

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100616\  
 Data File : BF090429.D  
 Acq On : 6 Oct 2016 20:20  
 Operator : UM/SJ  
 Sample : H5110-02  
 Misc :  
 ALS Vial : 8 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 BRAEN-AGGS-CLEAN-BORROW

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-BF100516.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         | 3.445       | 95            | 97          | 112          | rBV      | 92101          | 224554        | 2.91%           | 0.370%        |
| 2         | 5.194       | 247           | 250         | 258          | rVB      | 976011         | 1588238       | 20.58%          | 2.614%        |
| 3         | 5.606       | 283           | 286         | 288          | rBV      | 6091841        | 6156316       | 79.79%          | 10.131%       |
| 4         | 6.566       | 367           | 370         | 372          | rBV      | 50180          | 84860         | 1.10%           | 0.140%        |
| 5         | 6.623       | 372           | 375         | 377          | rVB      | 5880046        | 6921941       | 89.71%          | 11.391%       |
| 6         | 6.760       | 384           | 387         | 390          | rBV      | 5557529        | 6058708       | 78.52%          | 9.970%        |
| 7         | 6.989       | 405           | 407         | 410          | rBV      | 951014         | 1296329       | 16.80%          | 2.133%        |
| 8         | 7.149       | 419           | 421         | 423          | rVB      | 4167509        | 4655389       | 60.33%          | 7.661%        |
| 9         | 7.560       | 454           | 457         | 459          | rBV      | 4144064        | 4497613       | 58.29%          | 7.401%        |
| 10        | 8.280       | 518           | 520         | 522          | rBV      | 2071744        | 1803518       | 23.37%          | 2.968%        |
| 11        | 9.366       | 612           | 615         | 617          | rBV      | 7934544        | 7715902       | 100.00%         | 12.698%       |
| 12        | 9.755       | 646           | 649         | 651          | rBV      | 1970906        | 1587475       | 20.57%          | 2.612%        |
| 13        | 10.040      | 672           | 674         | 677          | rVB      | 2009218        | 1922843       | 24.92%          | 3.164%        |
| 14        | 10.829      | 741           | 743         | 746          | rBV2     | 3100581        | 4296845       | 55.69%          | 7.071%        |
| 15        | 10.955      | 751           | 754         | 759          | rVB      | 65876          | 114325        | 1.48%           | 0.188%        |
| 16        | 11.400      | 791           | 793         | 795          | rBV      | 117440         | 113518        | 1.47%           | 0.187%        |
| 17        | 11.538      | 802           | 805         | 807          | rBV      | 1846265        | 1947140       | 25.24%          | 3.204%        |
| 18        | 11.755      | 822           | 824         | 828          | rBV2     | 99688          | 119292        | 1.55%           | 0.196%        |
| 19        | 11.823      | 828           | 830         | 834          | rVB      | 75962          | 86138         | 1.12%           | 0.142%        |
| 20        | 12.052      | 848           | 850         | 853          | rBV      | 216509         | 269050        | 3.49%           | 0.443%        |
| 21        | 12.841      | 918           | 919         | 924          | rBV2     | 93555          | 150146        | 1.95%           | 0.247%        |
| 22        | 13.126      | 941           | 944         | 947          | rBV      | 6832692        | 6258988       | 81.12%          | 10.300%       |
| 23        | 14.018      | 1020          | 1022        | 1028         | rBV      | 222105         | 325533        | 4.22%           | 0.536%        |
| 24        | 14.178      | 1034          | 1036        | 1039         | rBV      | 1459649        | 1353256       | 17.54%          | 2.227%        |
| 25        | 15.687      | 1164          | 1168        | 1170         | rBV      | 755667         | 1218516       | 15.79%          | 2.005%        |

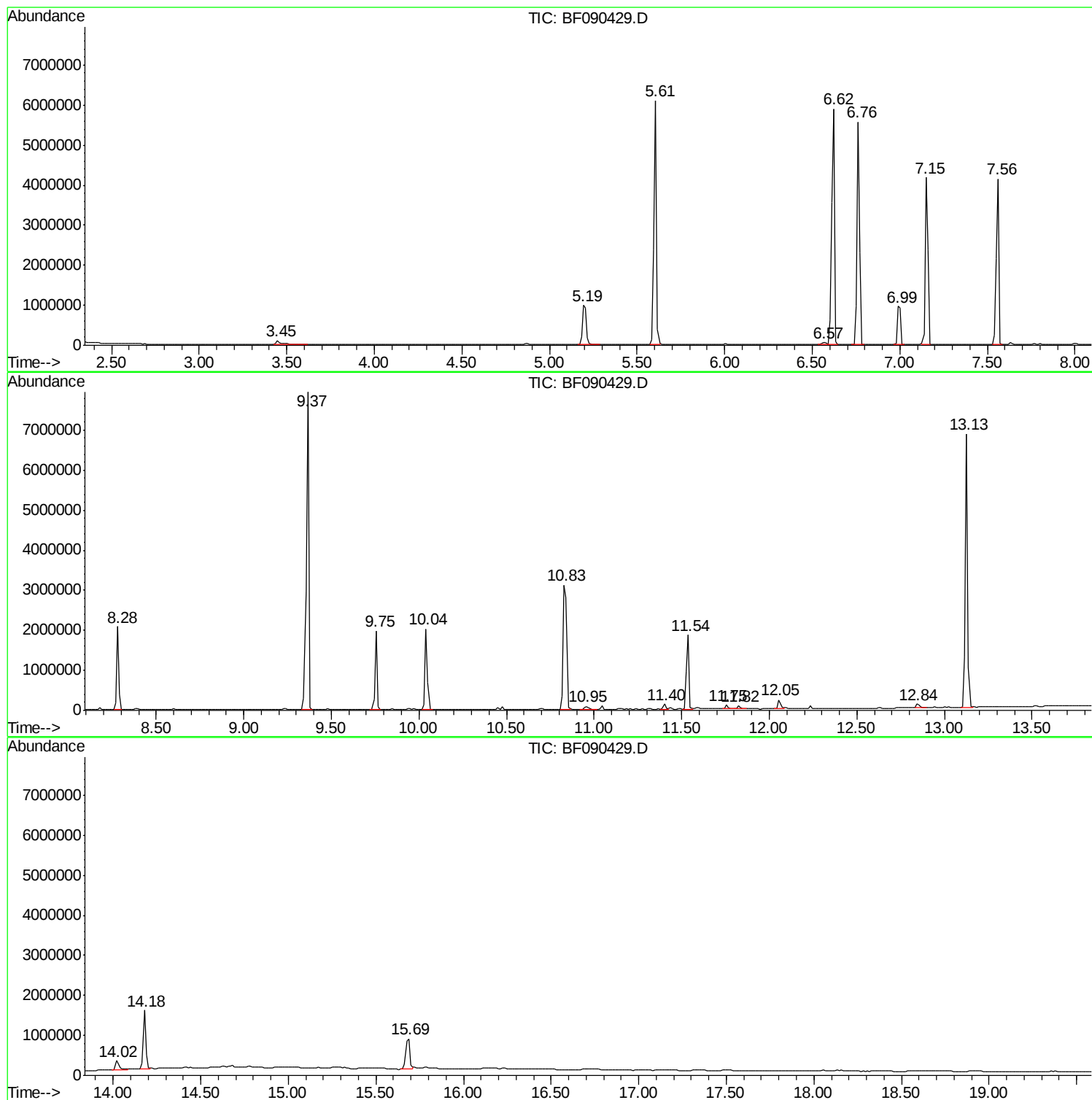
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Data File : BF090429.D  
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Misc :  
ALS Vial : 8 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
BRAEN-AGGS-CLEAN-BORROW

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF100516.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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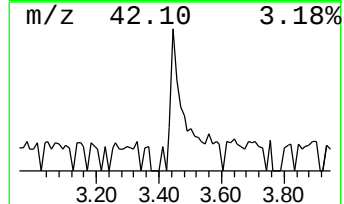
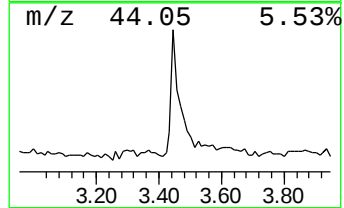
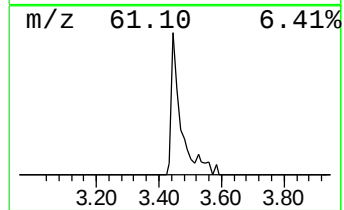
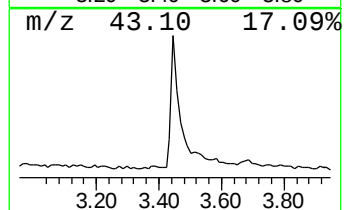
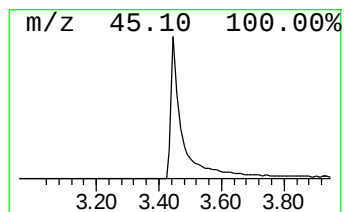
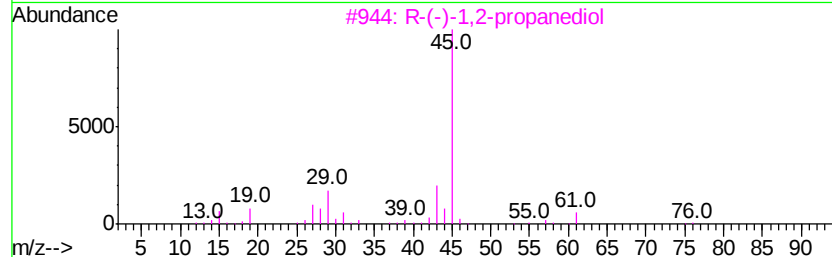
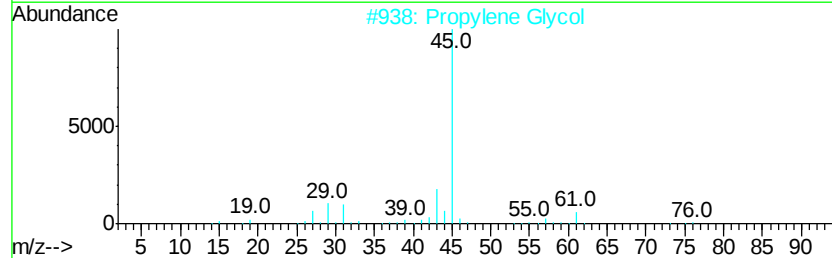
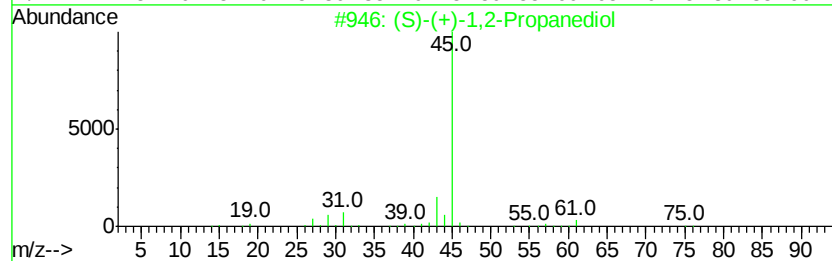
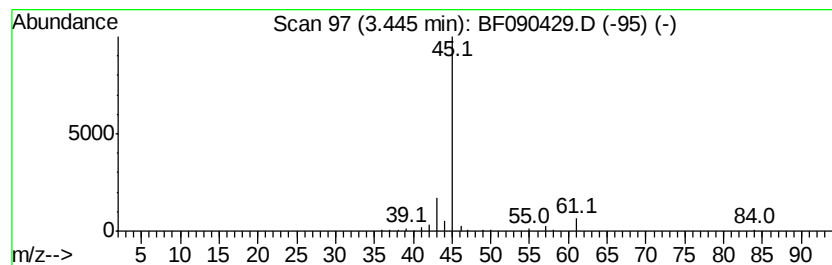
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 unknown3.45 Concentration Rank 5

| R.T. | EstConc | Area   | Relative to ISTD       | R.T. |
|------|---------|--------|------------------------|------|
| 3.45 | 3.46 ng | 224554 | 1,4-Dichlorobenzene-d4 | 7.00 |

| Hit# | of | Tentative ID            | MW | MolForm | CAS#        | Qual |
|------|----|-------------------------|----|---------|-------------|------|
| 1    | 5  | (S)-(+)-1,2-Propanediol | 76 | C3H8O2  | 004254-15-3 | 43   |
| 2    |    | Propylene Glycol        | 76 | C3H8O2  | 000057-55-6 | 43   |
| 3    |    | R-(-)-1,2-propanediol   | 76 | C3H8O2  | 004254-14-2 | 43   |
| 4    |    | 2-Pentanol              | 88 | C5H12O  | 006032-29-7 | 9    |
| 5    |    | Isopropyl Alcohol       | 60 | C3H8O   | 000067-63-0 | 9    |



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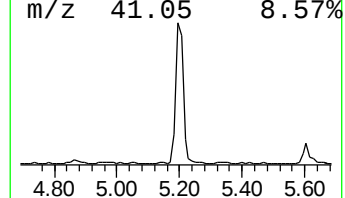
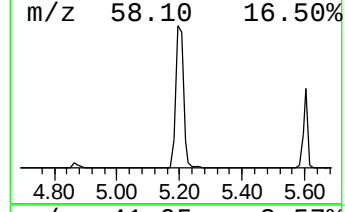
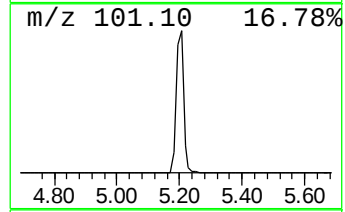
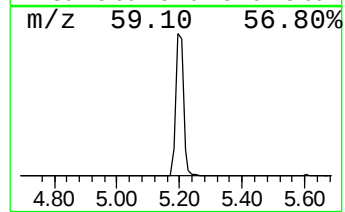
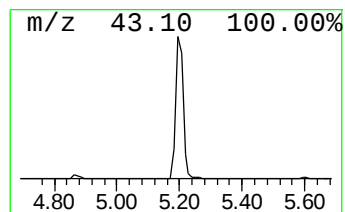
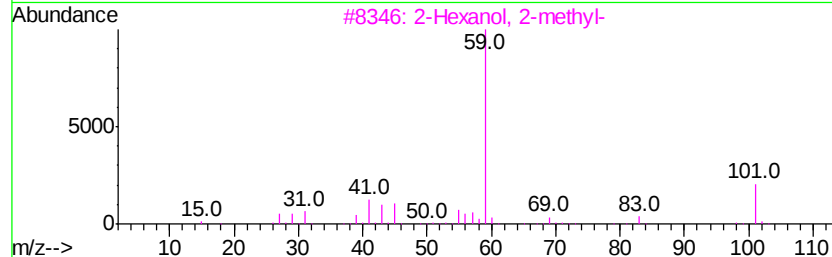
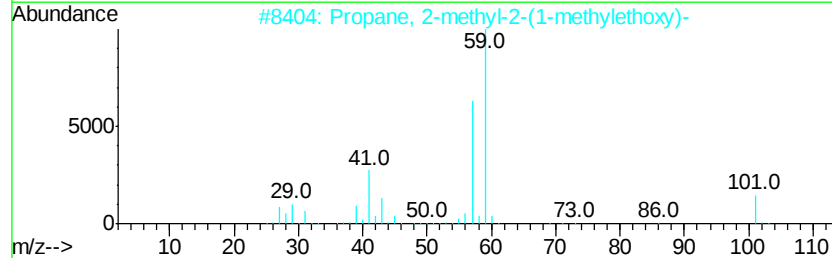
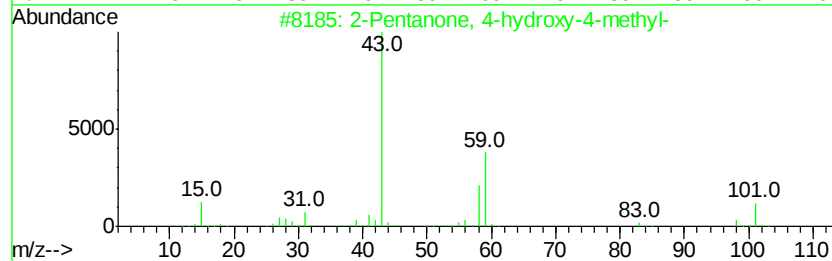
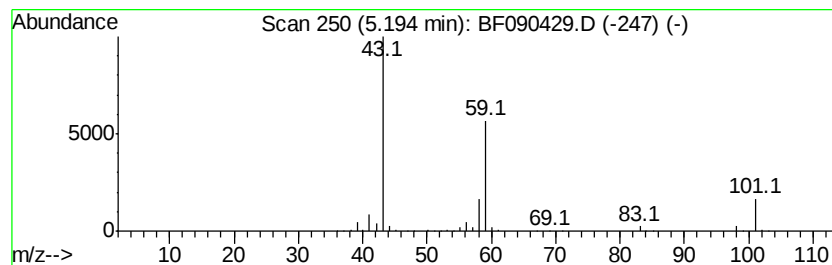
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 5.19 | 24.50 ng | 1588240 | 1,4-Dichlorobenzene-d4 | 7.00 |

| 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-methyleth... | 116 | C7H16O   | 017348-59-3 | 42   |
| 3    |    | 2-Hexanol, 2-methyl-                | 116 | C7H16O   | 000625-23-0 | 33   |
| 4    |    | 3-Hexanol, 4-methyl-                | 116 | C7H16O   | 000615-29-2 | 33   |
| 5    |    | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 23   |



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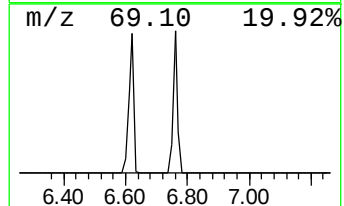
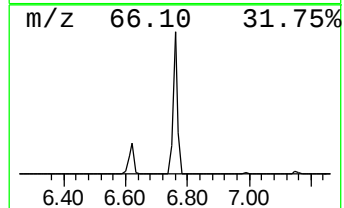
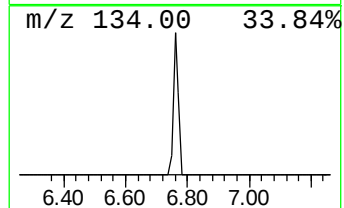
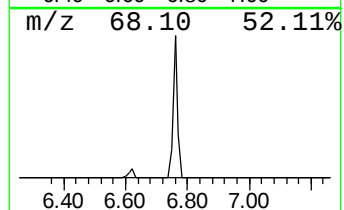
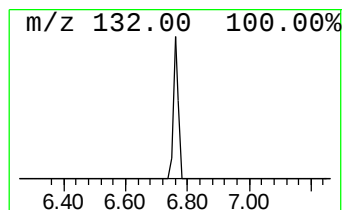
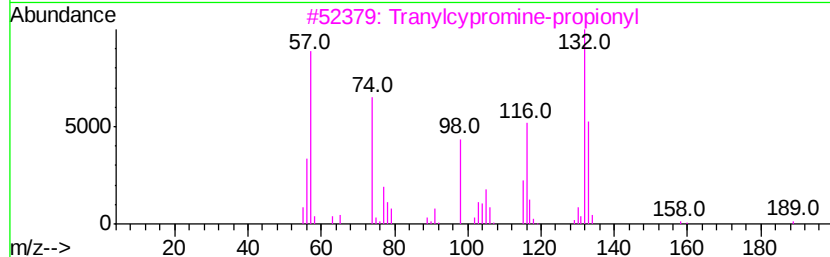
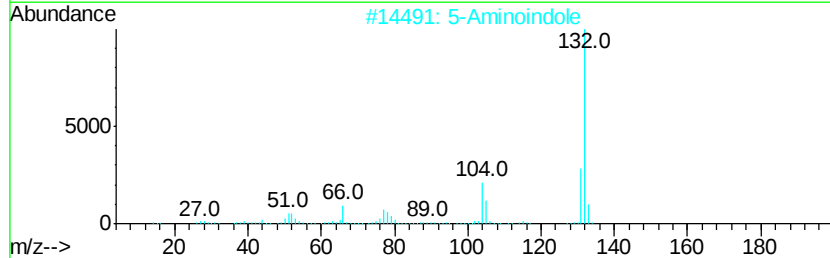
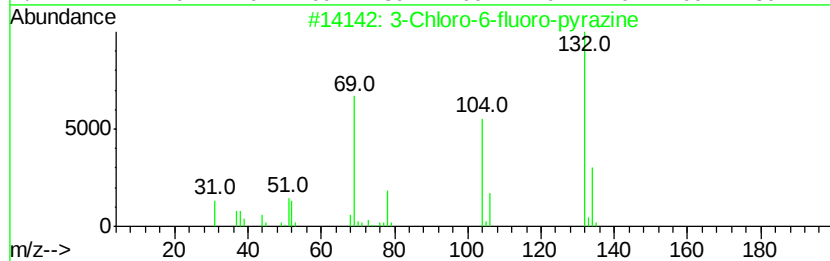
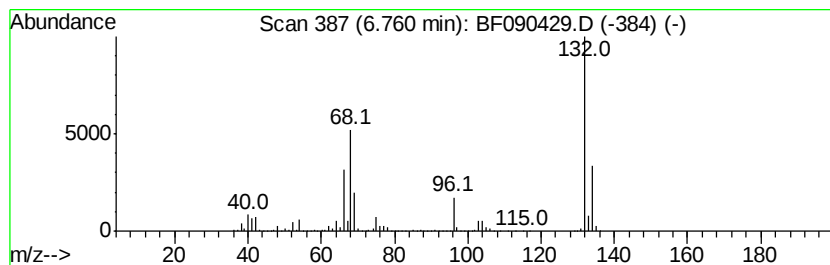
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF100516.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 3 unknown6.76 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.76 | 93.47 ng | 6058710 | 1,4-Dichlorobenzene-d4 | 7.00 |

| Hit# | of                             | Tentative ID | MW        | MolForm      | CAS# | Qual |
|------|--------------------------------|--------------|-----------|--------------|------|------|
| 1    | 3-Chloro-6-fluoro-pyrazine     | 132          | C4H2ClFN2 | 1000146-10-7 | 16   |      |
| 2    | 5-Aminoindole                  | 132          | C8H8N2    | 005192-03-0  | 12   |      |
| 3    | Tranvlcyproamine-propionyl     | 189          | C12H15NO  | 1000123-86-3 | 10   |      |
| 4    | Cyclopropanamine, 1-phenyl-    | 133          | C9H11N    | 1000351-26-2 | 9    |      |
| 5    | 1-Methylpyrrolo[1,2-a]pyrazine | 132          | C8H8N2    | 064608-59-9  | 9    |      |



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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

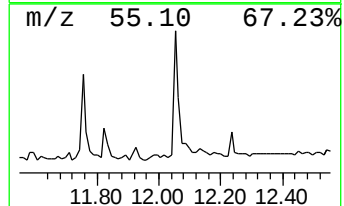
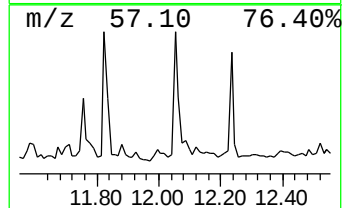
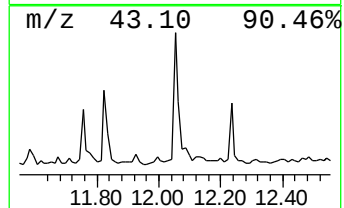
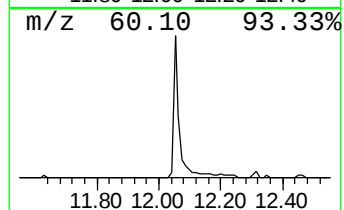
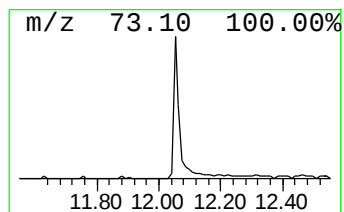
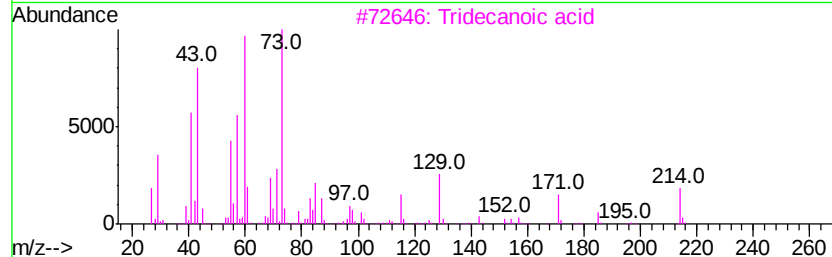
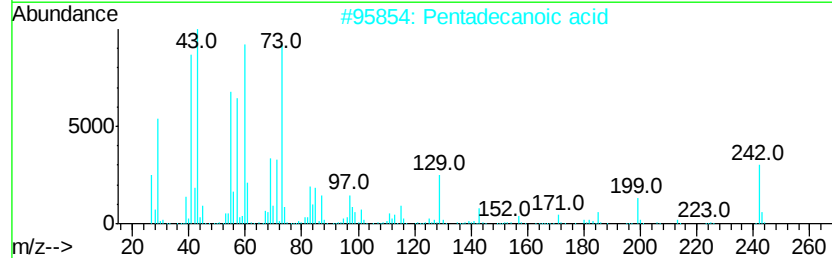
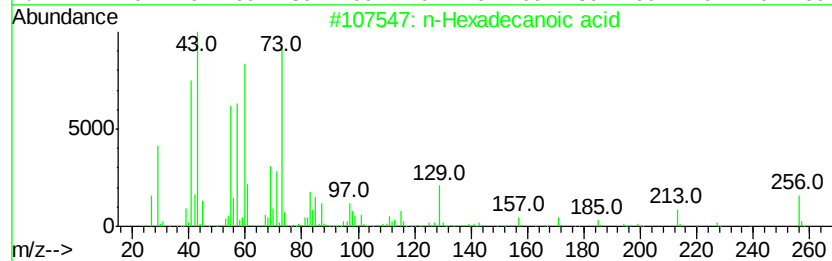
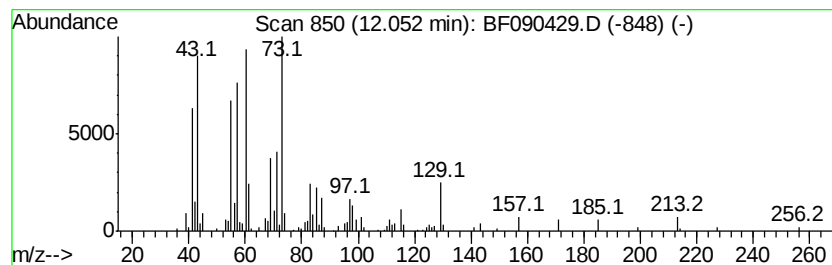
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 12.05 | 2.76 ng | 269050 | Phenanthrene-d10 | 11.54 |

| Hit# of | 5 | Tentative ID                        | MW  | MolForm   | CAS#        | Qual |
|---------|---|-------------------------------------|-----|-----------|-------------|------|
| 1       |   | n-Hexadecanoic acid                 | 256 | C16H32O2  | 000057-10-3 | 98   |
| 2       |   | Pentadecanoic acid                  | 242 | C15H30O2  | 001002-84-2 | 91   |
| 3       |   | Tridecanoic acid                    | 214 | C13H26O2  | 000638-53-9 | 80   |
| 4       |   | Tetradecanoic acid                  | 228 | C14H28O2  | 000544-63-8 | 80   |
| 5       |   | .alpha.-D-Glucopyranose, 4-O-.be... | 342 | C12H22O11 | 014641-93-1 | 50   |



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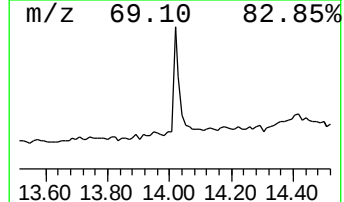
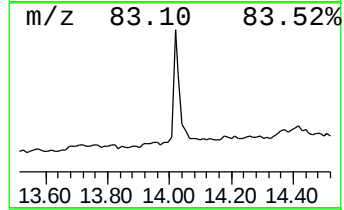
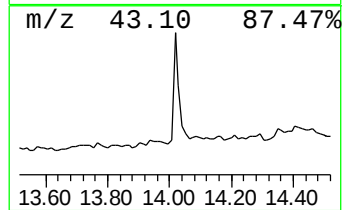
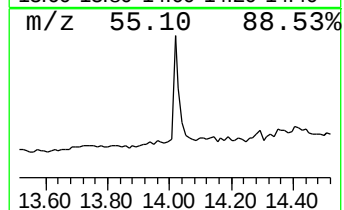
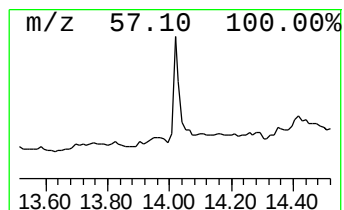
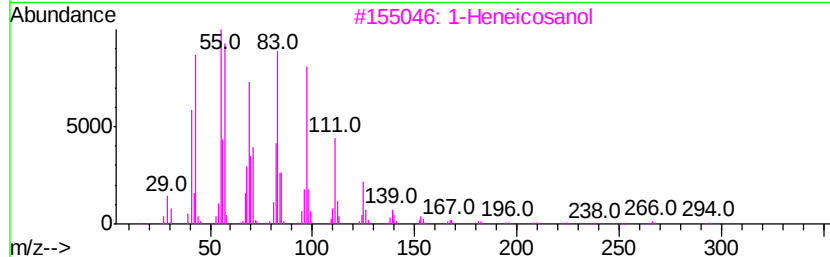
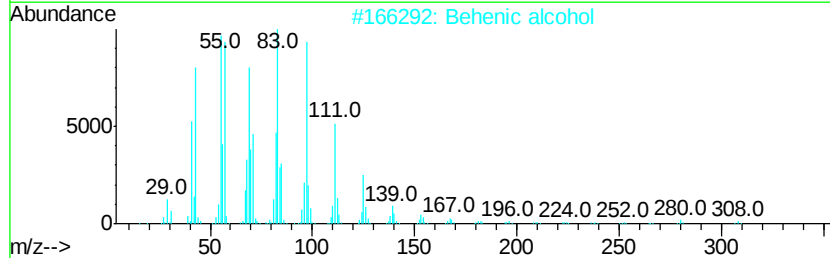
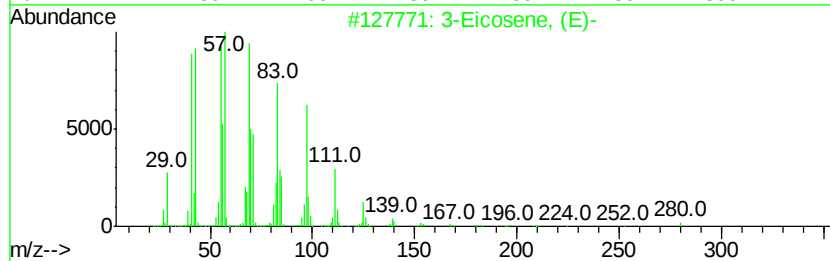
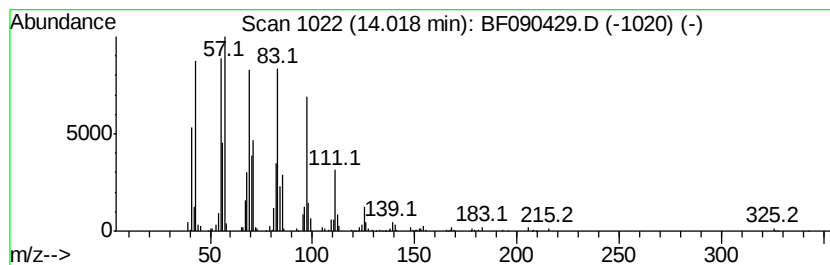
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 6 3-Eicosene, (E)- Concentration Rank 4

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 14.02 | 4.81 ng | 325533 | Chrysene-d12     | 14.18 |

| Hit# | of | Tentative ID                        | MW  | MolForm     | CAS#        | Qual |
|------|----|-------------------------------------|-----|-------------|-------------|------|
| 1    | 5  | 3-Eicosene, (E)-                    | 280 | C20H40      | 074685-33-9 | 95   |
| 2    |    | Behenic alcohol                     | 326 | C22H46O     | 000661-19-8 | 94   |
| 3    |    | 1-Heneicosanol                      | 312 | C21H44O     | 015594-90-8 | 91   |
| 4    |    | Trichloroacetic acid, tetradecyl... | 358 | C16H29Cl3O2 | 074339-52-9 | 91   |
| 5    |    | 1-Heneicosyl formate                | 340 | C22H44O2    | 077899-03-7 | 91   |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF100616\  
Data File : BF090429.D  
Acq On : 6 Oct 2016 20:20  
Operator : UM/SJ  
Sample : H5110-02  
Misc :  
ALS Vial : 8 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
BRAEN-AGGS-CLEAN-BORROW

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF100516.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |         |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|---------|------|
|                      |       |         |       |          | #                     | RT    | Resp    | Conc |
| unknown3.45          | 3.45  | 3.5     | ng    | 224554   | 1                     | 7.00  | 1296330 | 20.0 |
| 2-Pentanone, 4-hy... | 5.19  | 24.5    | ng    | 1588240  | 1                     | 7.00  | 1296330 | 20.0 |
| unknown6.76          | 6.76  | 93.5    | ng    | 6058710  | 1                     | 7.00  | 1296330 | 20.0 |
| n-Hexadecanoic acid  | 12.05 | 2.8     | ng    | 269050   | 4                     | 11.54 | 1947140 | 20.0 |
| 3-Eicosene, (E)-     | 14.02 | 4.8     | ng    | 325533   | 5                     | 14.18 | 1353260 | 20.0 |