

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061416\  
 Data File : BF088013.D  
 Acq On : 14 Jun 2016 22:25  
 Operator : UM/SJ  
 Sample : H3489-03 5X  
 Misc :  
 ALS Vial : 14 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 S7-B5(0-6)C

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-BF060716.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         | 1.724       | 11            | 12          | 21           | rVB      | 76722          | 162729        | 3.93%           | 1.158%        |
| 2         | 1.850       | 21            | 23          | 79           | rVB      | 1931498        | 4145904       | 100.00%         | 29.500%       |
| 3         | 4.250       | 230           | 233         | 237          | rBV      | 52616          | 63539         | 1.53%           | 0.452%        |
| 4         | 4.924       | 290           | 292         | 295          | rBV      | 185776         | 178913        | 4.32%           | 1.273%        |
| 5         | 5.359       | 328           | 330         | 333          | rBV      | 372604         | 442137        | 10.66%          | 3.146%        |
| 6         | 6.410       | 420           | 422         | 424          | rBV      | 626583         | 574410        | 13.85%          | 4.087%        |
| 7         | 6.547       | 431           | 434         | 436          | rBV      | 633949         | 610743        | 14.73%          | 4.346%        |
| 8         | 6.776       | 452           | 454         | 457          | rVB      | 557036         | 587906        | 14.18%          | 4.183%        |
| 9         | 6.936       | 466           | 468         | 470          | rVB      | 683156         | 551420        | 13.30%          | 3.924%        |
| 10        | 7.062       | 476           | 479         | 481          | rBV2     | 35157          | 48620         | 1.17%           | 0.346%        |
| 11        | 7.222       | 490           | 493         | 498          | rVV3     | 17584          | 50044         | 1.21%           | 0.356%        |
| 12        | 7.348       | 501           | 504         | 506          | rVV      | 340375         | 411704        | 9.93%           | 2.929%        |
| 13        | 8.068       | 565           | 567         | 570          | rBV      | 955265         | 808220        | 19.49%          | 5.751%        |
| 14        | 9.142       | 659           | 661         | 664          | rBV      | 660203         | 763134        | 18.41%          | 5.430%        |
| 15        | 9.542       | 692           | 696         | 698          | rBV      | 155987         | 150764        | 3.64%           | 1.073%        |
| 16        | 9.828       | 718           | 721         | 723          | rBV      | 713741         | 825030        | 19.90%          | 5.870%        |
| 17        | 10.605      | 787           | 789         | 791          | rBV      | 87000          | 78233         | 1.89%           | 0.557%        |
| 18        | 10.731      | 799           | 800         | 805          | rVB      | 31699          | 51620         | 1.25%           | 0.367%        |
| 19        | 11.302      | 848           | 850         | 854          | rBV      | 759940         | 731006        | 17.63%          | 5.201%        |
| 20        | 12.514      | 954           | 956         | 958          | rBV      | 177512         | 153869        | 3.71%           | 1.095%        |
| 21        | 12.742      | 973           | 976         | 977          | rBV      | 128239         | 141000        | 3.40%           | 1.003%        |
| 22        | 12.891      | 986           | 989         | 991          | rVB      | 603288         | 633528        | 15.28%          | 4.508%        |
| 23        | 13.794      | 1066          | 1068        | 1071         | rBV3     | 29342          | 47619         | 1.15%           | 0.339%        |
| 24        | 13.931      | 1078          | 1080        | 1082         | rBV      | 545702         | 814181        | 19.64%          | 5.793%        |
| 25        | 14.708      | 1146          | 1148        | 1153         | rVB      | 54481          | 109155        | 2.63%           | 0.777%        |
| 26        | 14.880      | 1161          | 1163        | 1165         | rBV      | 48526          | 73083         | 1.76%           | 0.520%        |
| 27        | 14.948      | 1167          | 1169        | 1173         | rVB2     | 90103          | 200875        | 4.85%           | 1.429%        |
| 28        | 15.348      | 1201          | 1204        | 1209         | rVB      | 481244         | 644490        | 15.55%          | 4.586%        |

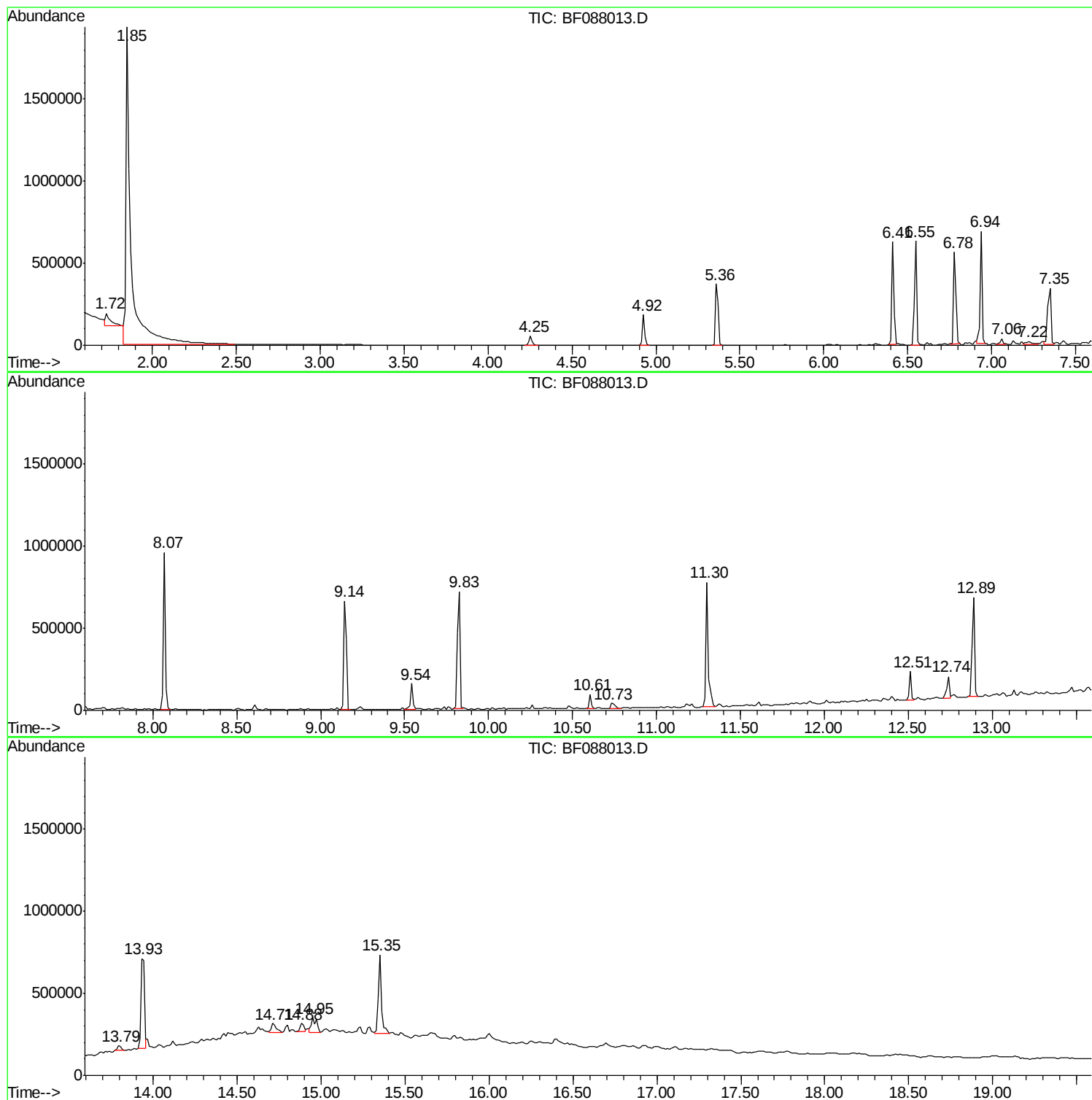
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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF060716.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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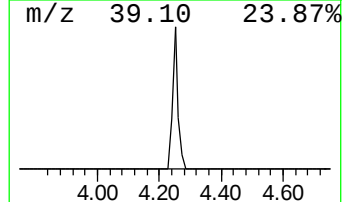
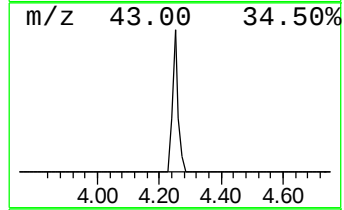
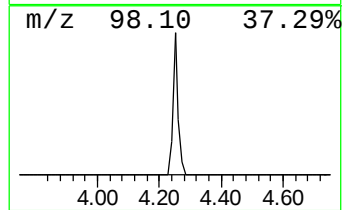
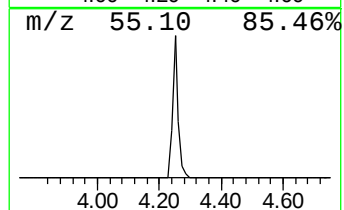
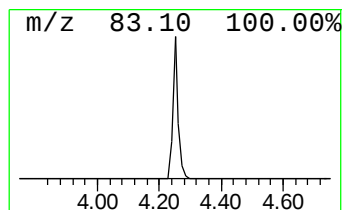
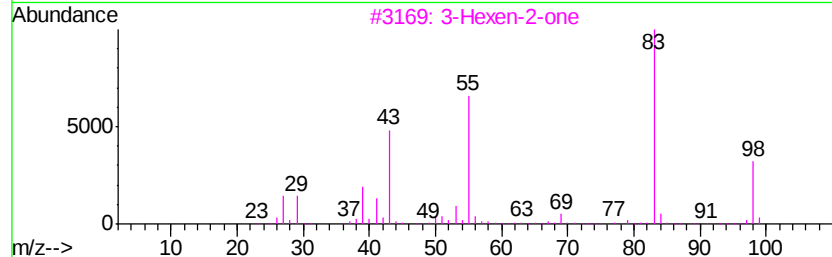
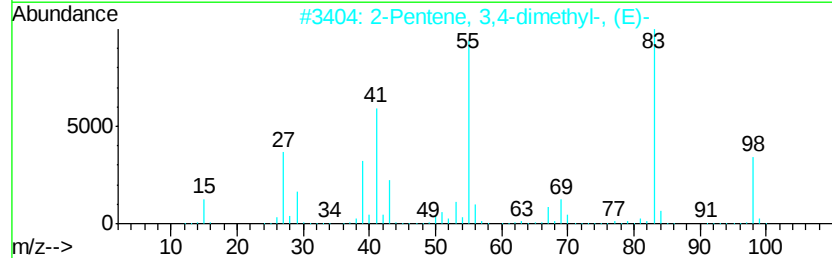
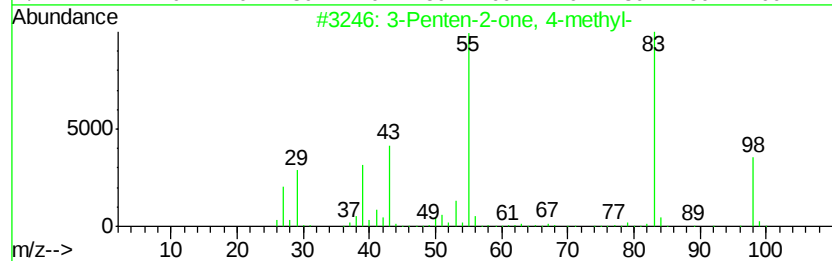
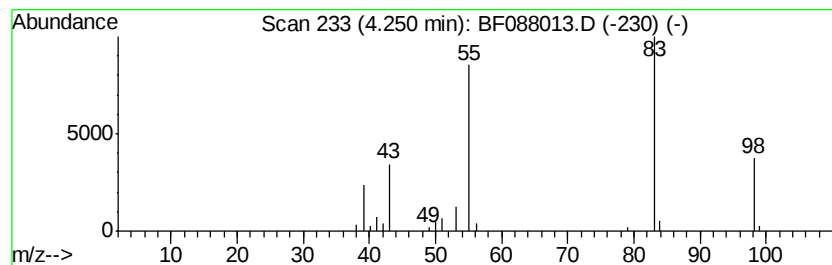
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 8

| R.T. | EstConc | Area  | Relative to ISTD       | R.T. |
|------|---------|-------|------------------------|------|
| 4.25 | 2.16 ng | 63539 | 1,4-Dichlorobenzene-d4 | 6.78 |

| Hit# | of | Tentative ID                   | MW | MolForm | CAS#        | Qual |
|------|----|--------------------------------|----|---------|-------------|------|
| 1    | 5  | 3-Penten-2-one, 4-methyl-      | 98 | C6H10O  | 000141-79-7 | 91   |
| 2    |    | 2-Pentene, 3,4-dimethyl-, (E)- | 98 | C7H14   | 004914-92-5 | 90   |
| 3    |    | 3-Hexen-2-one                  | 98 | C6H10O  | 000763-93-9 | 90   |
| 4    |    | 2-Pentene, 3,4-dimethyl-, (Z)- | 98 | C7H14   | 004914-91-4 | 86   |
| 5    |    | 2-Pentene, 4,4-dimethyl-, (Z)- | 98 | C7H14   | 000762-63-0 | 80   |



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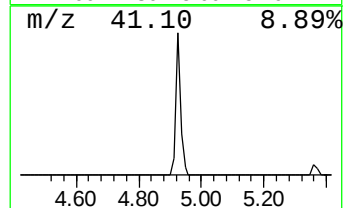
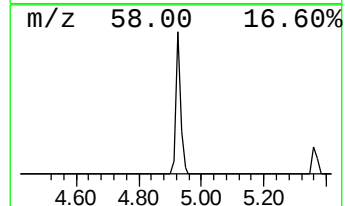
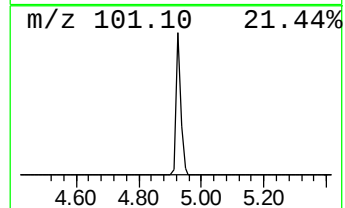
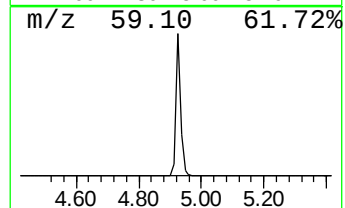
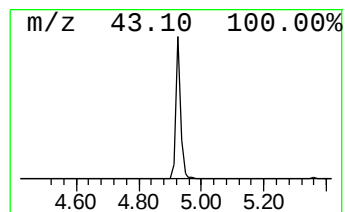
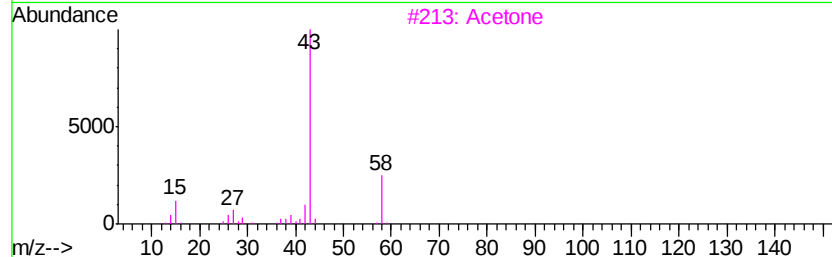
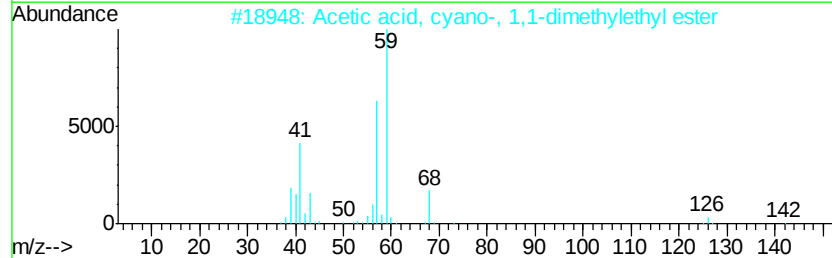
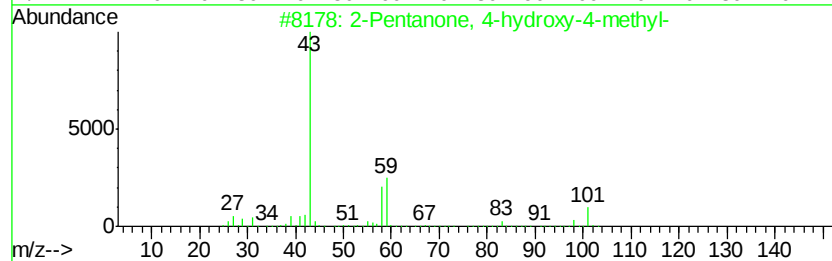
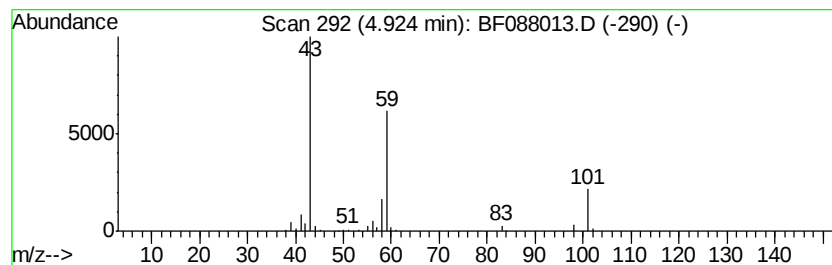
TIC Library : C:\Database\NIST11.L  
TIC Integration Parameters: LSCINT.P

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

| R.T. | EstConc | Area   | Relative to ISTD       | R.T. |
|------|---------|--------|------------------------|------|
| 4.92 | 6.09 ng | 178913 | 1,4-Dichlorobenzene-d4 | 6.78 |

| Hit# | of | Tentative ID                         | MW  | MolForm  | CAS#        | Qual |
|------|----|--------------------------------------|-----|----------|-------------|------|
| 1    | 5  | 2-Pentanone, 4-hydroxy-4-methyl-     | 116 | C6H12O2  | 000123-42-2 | 64   |
| 2    |    | Acetic acid, cyano-, 1,1-dimethyl... | 141 | C7H11NO2 | 001116-98-9 | 17   |
| 3    |    | Acetone                              | 58  | C3H6O    | 000067-64-1 | 9    |
| 4    |    | 2,3-Butanedione, monooxime           | 101 | C4H7NO2  | 000057-71-6 | 9    |
| 5    |    | Morpholine, 4-methyl-                | 101 | C5H11NO  | 000109-02-4 | 9    |



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ClientSampleId :  
S7-B5(0-6)C

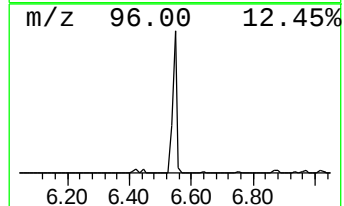
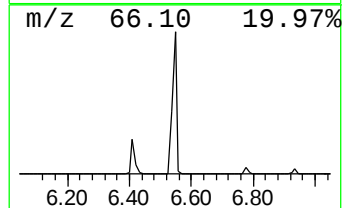
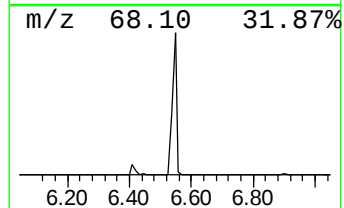
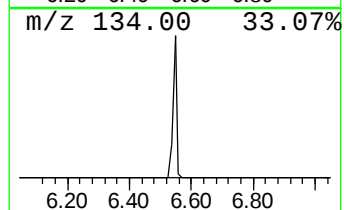
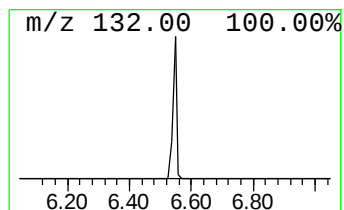
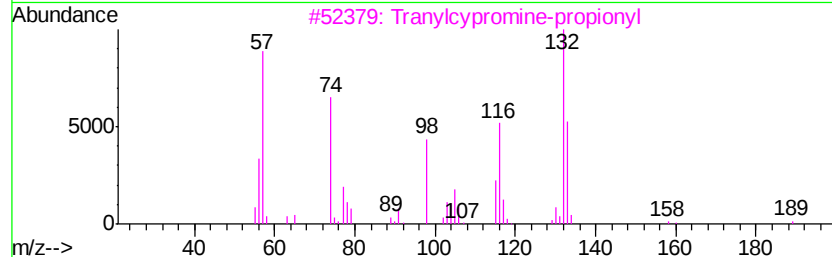
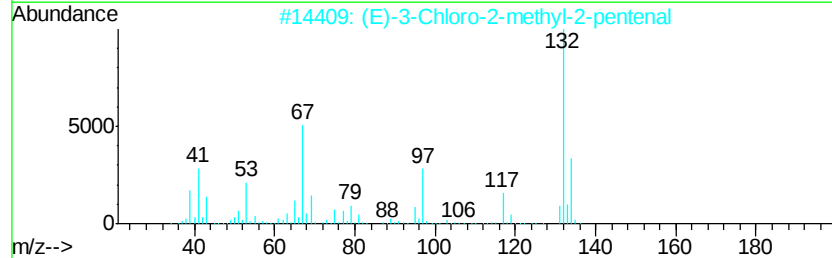
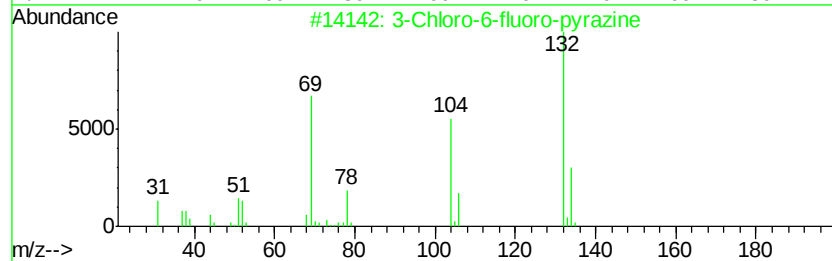
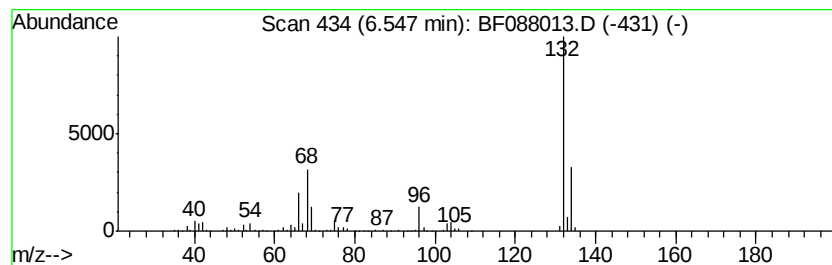
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 5 unknown6.55 Concentration Rank 2

| R.T. | EstConc  | Area   | Relative to ISTD       | R.T. |
|------|----------|--------|------------------------|------|
| 6.55 | 20.78 ng | 610743 | 1,4-Dichlorobenzene-d4 | 6.78 |

| 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  | 17   |
| 3    |    | Tranvlcypropine-propionyl        | 189 | C12H15NO  | 1000123-86-3 | 12   |
| 4    |    | 4-Chloro-6-fluoro-pyrimidine     | 132 | C4H2ClFN2 | 051422-01-6  | 9    |
| 5    |    | 4-Chloro-2-fluoro-pyrimidine     | 132 | C4H2ClFN2 | 051422-00-5  | 9    |



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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF060716.M  
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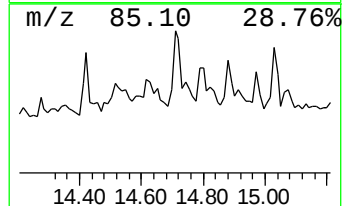
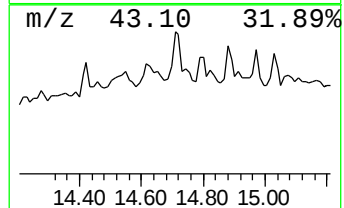
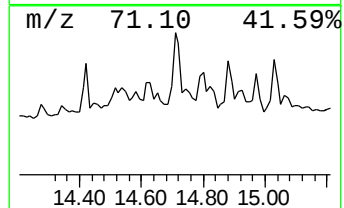
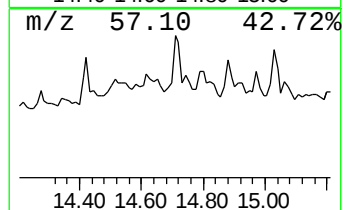
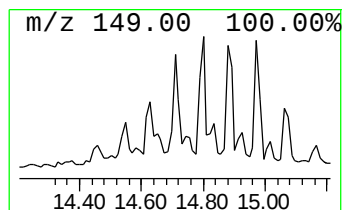
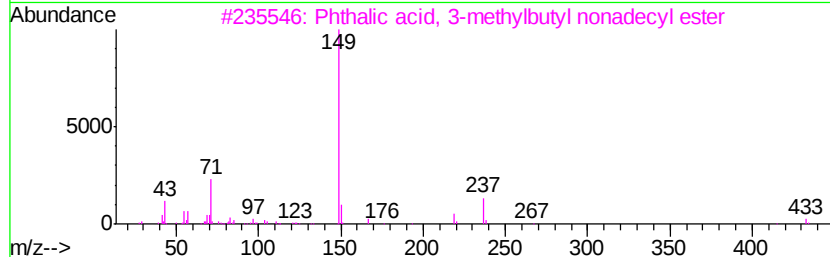
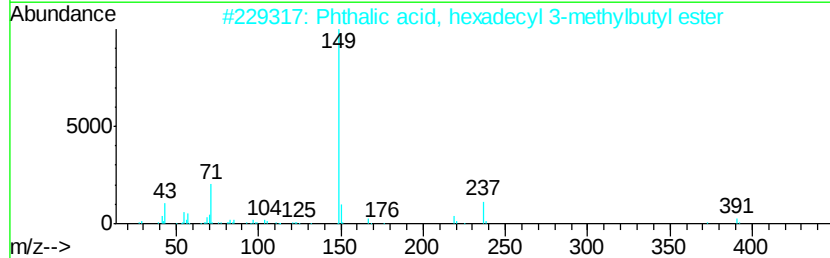
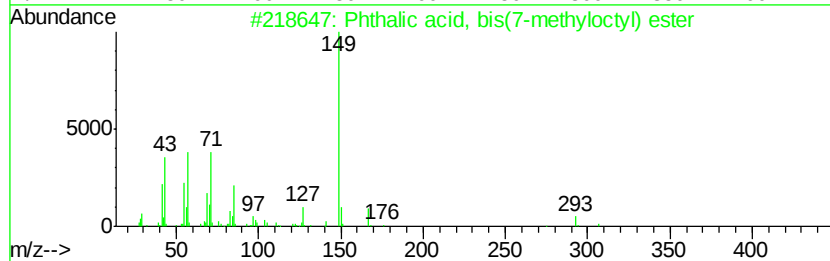
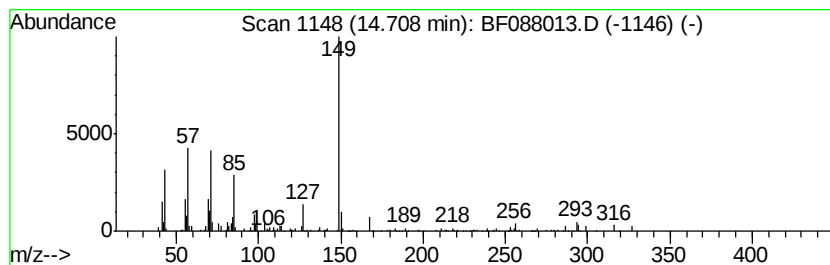
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\*\*\*\*\*  
Peak Number 7 Phthalic acid, bis(7-methyl... Concentration Rank 6

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|-------|---------|--------|------------------|-------|
| 14.71 | 3.39 ng | 109155 | Perylene-d12     | 15.35 |

| Hit# | of | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|------|----|-------------------------------------|-----|----------|--------------|------|
| 1    | 5  | Phthalic acid, bis(7-methyloctyl... | 418 | C26H42O4 | 020548-62-3  | 83   |
| 2    |    | Phthalic acid, hexadecyl 3-methy... | 460 | C29H48O4 | 1000356-81-7 | 59   |
| 3    |    | Phthalic acid, 3-methylbutyl non... | 502 | C32H54O4 | 1000356-82-0 | 59   |
| 4    |    | Phthalic acid, octyl tridec-2-yn... | 456 | C29H44O4 | 1000315-44-1 | 59   |
| 5    |    | 2,4,7-Trioxabicyclo[4.4.0]dec-9-... | 374 | C23H34O4 | 1000161-14-6 | 47   |



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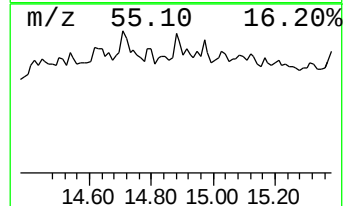
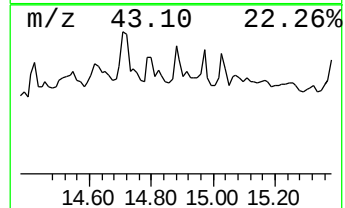
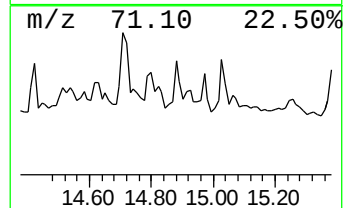
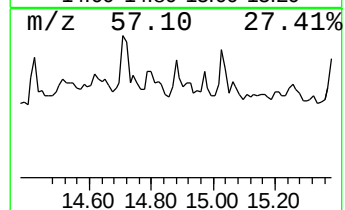
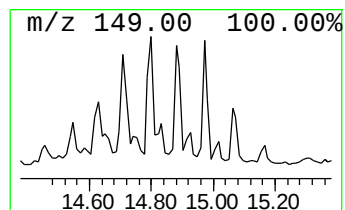
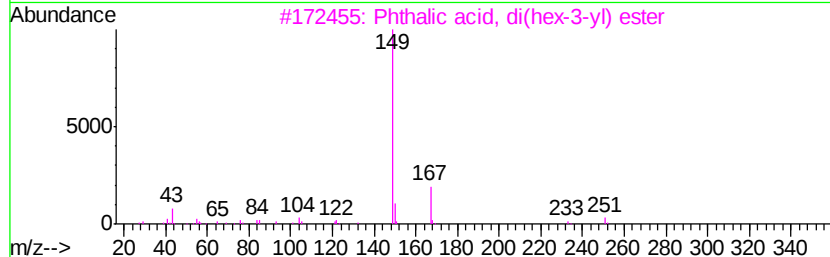
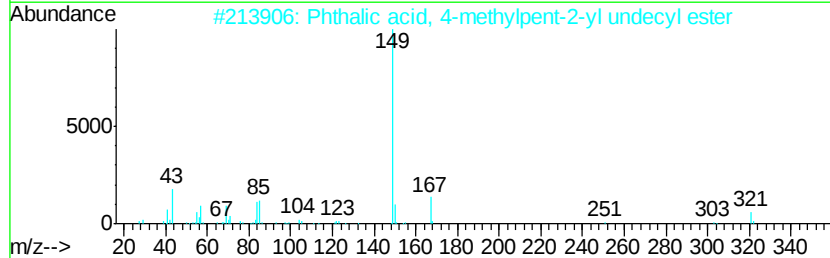
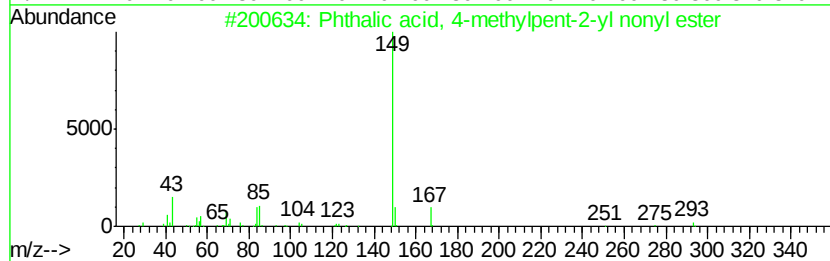
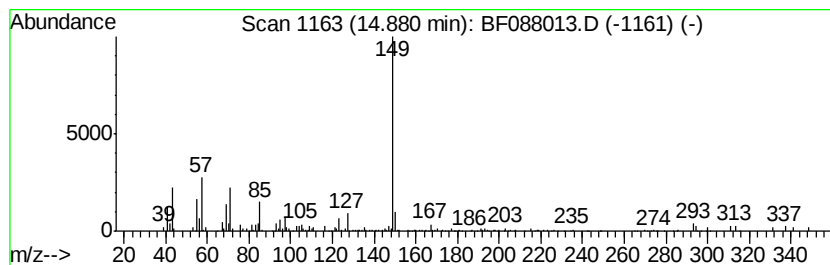
TIC Library : C:\Database\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 8 Phthalic acid, 4-methylpent... Concentration Rank 7

| R.T.  | EstConc | Area  | Relative to ISTD | R.T.  |
|-------|---------|-------|------------------|-------|
| 14.88 | 2.27 ng | 73083 | Perylene-d12     | 15.35 |

| Hit# | of | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|------|----|-------------------------------------|-----|----------|--------------|------|
| 1    | 5  | Phthalic acid, 4-methylpent-2-yl... | 376 | C23H36O4 | 1000356-87-9 | 59   |
| 2    |    | Phthalic acid, 4-methylpent-2-yl... | 404 | C25H40O4 | 1000356-88-1 | 53   |
| 3    |    | Phthalic acid, di(hex-3-yl) ester   | 334 | C20H30O4 | 1000356-96-7 | 50   |
| 4    |    | 1,2-Benzenedicarboxylic acid, bi... | 334 | C20H30O4 | 000146-50-9  | 50   |
| 5    |    | Phthalic acid, hex-3-yl isohexyl... | 334 | C20H30O4 | 1000356-95-6 | 50   |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF061416\  
Data File : BF088013.D  
Acq On : 14 Jun 2016 22:25  
Operator : UM/SJ  
Sample : H3489-03 5X  
Misc :  
ALS Vial : 14 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
S7-B5(0-6)C

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF060716.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 |
| 3-Penten-2-one, 4... | 4.25  | 2.2     | ng    | 63539    | 1                     | 6.78  | 587906 | 20.0 |
| 2-Pentanone, 4-hy... | 4.92  | 6.1     | ng    | 178913   | 1                     | 6.78  | 587906 | 20.0 |
| unknown6.55          | 6.55  | 20.8    | ng    | 610743   | 1                     | 6.78  | 587906 | 20.0 |
| Phthalic acid, bi... | 14.71 | 3.4     | ng    | 109155   | 6                     | 15.35 | 644490 | 20.0 |
| Phthalic acid, 4-... | 14.88 | 2.3     | ng    | 73083    | 6                     | 15.35 | 644490 | 20.0 |