

Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF080817\  
 Data File : BF097495.D  
 Acq On : 9 Aug 2017 3:43  
 Operator : SJ/JU  
 Sample : I4604-01  
 Misc :  
 ALS Vial : 21 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 MW-3A-080217

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-BF072517.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         | 2.316       | 87            | 90          | 96           | rVB4     | 13505          | 23875         | 1.00%           | 0.136%        |
| 2         | 4.528       | 463           | 466         | 474          | rBV      | 55938          | 98617         | 4.14%           | 0.563%        |
| 3         | 5.004       | 543           | 547         | 568          | rBV      | 962262         | 1458770       | 61.19%          | 8.332%        |
| 4         | 5.146       | 568           | 571         | 578          | rVB      | 20710          | 29430         | 1.23%           | 0.168%        |
| 5         | 5.645       | 653           | 656         | 665          | rBV      | 22597          | 31836         | 1.34%           | 0.182%        |
| 6         | 6.081       | 727           | 730         | 743          | rVB      | 607756         | 796672        | 33.42%          | 4.550%        |
| 7         | 6.181       | 743           | 747         | 756          | rVB      | 2257891        | 2252556       | 94.49%          | 12.866%       |
| 8         | 6.404       | 782           | 785         | 794          | rBV      | 619271         | 584260        | 24.51%          | 3.337%        |
| 9         | 6.563       | 808           | 812         | 819          | rBV      | 2107248        | 2062519       | 86.52%          | 11.781%       |
| 10        | 6.981       | 879           | 883         | 888          | rBV      | 1755870        | 1686311       | 70.74%          | 9.632%        |
| 11        | 7.687       | 1000          | 1003        | 1010         | rBV      | 645567         | 617027        | 25.88%          | 3.524%        |
| 12        | 8.098       | 1069          | 1073        | 1077         | rBV2     | 39724          | 66040         | 2.77%           | 0.377%        |
| 13        | 8.769       | 1182          | 1187        | 1190         | rBV      | 2504938        | 2383898       | 100.00%         | 13.616%       |
| 14        | 9.169       | 1252          | 1255        | 1264         | rVB      | 117993         | 105715        | 4.43%           | 0.604%        |
| 15        | 9.433       | 1296          | 1300        | 1307         | rBV      | 633515         | 572781        | 24.03%          | 3.272%        |
| 16        | 10.222      | 1430          | 1434        | 1454         | rVB      | 1118952        | 1093069       | 45.85%          | 6.243%        |
| 17        | 10.804      | 1529          | 1533        | 1540         | rBV3     | 17201          | 24649         | 1.03%           | 0.141%        |
| 18        | 10.904      | 1547          | 1550        | 1556         | rBV      | 538962         | 503629        | 21.13%          | 2.877%        |
| 19        | 11.469      | 1643          | 1646        | 1647         | rBV      | 30227          | 26650         | 1.12%           | 0.152%        |
| 20        | 12.245      | 1774          | 1778        | 1780         | rBV2     | 25199          | 29344         | 1.23%           | 0.168%        |
| 21        | 12.333      | 1790          | 1793        | 1800         | rVB      | 55966          | 51506         | 2.16%           | 0.294%        |
| 22        | 12.492      | 1815          | 1820        | 1823         | rBV      | 1860878        | 1843691       | 77.34%          | 10.531%       |
| 23        | 13.033      | 1909          | 1912        | 1916         | rBV      | 38913          | 38529         | 1.62%           | 0.220%        |
| 24        | 13.439      | 1975          | 1981        | 1988         | rVB6     | 29197          | 64036         | 2.69%           | 0.366%        |
| 25        | 13.533      | 1993          | 1997        | 2002         | rBV      | 487276         | 462044        | 19.38%          | 2.639%        |
| 26        | 13.951      | 2065          | 2068        | 2070         | rBV4     | 23779          | 35883         | 1.51%           | 0.205%        |
| 27        | 14.874      | 2221          | 2225        | 2229         | rBV      | 303128         | 359829        | 15.09%          | 2.055%        |
| 28        | 15.645      | 2353          | 2356        | 2359         | rVB4     | 29019          | 37674         | 1.58%           | 0.215%        |
| 29        | 16.257      | 2457          | 2460        | 2462         | rBV4     | 24340          | 31527         | 1.32%           | 0.180%        |
| 30        | 16.715      | 2535          | 2538        | 2540         | rBV4     | 21328          | 28769         | 1.21%           | 0.164%        |
| 31        | 17.168      | 2612          | 2615        | 2616         | rBV2     | 22174          | 27059         | 1.14%           | 0.155%        |
| 32        | 17.256      | 2628          | 2630        | 2636         | rVB6     | 22665          | 42187         | 1.77%           | 0.241%        |
| 33        | 17.404      | 2651          | 2655        | 2656         | rBV3     | 25603          | 37169         | 1.56%           | 0.212%        |

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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-BF072517.M  
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

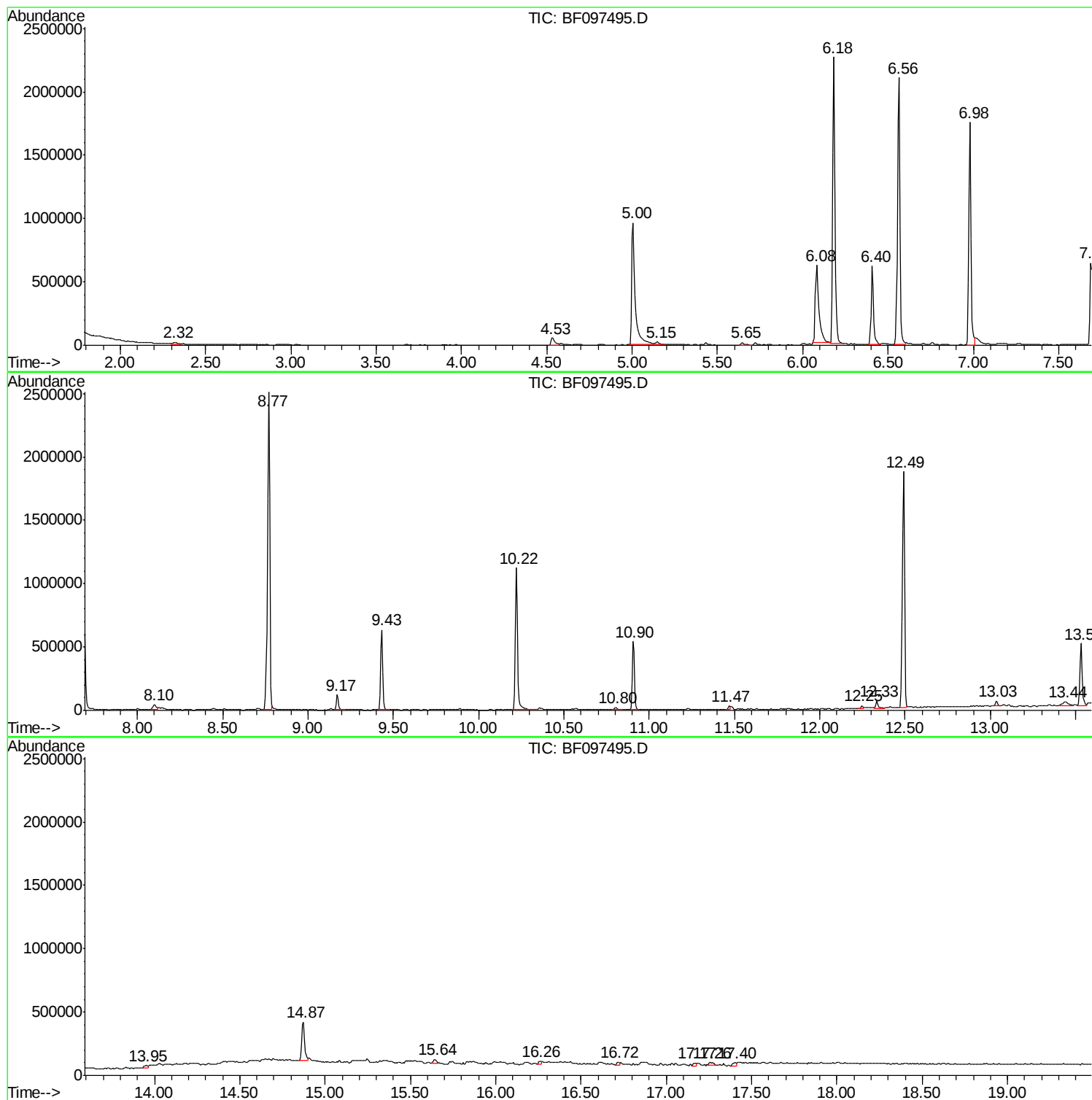
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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF072517.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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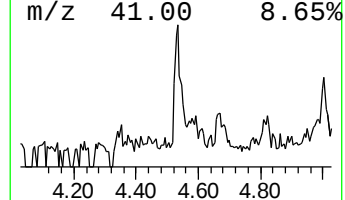
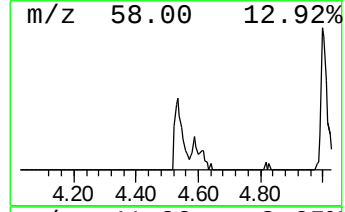
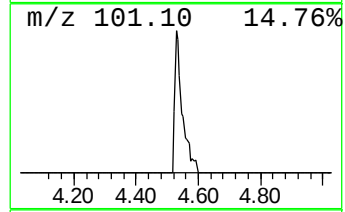
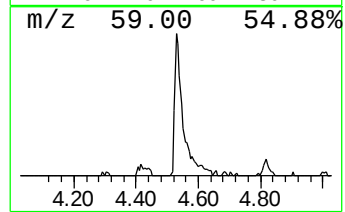
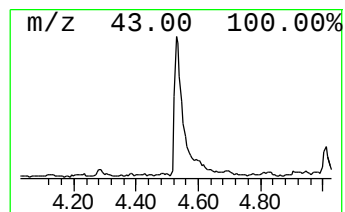
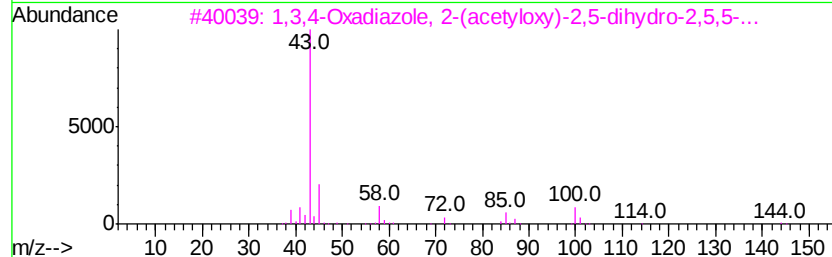
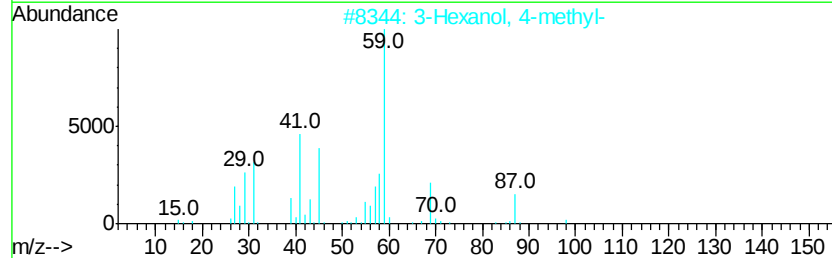
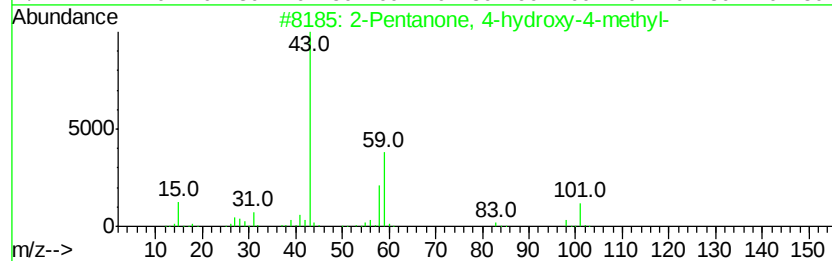
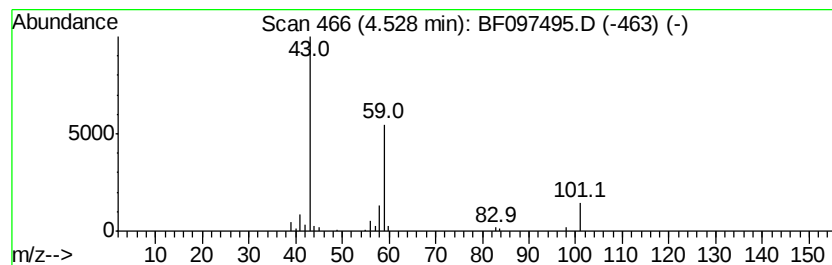
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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 3

| R.T. | EstConc | Area  | Relative to ISTD       | R.T. |
|------|---------|-------|------------------------|------|
| 4.53 | 3.38 ng | 98617 | 1,4-Dichlorobenzene-d4 | 6.40 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm   | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|-----------|-------------|------|
| 1    |    |   | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2   | 000123-42-2 | 64   |
| 2    |    |   | 3-Hexanol, 4-methyl-                | 116 | C7H16O    | 000615-29-2 | 28   |
| 3    |    |   | 1,3,4-Oxadiazole, 2-(acetyloxy)-... | 172 | C7H12N2O3 | 066398-57-0 | 10   |
| 4    |    |   | 2,3-Butanedione, monooxime          | 101 | C4H7NO2   | 000057-71-6 | 9    |
| 5    |    |   | Diacetamide                         | 101 | C4H7NO2   | 000625-77-4 | 9    |



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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF072517.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

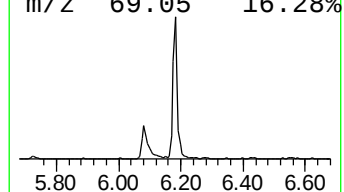
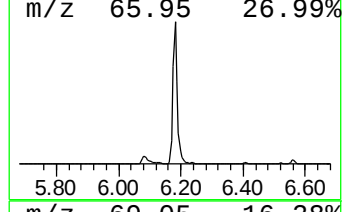
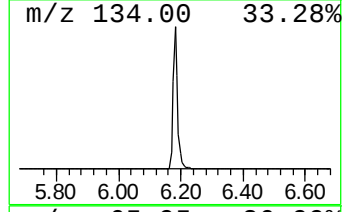
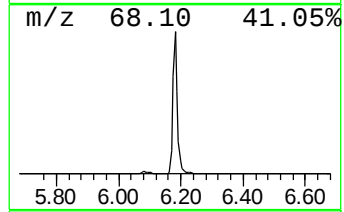
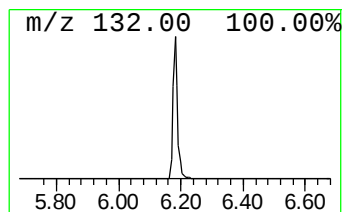
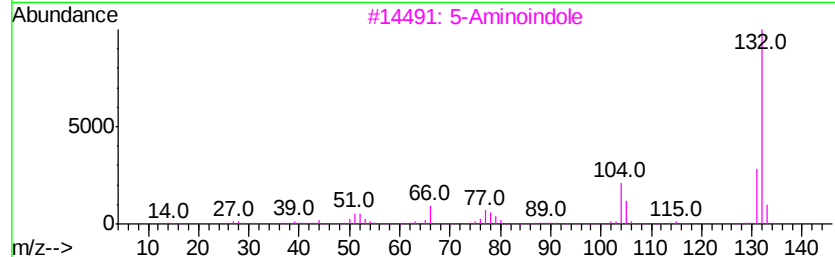
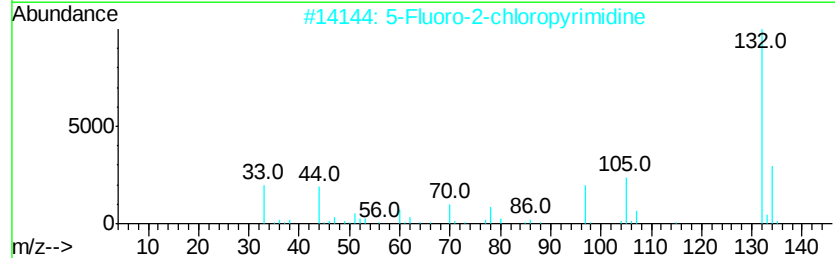
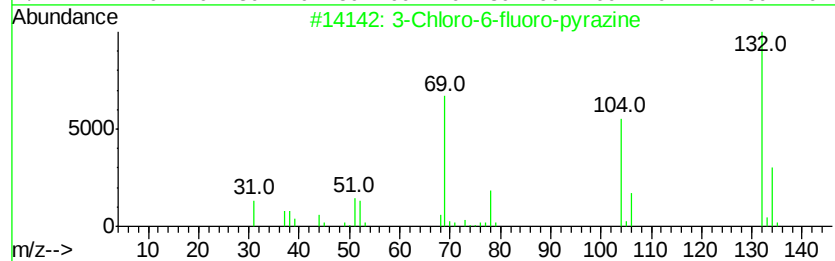
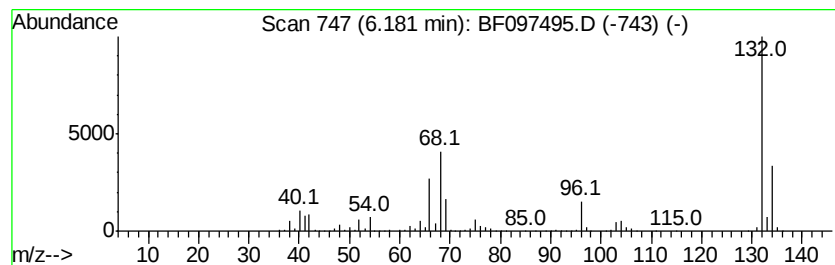
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 unknown6.18 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.18 | 77.11 ng | 2252560 | 1,4-Dichlorobenzene-d4 | 6.40 |

| Hit# | of | Tentative ID                | MW  | MolForm   | CAS#         | Qual |
|------|----|-----------------------------|-----|-----------|--------------|------|
| 1    | 5  | 3-Chloro-6-fluoro-pyrazine  | 132 | C4H2ClFN2 | 1000146-10-7 | 27   |
| 2    |    | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0  | 16   |
| 3    |    | 5-Aminoindole               | 132 | C8H8N2    | 005192-03-0  | 12   |
| 4    |    | Tranylcypromine-propionyl   | 189 | C12H15NO  | 1000123-86-3 | 10   |
| 5    |    | 1,3,5-Trifluorobenzene      | 132 | C6H3F3    | 000372-38-3  | 9    |



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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF072517.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

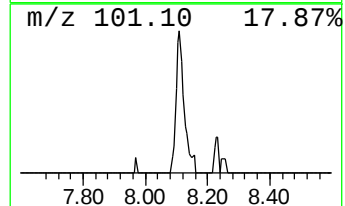
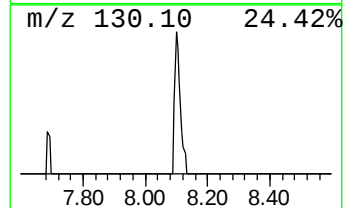
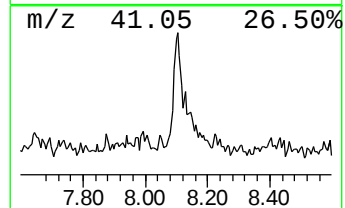
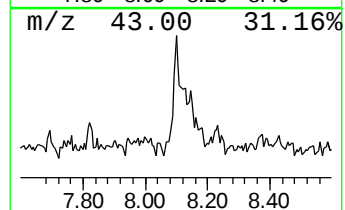
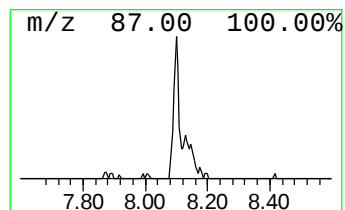
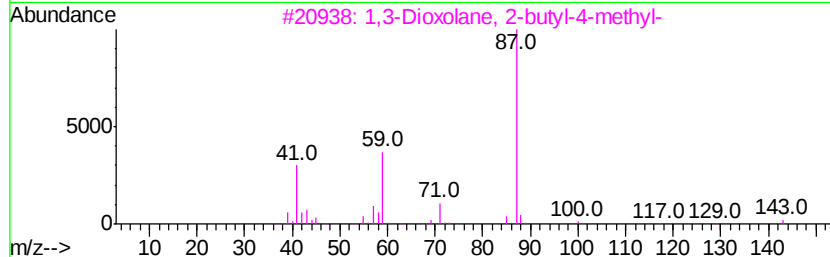
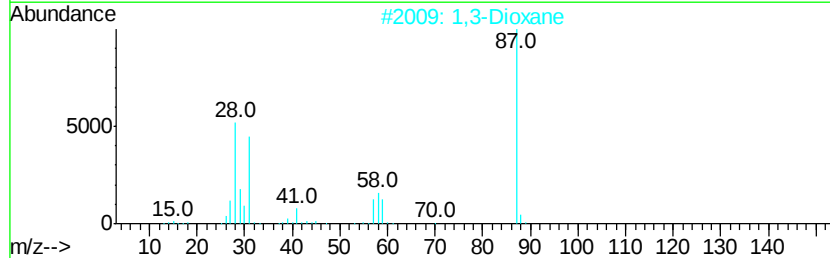
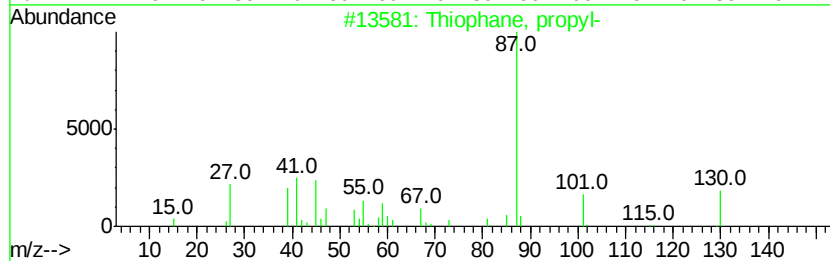
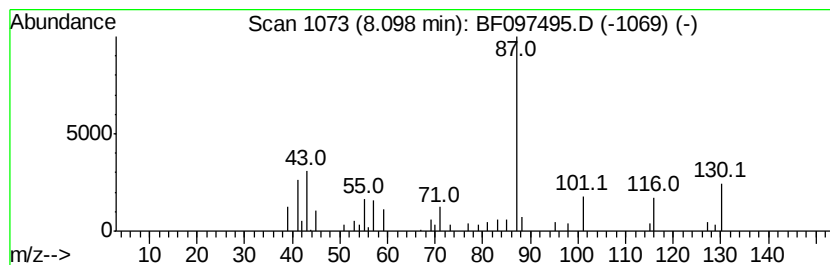
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 Thiophane, propyl- Concentration Rank 7

| R.T. | EstConc | Area  | Relative to ISTD | R.T. |
|------|---------|-------|------------------|------|
| 8.10 | 2.14 ng | 66040 | Naphthalene-d8   | 7.69 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|----------|--------------|------|
| 1    |    |   | Thiophane, propyl-                  | 130 | C7H14S   | 001551-34-4  | 72   |
| 2    |    |   | 1,3-Dioxane                         | 88  | C4H8O2   | 000505-22-6  | 38   |
| 3    |    |   | 1,3-Dioxolane, 2-butyl-4-methyl-    | 144 | C8H16O2  | 074094-60-3  | 37   |
| 4    |    |   | Diazene, butyl[1-(2,2-dimethylhy... | 172 | C8H20N4  | 061940-95-2  | 33   |
| 5    |    |   | 1,3-Dioxolane, 2-(3,4-dihydroxy-... | 214 | C11H18O4 | 1000162-73-6 | 28   |



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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF072517.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

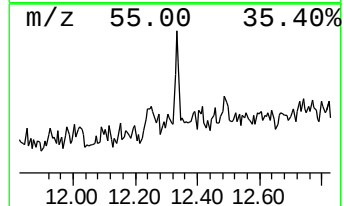
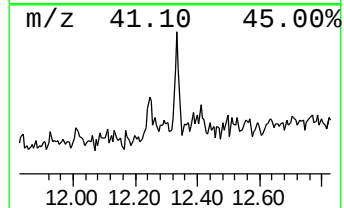
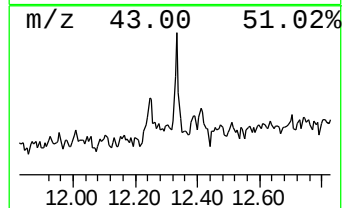
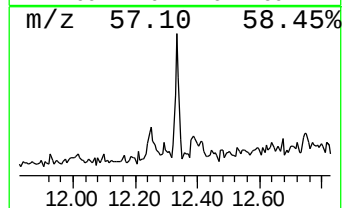
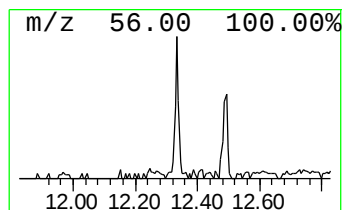
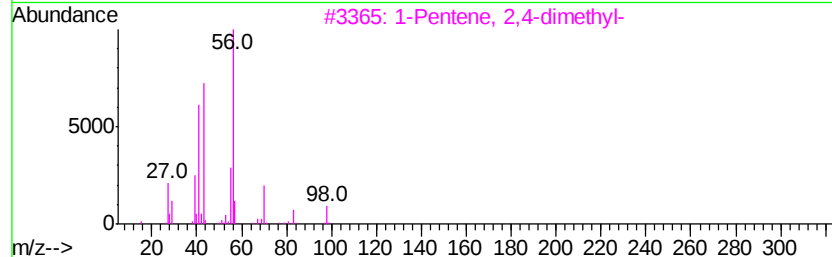
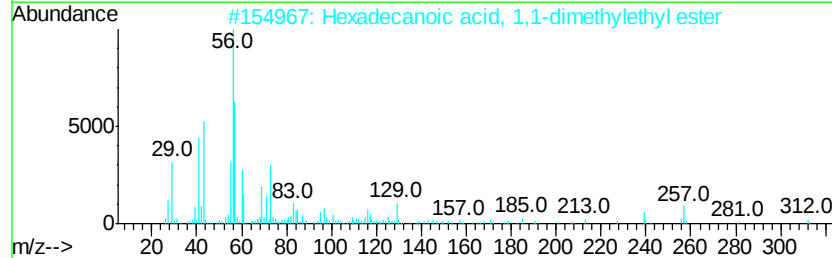
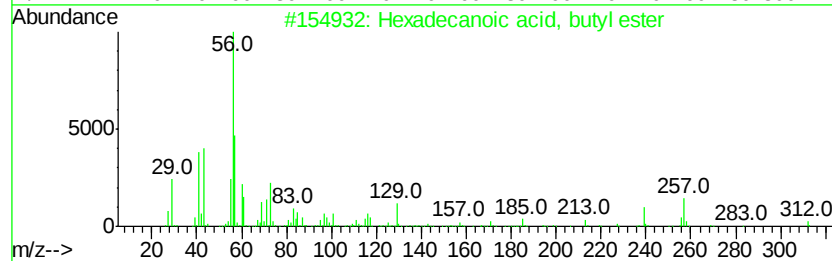
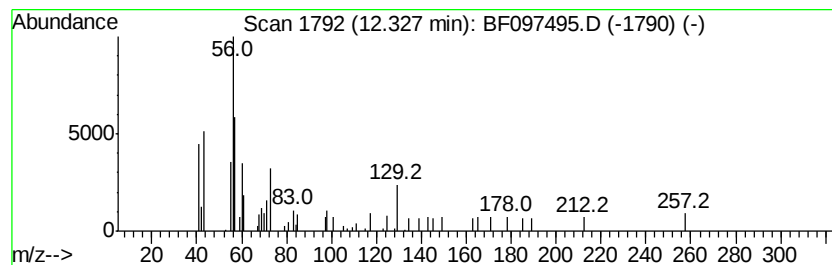
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 6

| R.T.  | EstConc | Area  | Relative to ISTD | R.T.  |
|-------|---------|-------|------------------|-------|
| 12.33 | 2.23 ng | 51506 | Chrysene-d12     | 13.53 |

| Hit# | of | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|-------------------------------------|-----|----------|-------------|------|
| 1    | 5  | Hexadecanoic acid, butyl ester      | 312 | C20H40O2 | 000111-06-8 | 83   |
| 2    |    | Hexadecanoic acid, 1,1-dimethyle... | 312 | C20H40O2 | 031158-91-5 | 83   |
| 3    |    | 1-Pentene, 2,4-dimethyl-            | 98  | C7H14    | 002213-32-3 | 35   |
| 4    |    | 4-Ethyl-4-methyl-5-methylene-1,...  | 142 | C7H10O3  | 080956-52-1 | 35   |
| 5    |    | Cyclobutane, 1,1-dimethyl-2-octyl-  | 196 | C14H28   | 062338-30-1 | 35   |



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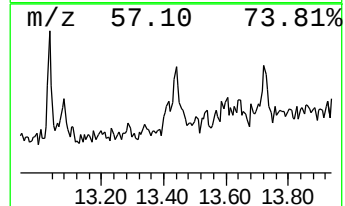
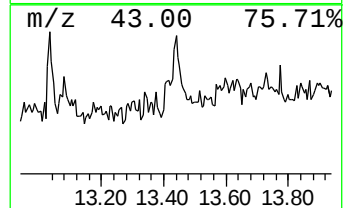
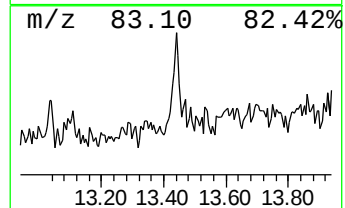
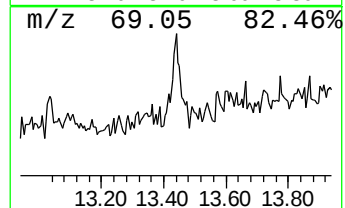
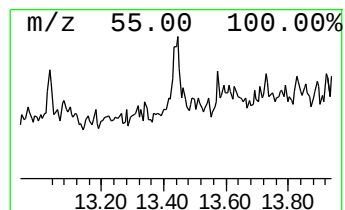
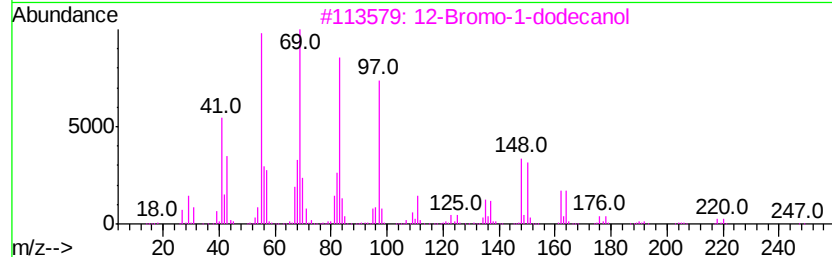
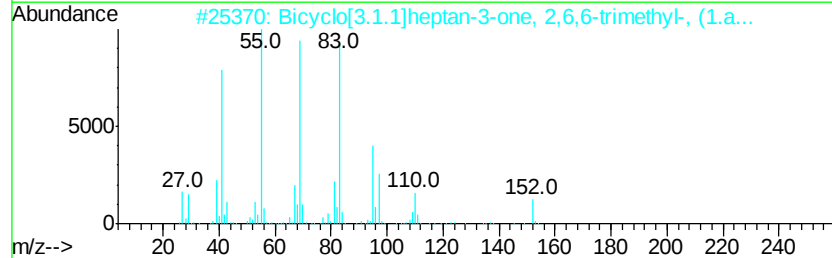
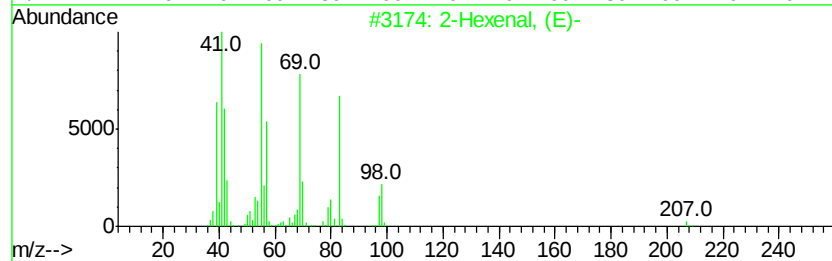
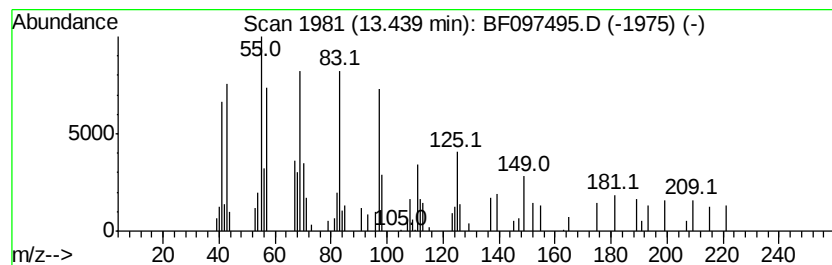
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 6 unknown13.44 Concentration Rank 4

| R.T.  | EstConc | Area  | Relative to ISTD |  | R.T.  |
|-------|---------|-------|------------------|--|-------|
| 13.44 | 2.77 ng | 64036 | Chrysene-d12     |  | 13.53 |

| Hit# | of                                  | 5 | Tentative ID | MW  | MolForm   | CAS#        | Qual |
|------|-------------------------------------|---|--------------|-----|-----------|-------------|------|
| 1    | 2-Hexenal, (E)-                     |   |              | 98  | C6H10O    | 006728-26-3 | 49   |
| 2    | Bicyclo[3.1.1]heptan-3-one, 2,6,... |   |              | 152 | C10H16O   | 000547-60-4 | 49   |
| 3    | 12-Bromo-1-dodecanol                |   |              | 264 | C12H25BrO | 003344-77-2 | 47   |
| 4    | Bicyclo[3.1.1]heptan-3-one, 2,6,... |   |              | 152 | C10H16O   | 015358-88-0 | 45   |
| 5    | 3-Hexene, 2,3-dimethyl-             |   |              | 112 | C8H16     | 007145-23-5 | 43   |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF080817\  
Data File : BF097495.D  
Acq On : 9 Aug 2017 3:43  
Operator : SJ/JU  
Sample : I4604-01  
Misc :  
ALS Vial : 21 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
MW-3A-080217

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF072517.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

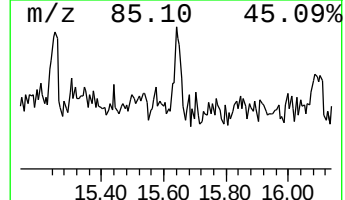
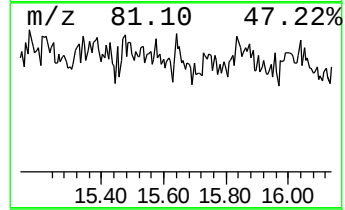
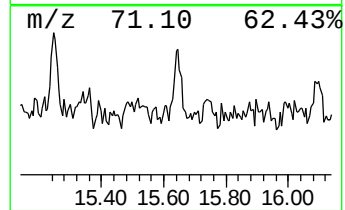
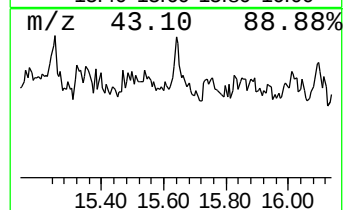
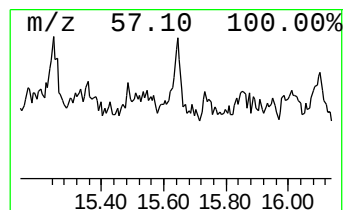
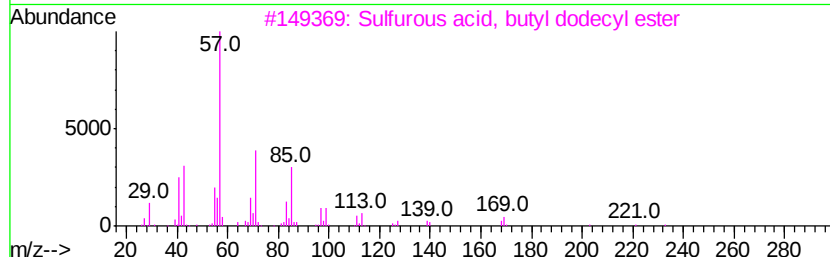
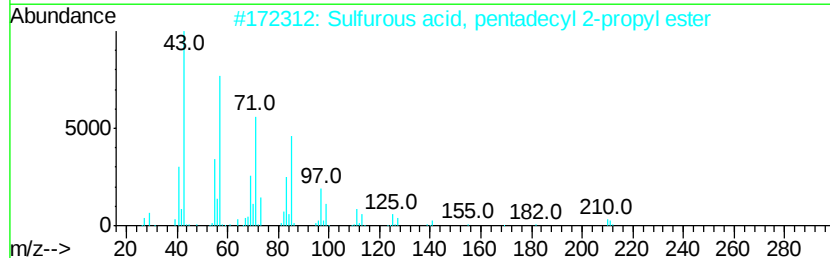
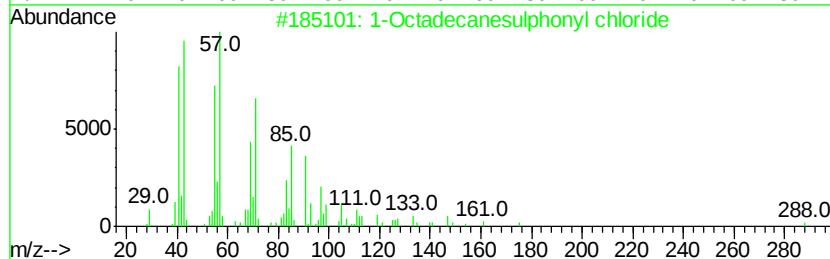
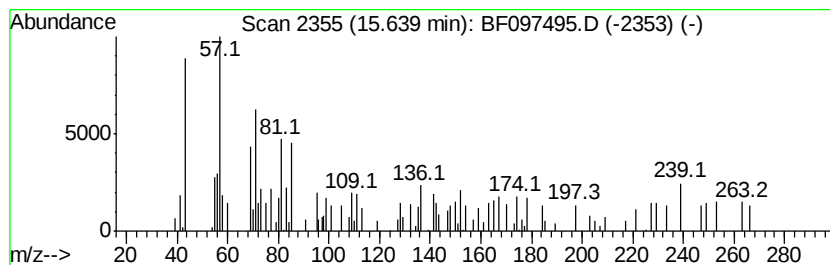
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 7 unknown15.64 Concentration Rank 8

| R.T.  | EstConc | Area  | Relative to ISTD | R.T.  |
|-------|---------|-------|------------------|-------|
| 15.64 | 2.09 ng | 37674 | Perylene-d12     | 14.87 |

| Hit# | of | Tentative ID                         | MW  | MolForm     | CAS#         | Qual |
|------|----|--------------------------------------|-----|-------------|--------------|------|
| 1    | 5  | 1-Octadecanesulphonyl chloride       | 352 | C18H37ClO2S | 1000342-70-4 | 10   |
| 2    |    | Sulfurous acid, pentadecyl 2-pro...  | 334 | C18H38O3S   | 1000309-12-6 | 10   |
| 3    |    | Sulfurous acid, butyl dodecyl ester  | 306 | C16H34O3S   | 1000309-17-9 | 10   |
| 4    |    | Sulfurous acid, 2-propyl tetradec... | 320 | C17H36O3S   | 1000309-12-5 | 10   |
| 5    |    | Sulfurous acid, hexadecyl 2-pent...  | 376 | C21H44O3S   | 1000309-16-5 | 10   |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF080817\  
Data File : BF097495.D  
Acq On : 9 Aug 2017 3:43  
Operator : SJ/JU  
Sample : I4604-01  
Misc :  
ALS Vial : 21 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
MW-3A-080217

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF072517.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

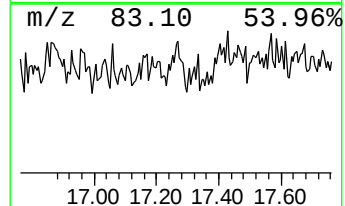
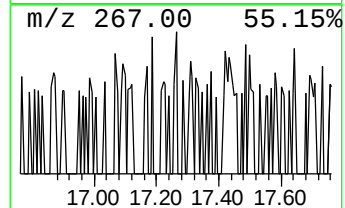
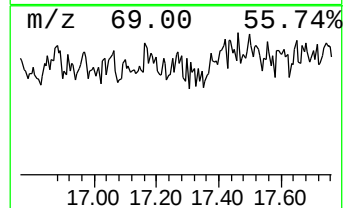
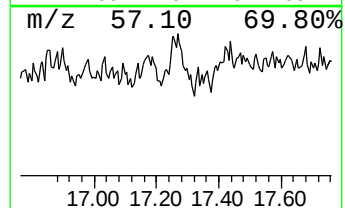
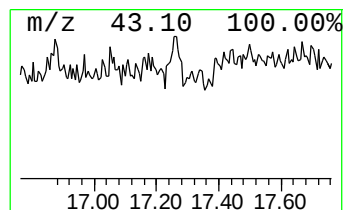
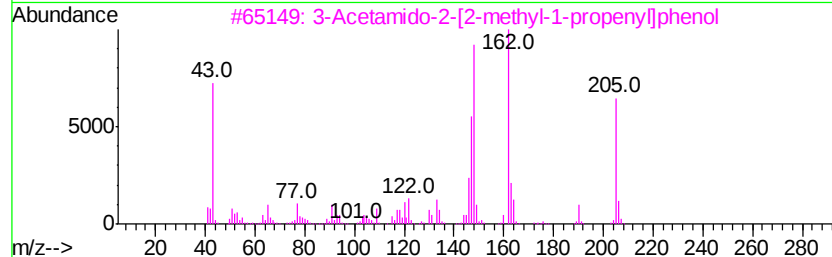
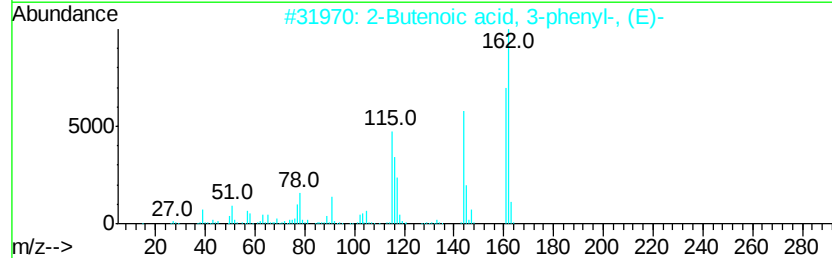
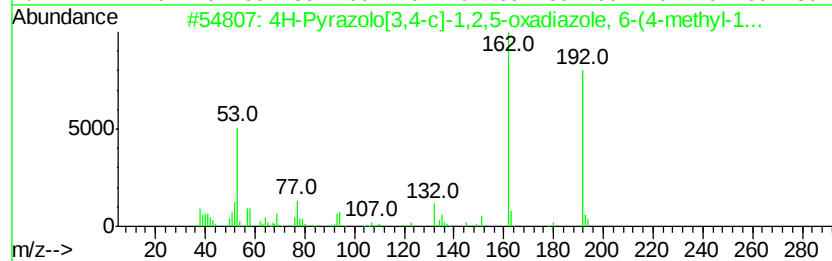
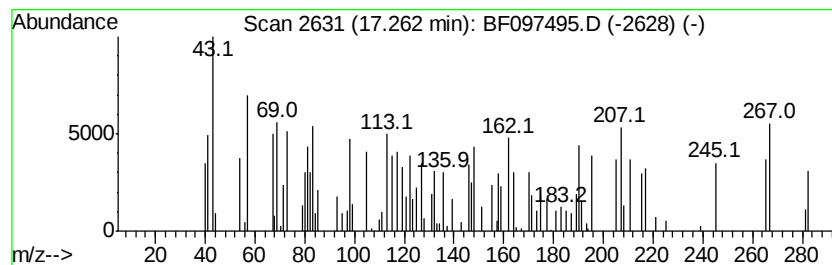
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 8 unknown17.26 Concentration Rank 5

| R.T.  | EstConc | Area  | Relative to ISTD | R.T.  |
|-------|---------|-------|------------------|-------|
| 17.26 | 2.34 ng | 42187 | Perylene-d12     | 14.87 |

| Hit# | of | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|-------------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 4H-Pyrazolo[3,4-c]-1,2,5-oxadiaz... | 192 | C6H4N6O2  | 1000277-10-5 | 9    |
| 2    |    | 2-Butenoic acid, 3-phenyl-, (E)-    | 162 | C10H10O2  | 000704-80-3  | 9    |
| 3    |    | 3-Acetamido-2-[2-methyl-1-propen... | 205 | C12H15NO2 | 031011-04-8  | 9    |
| 4    |    | Cyclopropanecarboxamide, 2-pheny... | 245 | C15H19NO2 | 1000302-84-8 | 9    |
| 5    |    | .beta.-Methylcinnamic acid          | 162 | C10H10O2  | 001199-20-8  | 7    |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF080817\  
Data File : BF097495.D  
Acq On : 9 Aug 2017 3:43  
Operator : SJ/JU  
Sample : I4604-01  
Misc :  
ALS Vial : 21 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
MW-3A-080217

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF072517.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

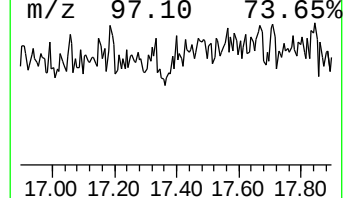
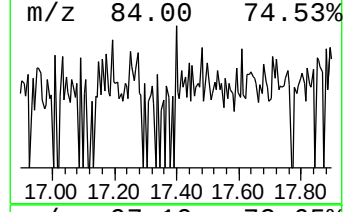
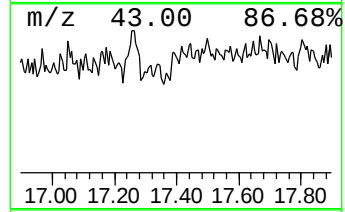
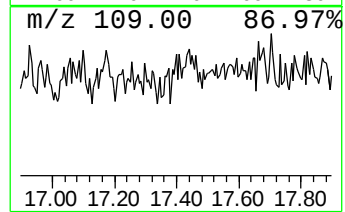
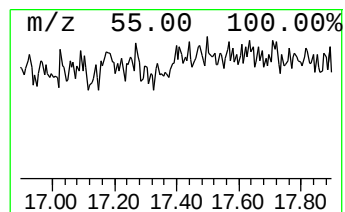
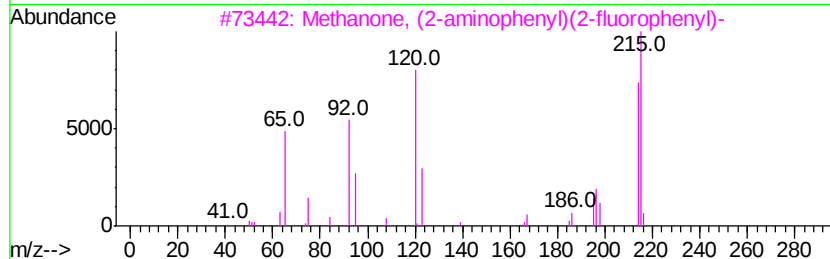
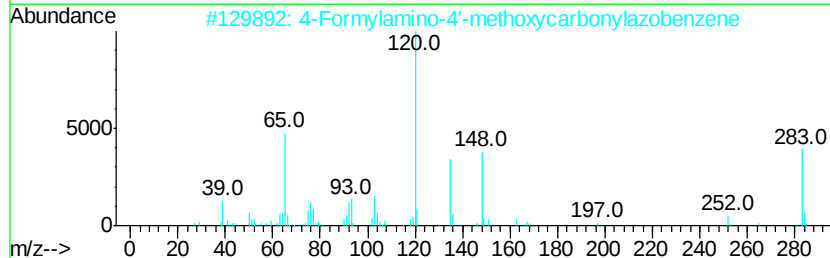
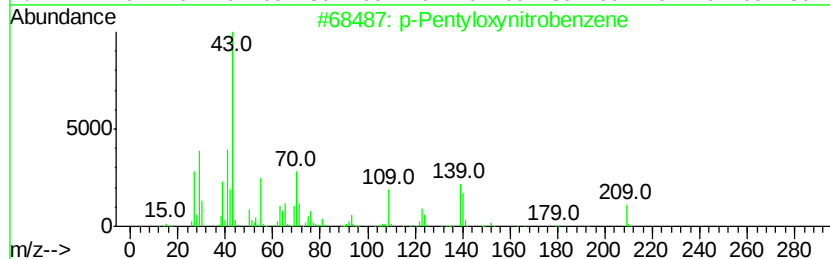
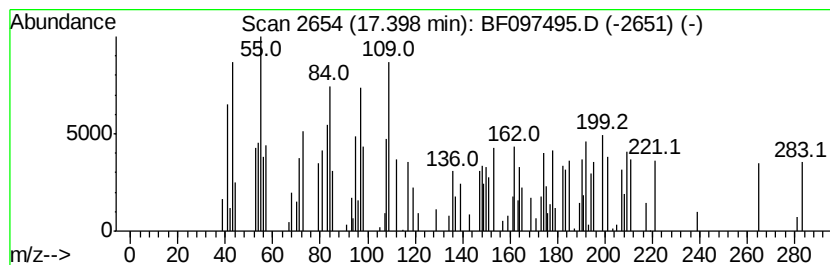
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 9 unknown17.40 Concentration Rank 9

| R.T.  | EstConc | Area  | Relative to ISTD | R.T.  |
|-------|---------|-------|------------------|-------|
| 17.40 | 2.07 ng | 37169 | Perylene-d12     | 14.87 |

| Hit# | of | Tentative ID                        | MW  | MolForm    | CAS#         | Qual |
|------|----|-------------------------------------|-----|------------|--------------|------|
| 1    | 5  | p-Pentyloxynitrobenzene             | 209 | C11H15N03  | 063469-11-4  | 18   |
| 2    |    | 4-Formylamino-4'-methoxycarbonyl... | 283 | C15H13N3O3 | 1000284-37-6 | 14   |
| 3    |    | Methanone, (2-aminophenyl)(2-flu... | 215 | C13H10FN0  | 001581-13-1  | 14   |
| 4    |    | Benzonitrile, 4-(1,2,3,4-tetrahy... | 249 | C15H11N3O  | 1000318-94-2 | 12   |
| 5    |    | Propan-1-one, 1-(4-hydroxyphenyl... | 223 | C10H13N3OS | 043221-09-6  | 12   |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF080817\  
Data File : BF097495.D  
Acq On : 9 Aug 2017 3:43  
Operator : SJ/JU  
Sample : I4604-01  
Misc :  
ALS Vial : 21 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
MW-3A-080217

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF072517.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 |
| 2-Pentanone, 4-hy... | 4.53  | 3.4     | ng    | 98617    | 1                     | 6.40  | 584260 | 20.0 |
| unknown6.18          | 6.18  | 77.1    | ng    | 2252560  | 1                     | 6.40  | 584260 | 20.0 |
| Thiophane, propyl-   | 8.10  | 2.1     | ng    | 66040    | 2                     | 7.69  | 617027 | 20.0 |
| Hexadecanoic acid... | 12.33 | 2.2     | ng    | 51506    | 5                     | 13.53 | 462044 | 20.0 |
| unknown13.44         | 13.44 | 2.8     | ng    | 64036    | 5                     | 13.53 | 462044 | 20.0 |
| unknown15.64         | 15.64 | 2.1     | ng    | 37674    | 6                     | 14.87 | 359829 | 20.0 |
| unknown17.26         | 17.26 | 2.3     | ng    | 42187    | 6                     | 14.87 | 359829 | 20.0 |
| unknown17.40         | 17.40 | 2.1     | ng    | 37169    | 6                     | 14.87 | 359829 | 20.0 |