

Data Path : Z:\HPCHEM1\BNA F\Data\BF030217\  
 Data File : BF093337.D  
 Acq On : 2 Mar 2017 22:50  
 Operator : SJ/MA  
 Sample : I2015-06  
 Misc :  
 ALS Vial : 21 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 38A-7-9

Integration Parameters: rteint.p  
 Integrator: RTE  
 Smoothing : ON  
 Sampling : 1  
 Start Thrs: 0.2  
 Stop Thrs : 0

Filtering: 5  
 Min Area: 3 % of largest Peak  
 Max Peaks: 100  
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >  
 Peak separation: 5

Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF013017.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         | 4.944       | 248           | 250         | 261          | rBV      | 1099669        | 1581991       | 41.19%          | 4.488%        |
| 2         | 5.390       | 286           | 289         | 310          | rBV      | 3232732        | 3840731       | 100.00%         | 10.897%       |
| 3         | 6.442       | 378           | 381         | 389          | rBV      | 3400560        | 3801984       | 98.99%          | 10.787%       |
| 4         | 6.567       | 389           | 392         | 394          | rVV      | 2647603        | 3497447       | 91.06%          | 9.923%        |
| 5         | 6.659       | 398           | 400         | 410          | rVB2     | 14320          | 46060         | 1.20%           | 0.131%        |
| 6         | 6.796       | 410           | 412         | 414          | rBV      | 865604         | 955273        | 24.87%          | 2.710%        |
| 7         | 6.944       | 423           | 425         | 428          | rBV      | 2173254        | 2380270       | 61.97%          | 6.753%        |
| 8         | 7.367       | 459           | 462         | 464          | rBV      | 2216729        | 2227912       | 58.01%          | 6.321%        |
| 9         | 8.087       | 523           | 525         | 527          | rBV      | 1320882        | 1240325       | 32.29%          | 3.519%        |
| 10        | 9.173       | 617           | 620         | 622          | rBV      | 2961679        | 3597904       | 93.68%          | 10.208%       |
| 11        | 9.573       | 652           | 655         | 657          | rBV      | 216170         | 287895        | 7.50%           | 0.817%        |
| 12        | 9.848       | 676           | 679         | 681          | rBV      | 1436964        | 1413972       | 36.82%          | 4.012%        |
| 13        | 10.271      | 715           | 716         | 718          | rVB      | 50558          | 50886         | 1.32%           | 0.144%        |
| 14        | 10.636      | 745           | 748         | 751          | rBV      | 1871936        | 1980526       | 51.57%          | 5.619%        |
| 15        | 10.751      | 756           | 758         | 762          | rVB      | 83609          | 111937        | 2.91%           | 0.318%        |
| 16        | 11.196      | 795           | 797         | 798          | rBV      | 83605          | 72439         | 1.89%           | 0.206%        |
| 17        | 11.334      | 807           | 809         | 811          | rBV      | 1550282        | 1464342       | 38.13%          | 4.155%        |
| 18        | 11.619      | 832           | 834         | 837          | rBV      | 48820          | 49840         | 1.30%           | 0.141%        |
| 19        | 12.739      | 930           | 932         | 934          | rBV      | 227934         | 196646        | 5.12%           | 0.558%        |
| 20        | 12.819      | 934           | 939         | 941          | rVB      | 27384          | 43549         | 1.13%           | 0.124%        |
| 21        | 12.922      | 945           | 948         | 950          | rBV      | 3186365        | 3350309       | 87.23%          | 9.505%        |
| 22        | 13.437      | 991           | 993         | 995          | rBV      | 121700         | 140434        | 3.66%           | 0.398%        |
| 23        | 13.814      | 1023          | 1026        | 1034         | rBV      | 113210         | 194429        | 5.06%           | 0.552%        |
| 24        | 13.974      | 1038          | 1040        | 1042         | rBV      | 1304466        | 1307647       | 34.05%          | 3.710%        |
| 25        | 14.728      | 1103          | 1106        | 1108         | rVB      | 28593          | 52755         | 1.37%           | 0.150%        |
| 26        | 14.797      | 1109          | 1112        | 1114         | rBV      | 59132          | 69394         | 1.81%           | 0.197%        |
| 27        | 15.037      | 1131          | 1133        | 1137         | rBV      | 34446          | 46737         | 1.22%           | 0.133%        |
| 28        | 15.391      | 1161          | 1164        | 1175         | rVB      | 744203         | 1044730       | 27.20%          | 2.964%        |
| 29        | 15.791      | 1197          | 1199        | 1202         | rVB      | 33255          | 51054         | 1.33%           | 0.145%        |
| 30        | 16.260      | 1237          | 1240        | 1246         | rVB      | 30084          | 57385         | 1.49%           | 0.163%        |
| 31        | 16.797      | 1284          | 1287        | 1292         | rBV      | 21491          | 49952         | 1.30%           | 0.142%        |
| 32        | 19.106      | 1486          | 1489        | 1495         | rVB8     | 11460          | 40247         | 1.05%           | 0.114%        |

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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-BF013017.M  
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

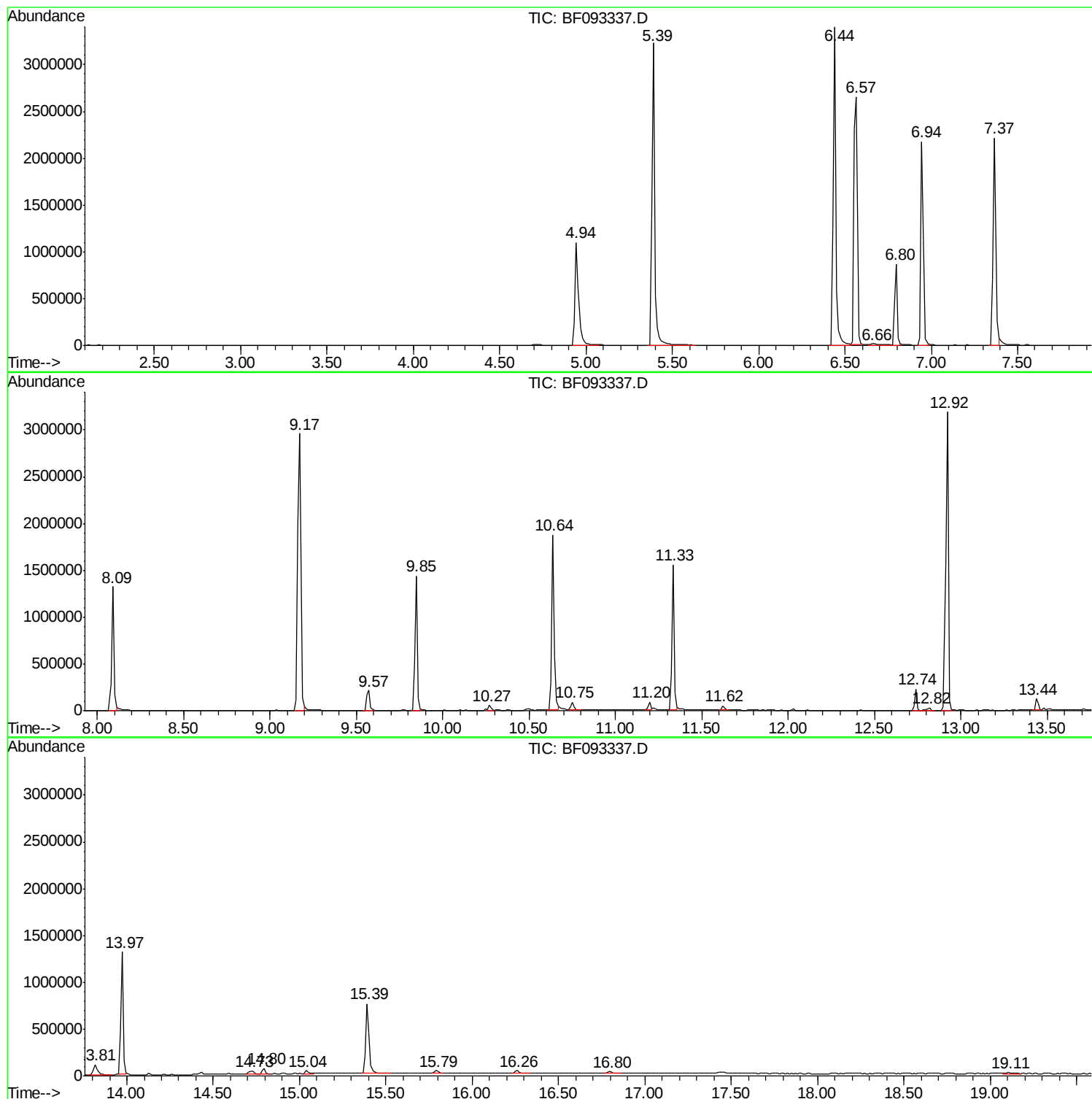
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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF013017.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P



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38A-7-9

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF013017.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

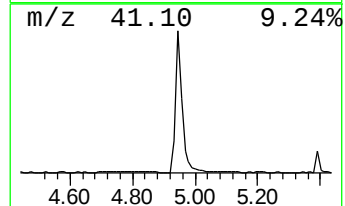
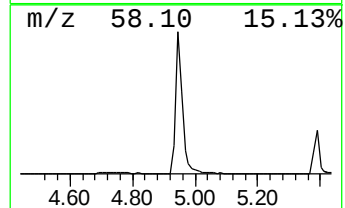
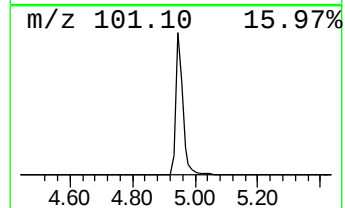
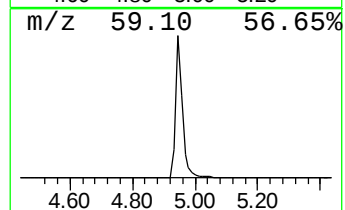
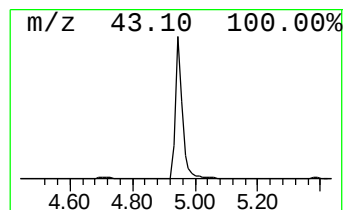
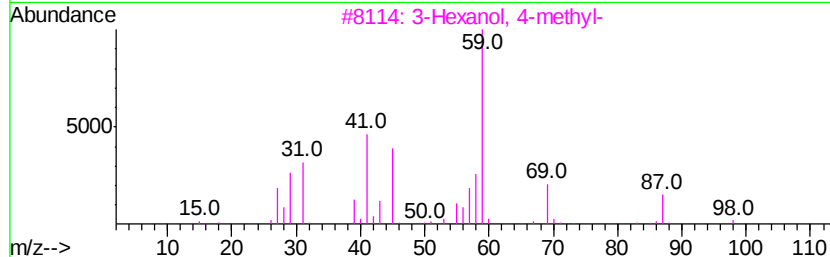
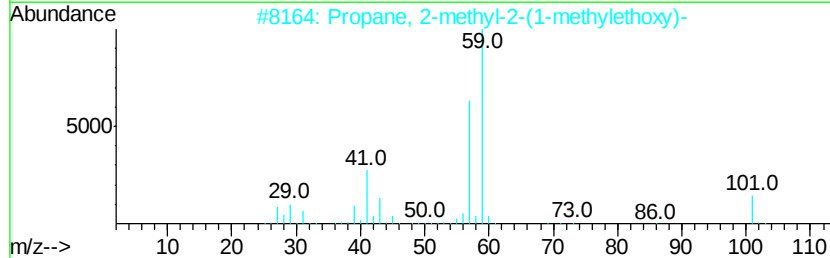
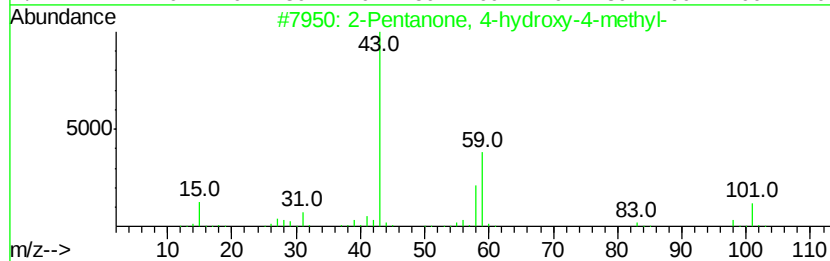
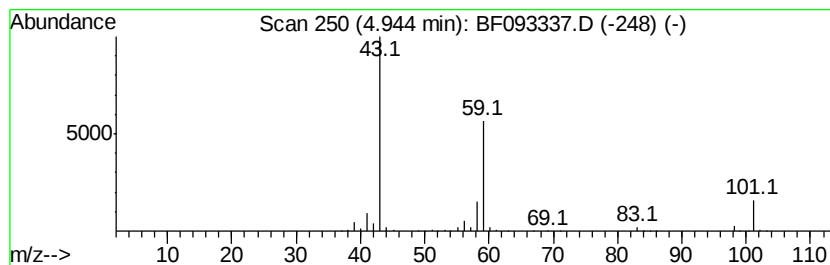
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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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. |
|------|----------|---------|------------------------|------|
| 4.94 | 33.12 ng | 1581990 | 1,4-Dichlorobenzene-d4 | 6.80 |

| Hit# | of | Tentative ID                          | MW  | MolForm  | CAS#        | Qual |
|------|----|---------------------------------------|-----|----------|-------------|------|
| 1    | 5  | 2-Pentanone, 4-hydroxy-4-methyl-      | 116 | C6H12O2  | 000123-42-2 | 59   |
| 2    |    | Propane, 2-methyl-2-(1-methylethoxy)- | 116 | C7H16O   | 017348-59-3 | 42   |
| 3    |    | 3-Hexanol, 4-methyl-                  | 116 | C7H16O   | 000615-29-2 | 33   |
| 4    |    | 2-Hexanol, 2-methyl-                  | 116 | C7H16O   | 000625-23-0 | 33   |
| 5    |    | Acetic acid, cyano-, 1,1-dimethyl-    | 141 | C7H11NO2 | 001116-98-9 | 32   |



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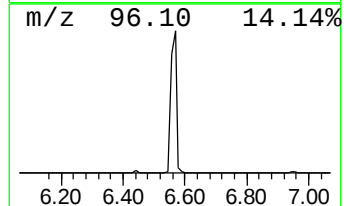
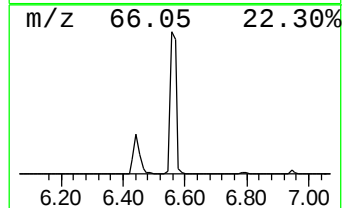
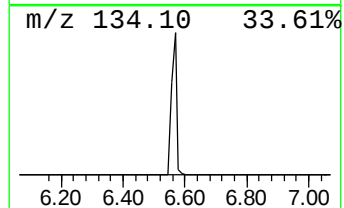
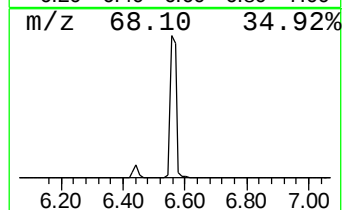
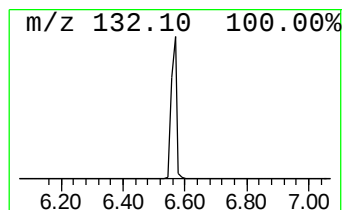
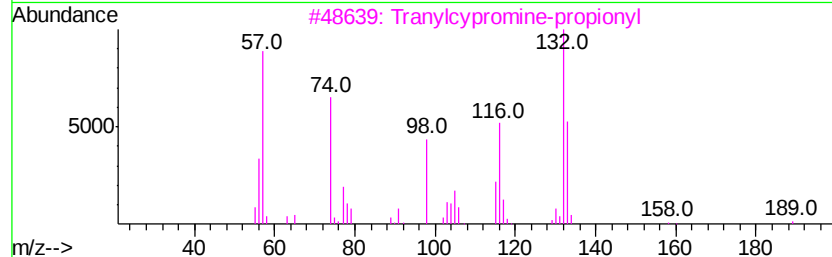
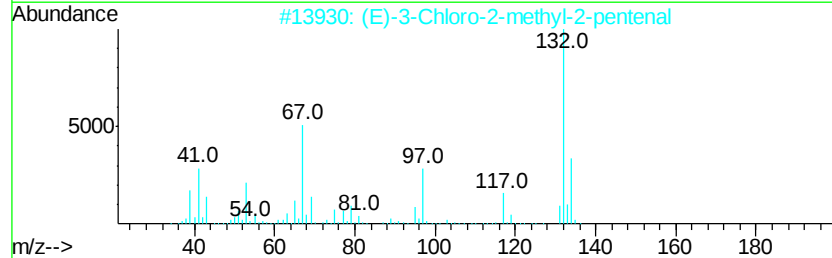
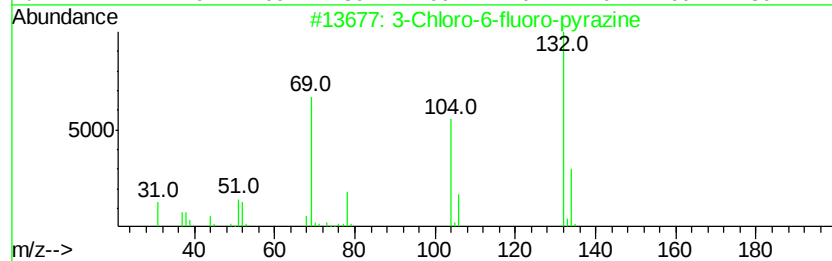
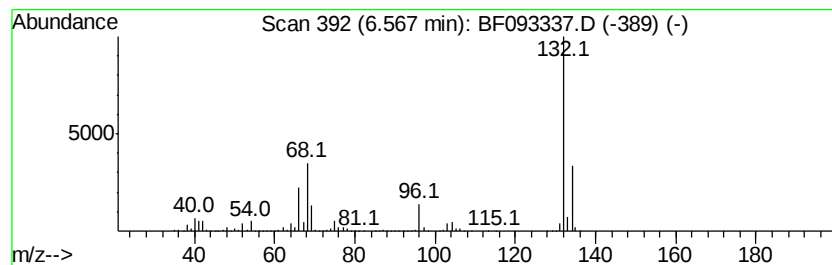
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF013017.M  
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TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 unknown6.57 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.57 | 73.22 ng | 3497450 | 1,4-Dichlorobenzene-d4 | 6.80 |

| Hit# | of | Tentative ID                     | MW  | MolForm   | CAS#         | Qual |
|------|----|----------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 3-Chloro-6-fluoro-pyrazine       | 132 | C4H2ClFN2 | 1000146-10-7 | 38   |
| 2    |    | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO   | 031357-76-3  | 25   |
| 3    |    | Tranvlcypropine-propionyl        | 189 | C12H15NO  | 1000123-86-3 | 16   |
| 4    |    | 5-Fluoro-2-chloropyrimidine      | 132 | C4H2ClFN2 | 062802-42-0  | 9    |
| 5    |    | 4-Chloro-2-fluoro-pyrimidine     | 132 | C4H2ClFN2 | 051422-00-5  | 9    |



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BNA\_F  
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38A-7-9

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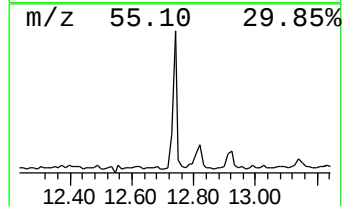
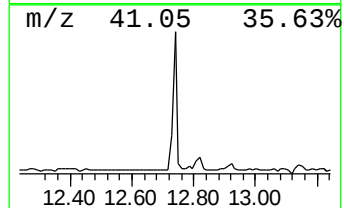
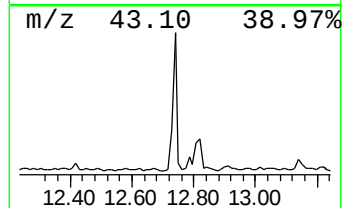
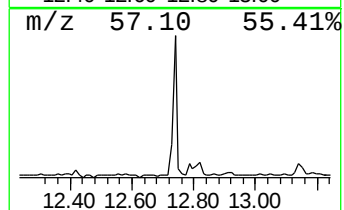
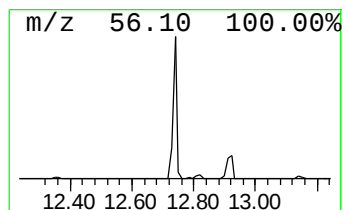
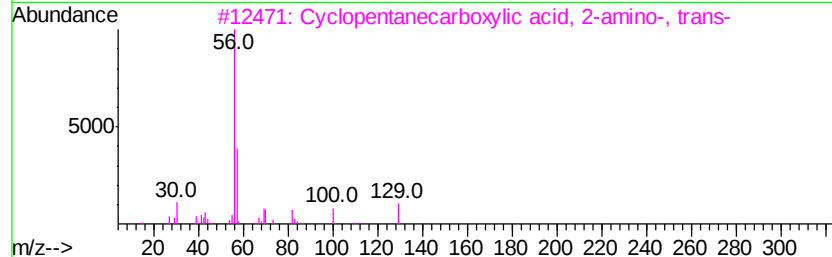
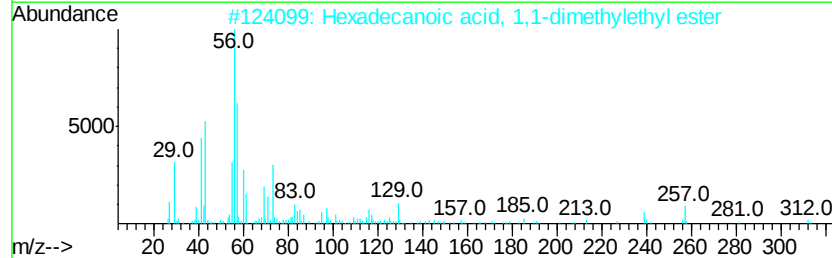
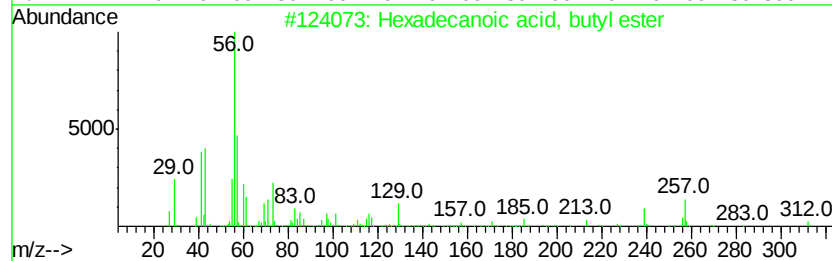
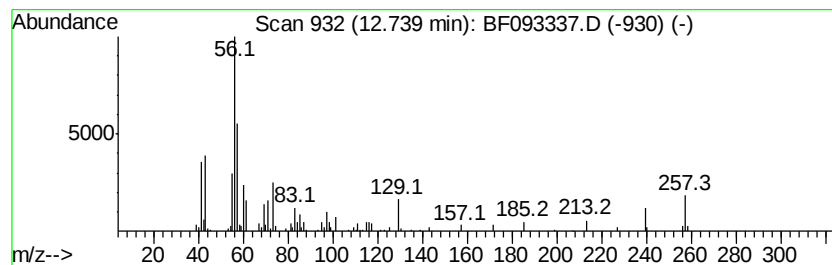
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 4 Hexadecanoic acid, butyl ester Concentration Rank 4

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 12.74 | 3.01 ng | 196646 | Chrysene-d12     | 13.97 |

| 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 | 52   |
| 3    |    | Cyclopentanecarboxylic acid, 2-a... | 129 | C6H11NO2 | 040482-05-1 | 43   |
| 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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ALS Vial : 21 Sample Multiplier: 1

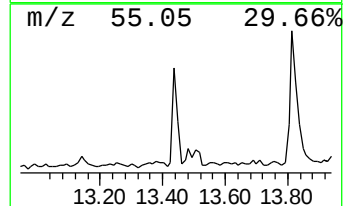
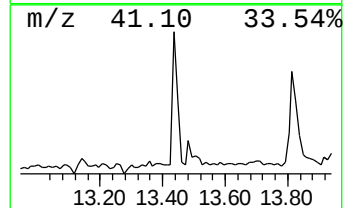
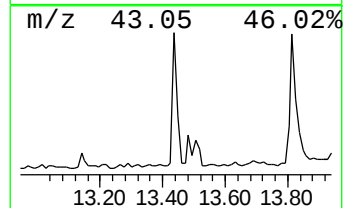
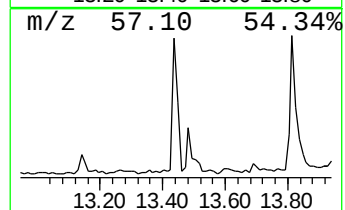
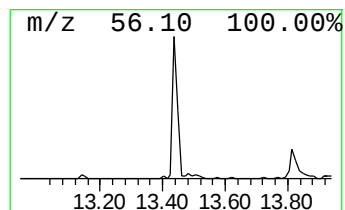
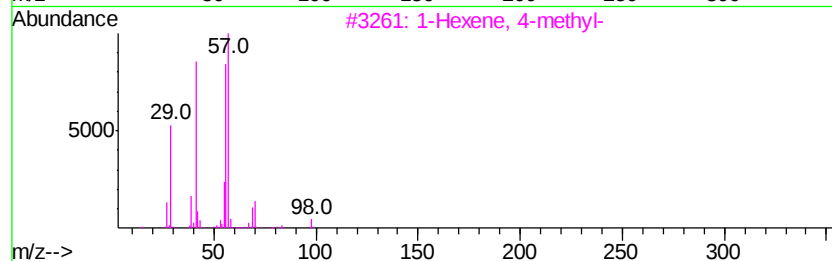
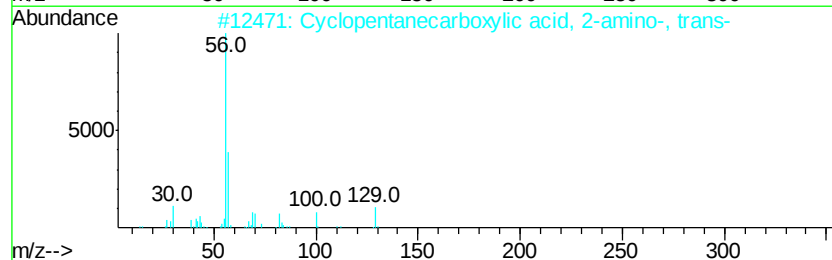
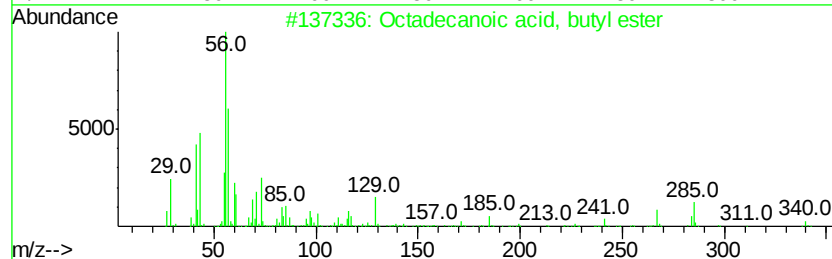
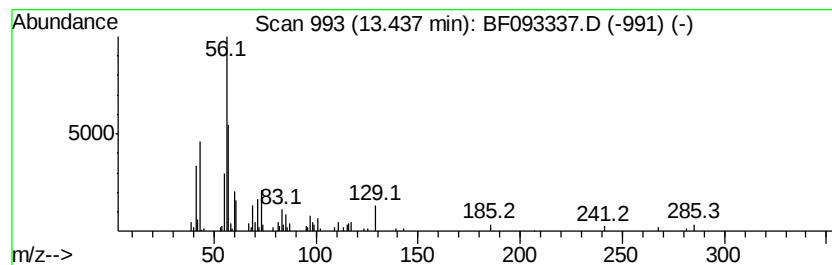
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TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 5 Octadecanoic acid, butyl ester Concentration Rank 6

| R.T.      | EstConc                                       | Area   | Relative to ISTD | R.T.        |      |
|-----------|-----------------------------------------------|--------|------------------|-------------|------|
| 13.44     | 2.15 ng                                       | 140434 | Chrysene-d12     | 13.97       |      |
| Hit# of 5 | Tentative ID                                  | MW     | MolForm          | CAS#        | Qual |
| 1         | Octadecanoic acid, butyl ester                | 340    | C22H44O2         | 000123-95-5 | 91   |
| 2         | Cyclopentanecarboxylic acid, 2-amino-, trans- | 129    | C6H11NO2         | 040482-05-1 | 46   |
| 3         | 1-Hexene, 4-methyl-                           | 98     | C7H14            | 003769-23-1 | 43   |
| 4         | 1-Hexene, 2,5-dimethyl-                       | 112    | C8H16            | 006975-92-4 | 38   |
| 5         | 1-Hexene, 2-methyl-                           | 98     | C7H14            | 006094-02-6 | 38   |



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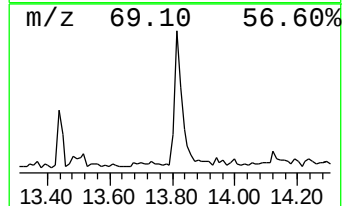
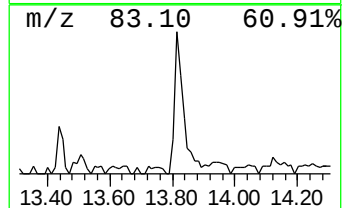
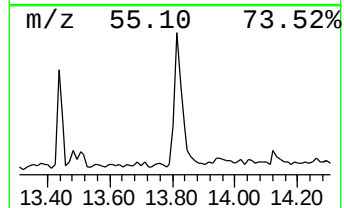
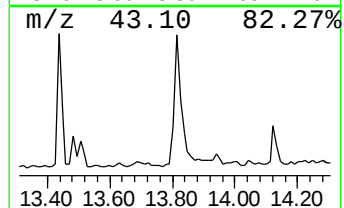
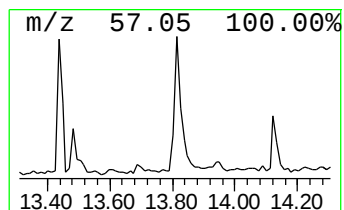
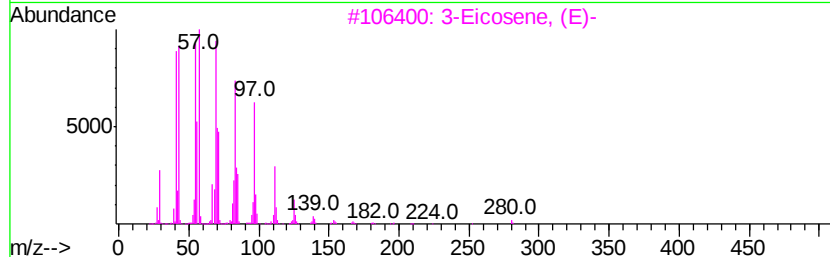
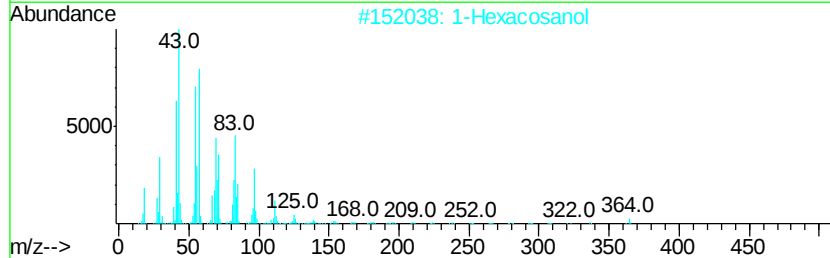
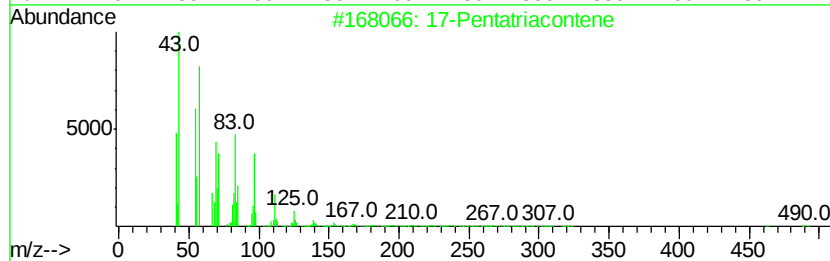
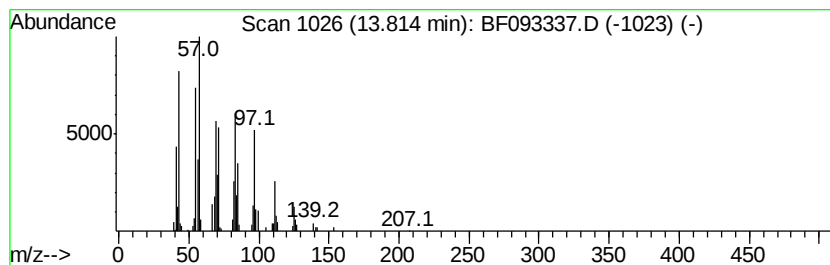
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 6 17-Pentatriacontene Concentration Rank 5

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 13.81 | 2.97 ng | 194429 | Chrysene-d12     | 13.97 |

| Hit# | of | Tentative ID                        | MW  | MolForm    | CAS#        | Qual |
|------|----|-------------------------------------|-----|------------|-------------|------|
| 1    | 5  | 17-Pentatriacontene                 | 491 | C35H70     | 006971-40-0 | 91   |
| 2    |    | 1-Hexacosanol                       | 382 | C26H54O    | 000506-52-5 | 87   |
| 3    |    | 3-Eicosene, (E)-                    | 280 | C20H40     | 074685-33-9 | 81   |
| 4    |    | 1-Decanol, 2-hexyl-                 | 242 | C16H34O    | 002425-77-6 | 74   |
| 5    |    | Pentafluoropropionic acid, hexad... | 388 | C19H33F5O2 | 006222-07-7 | 72   |



Data Path : Z:\HPCHEM1\BNA\_F\Data\BF030217\  
Data File : BF093337.D  
Acq On : 2 Mar 2017 22:50  
Operator : SJ/MA  
Sample : I2015-06  
Misc :  
ALS Vial : 21 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
38A-7-9

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF013017.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |         |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|---------|------|
|                      |       |         |       |          | #                     | RT    | Resp    | Conc |
| 2-Pentanone, 4-hy... | 4.94  | 33.1    | ng    | 1581990  | 1                     | 6.80  | 955273  | 20.0 |
| unknown6.57          | 6.57  | 73.2    | ng    | 3497450  | 1                     | 6.80  | 955273  | 20.0 |
| Hexadecanoic acid... | 12.74 | 3.0     | ng    | 196646   | 5                     | 13.97 | 1307650 | 20.0 |
| Octadecanoic acid... | 13.44 | 2.1     | ng    | 140434   | 5                     | 13.97 | 1307650 | 20.0 |
| 17-Pentatriacontene  | 13.81 | 3.0     | ng    | 194429   | 5                     | 13.97 | 1307650 | 20.0 |