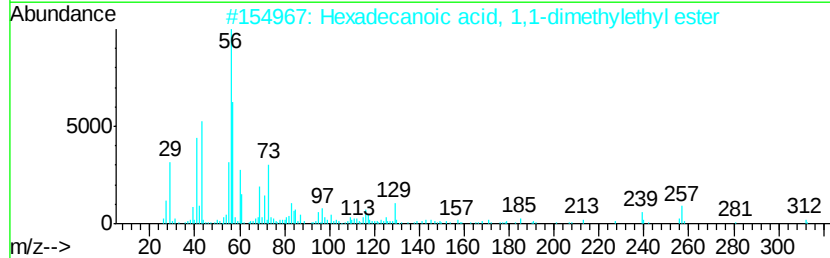
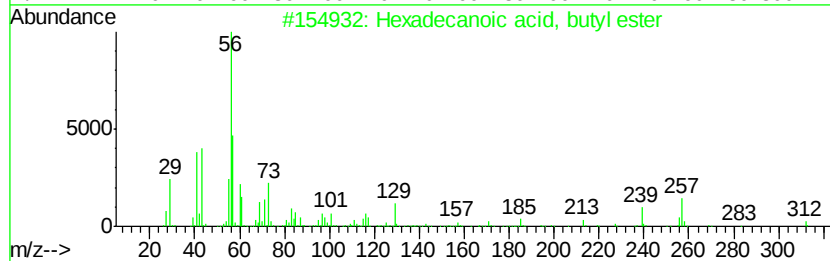
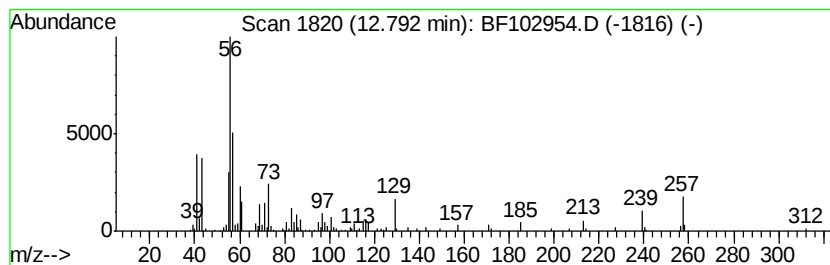
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TIC Integration Parameters: LSCINT.P

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Peak Number 4 Hexadecanoic acid, butyl ester Concentration Rank 3

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 12.79 | 2.81 ng | 199940 | Chrysene-d12     | 14.03 |

| Hit# | of | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|-------------------------------------|-----|----------|-------------|------|
| 1    | 5  | Hexadecanoic acid, butyl ester      | 312 | C20H40O2 | 000111-06-8 | 91   |
| 2    |    | Hexadecanoic acid, 1,1-dimethyle... | 312 | C20H40O2 | 031158-91-5 | 91   |
| 3    |    | 1-Pentene, 2,4-dimethyl-            | 98  | C7H14    | 002213-32-3 | 35   |
| 4    |    | 1-Hexene, 2,5-dimethyl-             | 112 | C8H16    | 006975-92-4 | 35   |
| 5    |    | 1-Hexene, 2-methyl-                 | 98  | C7H14    | 006094-02-6 | 35   |



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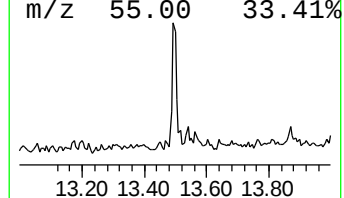
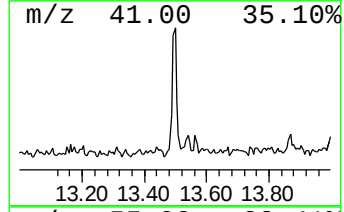
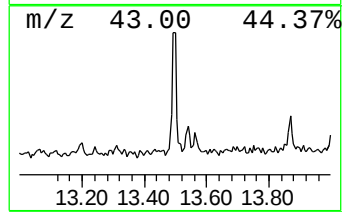
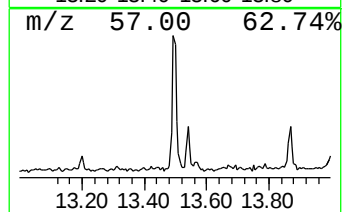
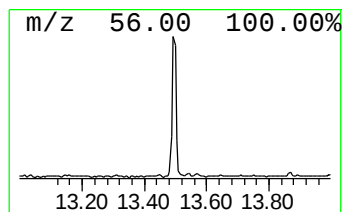
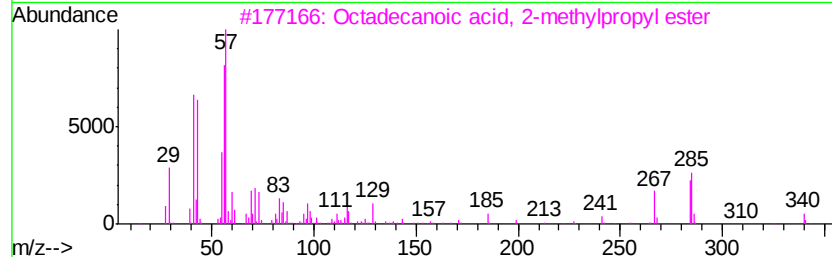
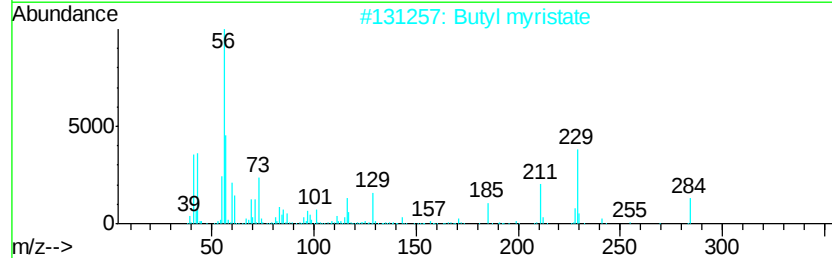
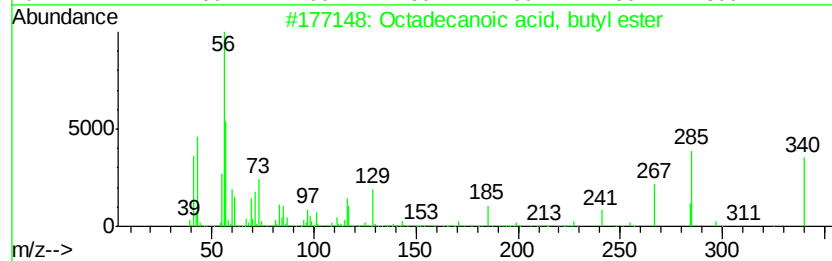
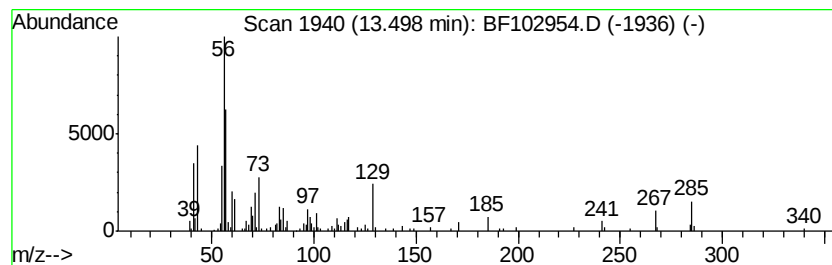
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Peak Number 5 Octadecanoic acid, butyl ester Concentration Rank 5

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 13.50 | 2.29 ng | 163068 | Chrysene-d12     | 14.03 |

| Hit# | of | Tentative ID                            | MW  | MolForm  | CAS#        | Qual |
|------|----|-----------------------------------------|-----|----------|-------------|------|
| 1    | 5  | Octadecanoic acid, butyl ester          | 340 | C22H44O2 | 000123-95-5 | 91   |
| 2    |    | Butyl myristate                         | 284 | C18H36O2 | 000110-36-1 | 53   |
| 3    |    | Octadecanoic acid, 2-methylpropyl ester | 340 | C22H44O2 | 000646-13-9 | 50   |
| 4    |    | Pentanal, 3-methyl-                     | 100 | C6H12O   | 015877-57-3 | 38   |
| 5    |    | Decane, 2,2,3-trimethyl-                | 184 | C13H28   | 062338-09-4 | 37   |



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| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |         |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|---------|------|
|                      |       |         |       |          | #                     | RT    | Resp    | Conc |
| 2-Pentanone, 4-hy... | 5.12  | 2.6     | ng    | 134044   | 1                     | 6.87  | 1047790 | 20.0 |
| unknown6.64          | 6.64  | 76.9    | ng    | 4028470  | 1                     | 6.87  | 1047790 | 20.0 |
| Hexadecanoic acid... | 12.79 | 2.8     | ng    | 199940   | 5                     | 14.03 | 1423590 | 20.0 |
| Octadecanoic acid... | 13.50 | 2.3     | ng    | 163068   | 5                     | 14.03 | 1423590 | 20.0 |