

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092716\  
 Data File : BF090272.D  
 Acq On : 28 Sep 2016 00:32  
 Operator : UM/SJ  
 Sample : H4949-11  
 Misc :  
 ALS Vial : 25 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 S-6-1-LOC-6(0-5)

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-BF092016.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         | 1.644       | 4             | 5           | 48           | rVB      | 2135304        | 5683335       | 100.00%         | 15.713%       |
| 2         | 4.559       | 257           | 260         | 270          | rBV      | 356839         | 612833        | 10.78%          | 1.694%        |
| 3         | 5.039       | 299           | 302         | 304          | rBV      | 2498296        | 2818468       | 49.59%          | 7.792%        |
| 4         | 6.136       | 395           | 398         | 401          | rBV      | 2271725        | 2730850       | 48.05%          | 7.550%        |
| 5         | 6.239       | 405           | 407         | 410          | rVV      | 2352179        | 2828549       | 49.77%          | 7.820%        |
| 6         | 6.479       | 425           | 428         | 430          | rBV      | 673351         | 797568        | 14.03%          | 2.205%        |
| 7         | 6.627       | 439           | 441         | 444          | rBV      | 1864849        | 2153010       | 37.88%          | 5.952%        |
| 8         | 7.050       | 475           | 478         | 480          | rBV      | 1804309        | 1859393       | 32.72%          | 5.141%        |
| 9         | 7.759       | 538           | 540         | 543          | rBV      | 946319         | 1042151       | 18.34%          | 2.881%        |
| 10        | 8.845       | 632           | 635         | 637          | rBV      | 2843517        | 3065911       | 53.95%          | 8.476%        |
| 11        | 9.245       | 667           | 670         | 672          | rBV      | 1133711        | 1088166       | 19.15%          | 3.008%        |
| 12        | 9.359       | 678           | 680         | 683          | rVB      | 80936          | 69433         | 1.22%           | 0.192%        |
| 13        | 9.496       | 690           | 692         | 694          | rVV      | 911323         | 1139736       | 20.05%          | 3.151%        |
| 14        | 9.965       | 731           | 733         | 734          | rVB      | 81120          | 73471         | 1.29%           | 0.203%        |
| 15        | 10.285      | 758           | 761         | 763          | rBV      | 1666005        | 1634565       | 28.76%          | 4.519%        |
| 16        | 10.433      | 771           | 774         | 778          | rVB      | 93379          | 116039        | 2.04%           | 0.321%        |
| 17        | 10.879      | 810           | 813         | 814          | rVB2     | 45951          | 59799         | 1.05%           | 0.165%        |
| 18        | 10.971      | 818           | 821         | 825          | rBV2     | 980724         | 1309886       | 23.05%          | 3.621%        |
| 19        | 11.039      | 825           | 827         | 830          | rVB      | 85104          | 88229         | 1.55%           | 0.244%        |
| 20        | 11.233      | 839           | 844         | 846          | rBV2     | 36777          | 81334         | 1.43%           | 0.225%        |
| 21        | 11.531      | 869           | 870         | 872          | rVV2     | 61866          | 90643         | 1.59%           | 0.251%        |
| 22        | 11.576      | 872           | 874         | 878          | rVB2     | 75956          | 126077        | 2.22%           | 0.349%        |
| 23        | 11.782      | 889           | 892         | 896          | rVB2     | 42226          | 73958         | 1.30%           | 0.204%        |
| 24        | 12.171      | 923           | 926         | 928          | rBV      | 366205         | 526958        | 9.27%           | 1.457%        |
| 25        | 12.308      | 936           | 938         | 941          | rBV2     | 37157          | 64236         | 1.13%           | 0.178%        |
| 26        | 12.388      | 942           | 945         | 947          | rBV      | 512504         | 574937        | 10.12%          | 1.590%        |
| 27        | 12.548      | 957           | 959         | 962          | rVV      | 1553985        | 1505446       | 26.49%          | 4.162%        |
| 28        | 12.616      | 962           | 965         | 966          | rVV2     | 34556          | 61279         | 1.08%           | 0.169%        |
| 29        | 12.719      | 970           | 974         | 976          | rVB2     | 51949          | 100988        | 1.78%           | 0.279%        |
| 30        | 12.822      | 981           | 983         | 987          | rVB2     | 53880          | 71825         | 1.26%           | 0.199%        |
| 31        | 13.028      | 999           | 1001        | 1005         | rBV2     | 28800          | 58386         | 1.03%           | 0.161%        |
| 32        | 13.142      | 1009          | 1011        | 1014         | rVV2     | 38300          | 57013         | 1.00%           | 0.158%        |
| 33        | 13.325      | 1025          | 1027        | 1028         | rBV      | 54032          | 61192         | 1.08%           | 0.169%        |
| 34        | 13.405      | 1032          | 1034        | 1035         | rVV      | 123715         | 123836        | 2.18%           | 0.342%        |

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ALS Vial : 25 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
S-6-1-LOC-6(0-5)

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-BF092016.M  
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

|    |        |      |      |      |      |        |         |        |        |
|----|--------|------|------|------|------|--------|---------|--------|--------|
| 35 | 13.462 | 1038 | 1039 | 1044 | rVV3 | 134604 | 192690  | 3.39%  | 0.533% |
| 36 | 13.577 | 1046 | 1049 | 1055 | rVV2 | 897940 | 1392584 | 24.50% | 3.850% |
| 37 | 14.102 | 1093 | 1095 | 1099 | rVB4 | 49474  | 62205   | 1.09%  | 0.172% |
| 38 | 14.560 | 1133 | 1135 | 1140 | rBV  | 237349 | 482696  | 8.49%  | 1.334% |
| 39 | 14.800 | 1154 | 1156 | 1159 | rBV  | 137411 | 149835  | 2.64%  | 0.414% |
| 40 | 14.845 | 1159 | 1160 | 1163 | rBV  | 142272 | 182901  | 3.22%  | 0.506% |
| 41 | 14.902 | 1163 | 1165 | 1170 | rVB  | 536328 | 653086  | 11.49% | 1.806% |
| 42 | 16.034 | 1262 | 1264 | 1269 | rVB2 | 75286  | 163927  | 2.88%  | 0.453% |
| 43 | 16.377 | 1292 | 1294 | 1301 | rVB  | 67170  | 141227  | 2.48%  | 0.390% |

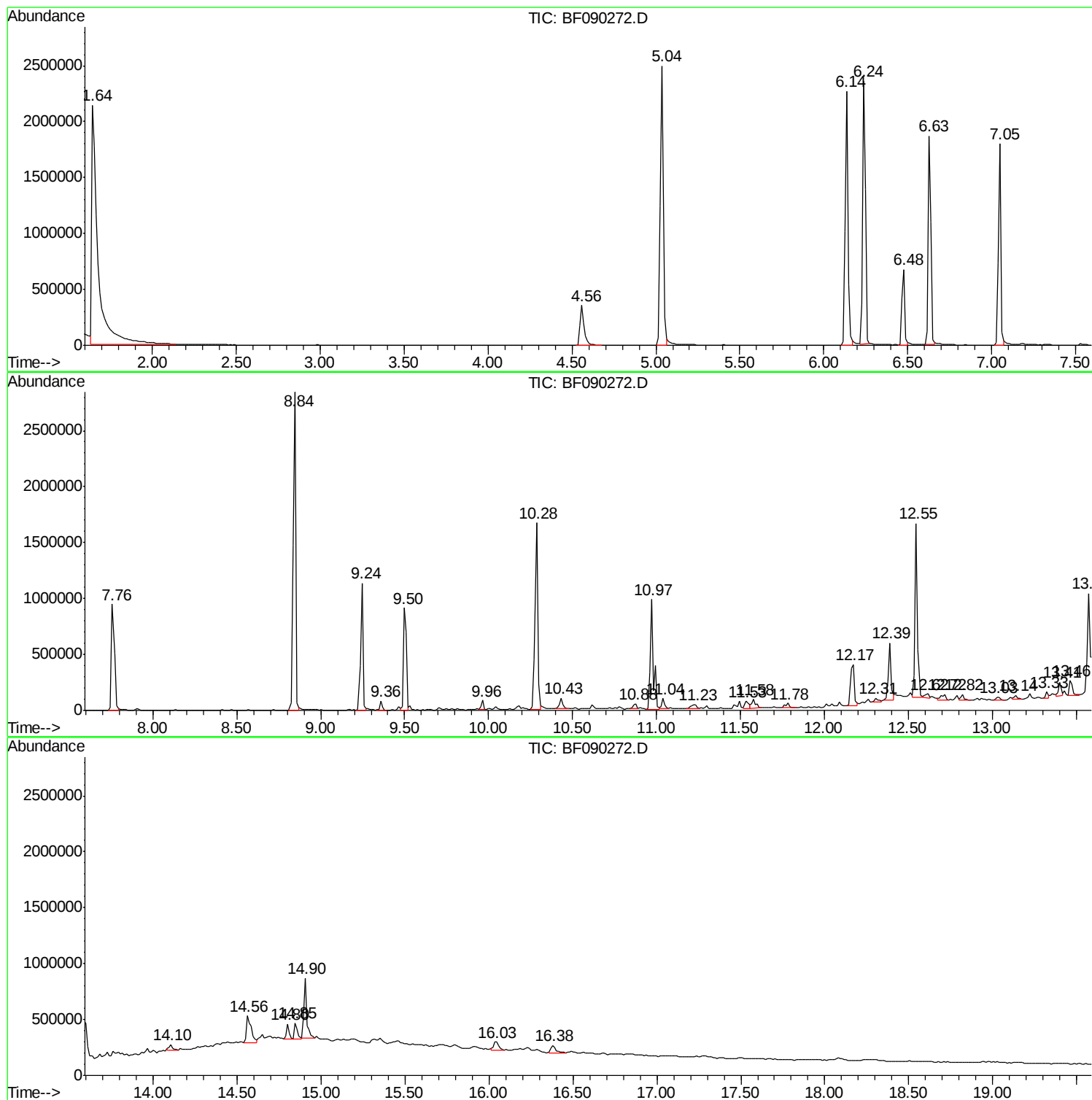
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Instrument :  
BNA\_F  
ClientSampled :  
S-6-1-LOC-6(0-5)

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF092016.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF092716\  
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Acq On : 28 Sep 2016 00:32  
Operator : UM/SJ  
Sample : H4949-11  
Misc :  
ALS Vial : 25 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
S-6-1-LOC-6(0-5)

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF092016.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

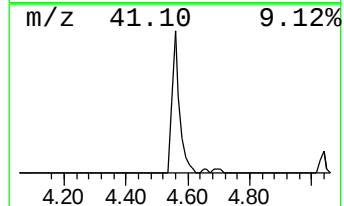
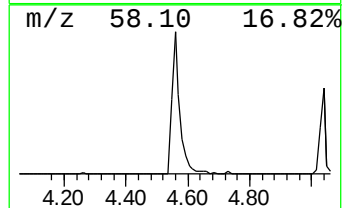
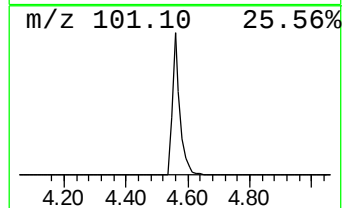
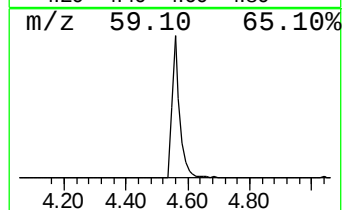
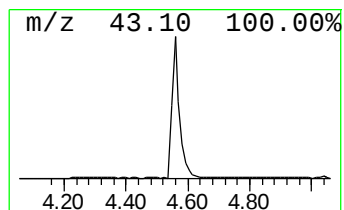
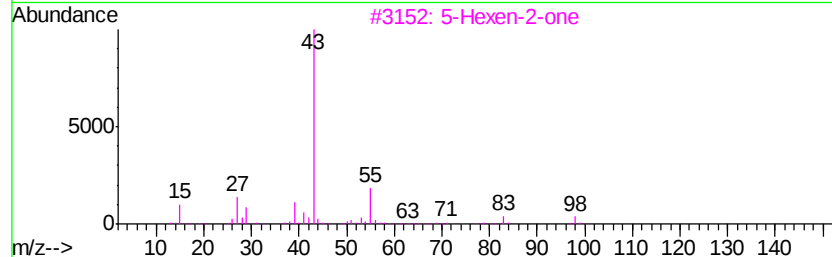
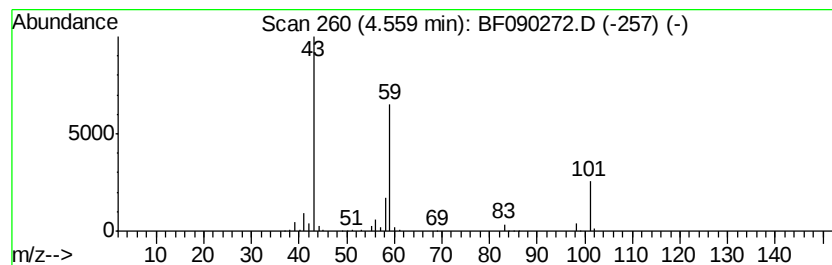
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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

| R.T. | EstConc  | Area   | Relative to ISTD       | R.T. |
|------|----------|--------|------------------------|------|
| 4.56 | 15.37 ng | 612833 | 1,4-Dichlorobenzene-d4 | 6.48 |

| Hit# | of | Tentative ID                         | MW  | MolForm  | CAS#        | Qual |
|------|----|--------------------------------------|-----|----------|-------------|------|
| 1    | 5  | 2-Pentanone, 4-hydroxy-4-methyl-     | 116 | C6H12O2  | 000123-42-2 | 50   |
| 2    |    | Acetic acid, cyano-, 1,1-dimethyl... | 141 | C7H11NO2 | 001116-98-9 | 25   |
| 3    |    | 5-Hexen-2-one                        | 98  | C6H10O   | 000109-49-9 | 9    |
| 4    |    | Acetone                              | 58  | C3H6O    | 000067-64-1 | 9    |
| 5    |    | Butane, 1-ethoxy-                    | 102 | C6H14O   | 000628-81-9 | 9    |



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Misc :  
ALS Vial : 25 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
S-6-1-LOC-6(0-5)

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092016.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

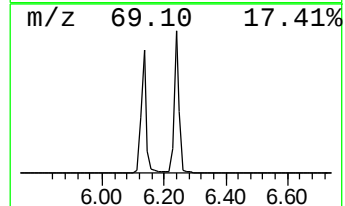
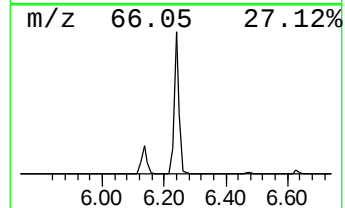
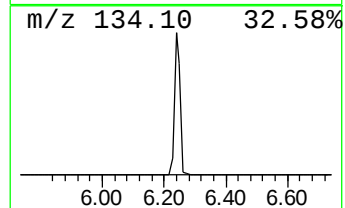
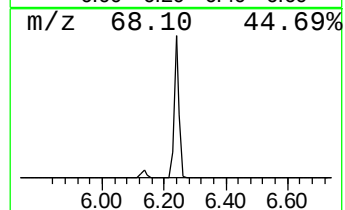
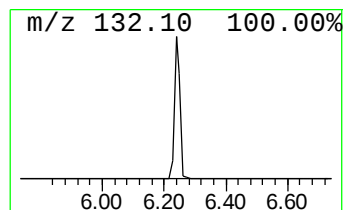
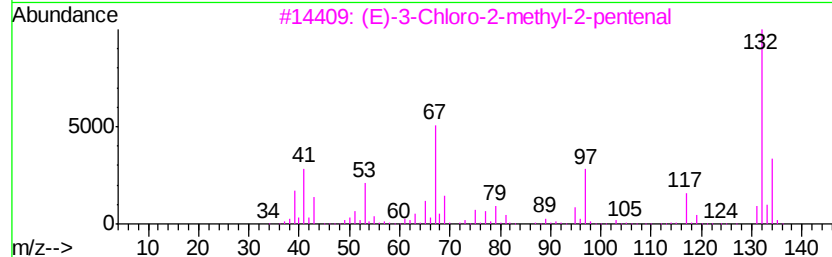
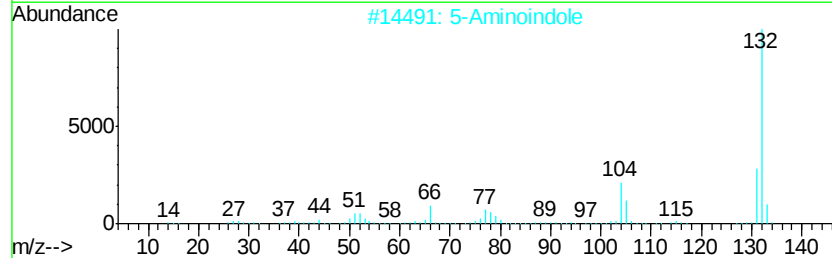
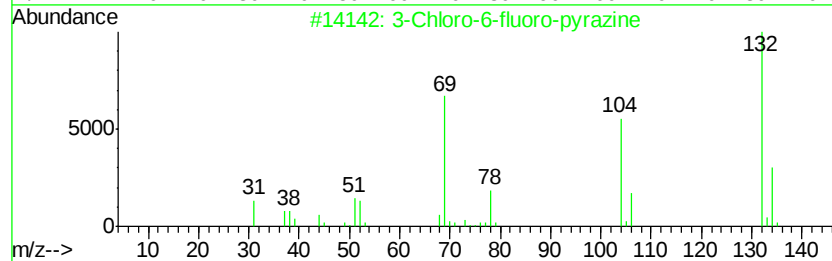
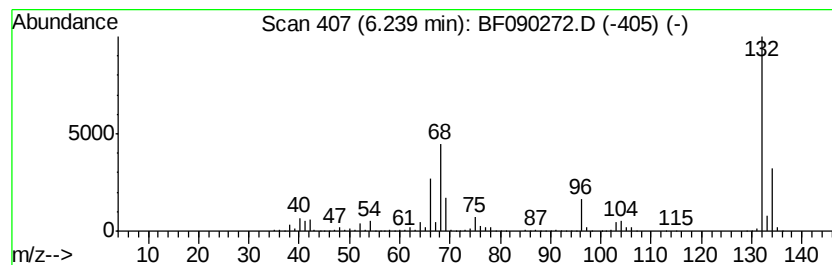
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 3 unknown6.24 Concentration Rank 2

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.24 | 70.93 ng | 2828550 | 1,4-Dichlorobenzene-d4 | 6.48 |

| Hit# | of | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|-------------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 3-Chloro-6-fluoro-pyrazine          | 132 | C4H2ClFN2 | 1000146-10-7 | 27   |
| 2    |    | 5-Aminoindole                       | 132 | C8H8N2    | 005192-03-0  | 12   |
| 3    |    | (E)-3-Chloro-2-methyl-2-pentenal    | 132 | C6H9ClO   | 031357-76-3  | 9    |
| 4    |    | 1-Methylpyrrolo[1,2-a]pyrazine      | 132 | C8H8N2    | 064608-59-9  | 9    |
| 5    |    | 2H-Cyclopenta[d]pyridazine, 2-me... | 132 | C8H8N2    | 022291-85-6  | 9    |



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Instrument :  
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ClientSampleId :  
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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF092016.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

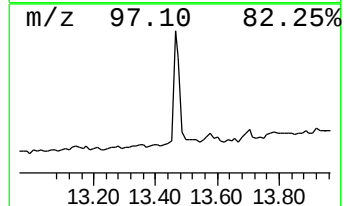
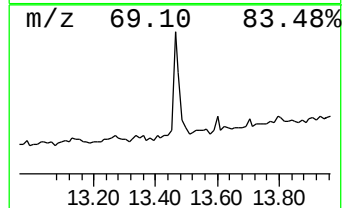
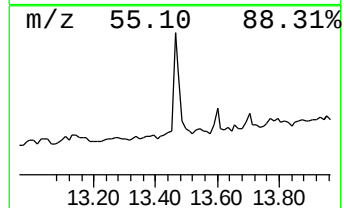
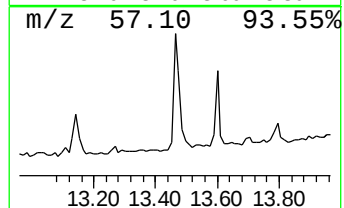
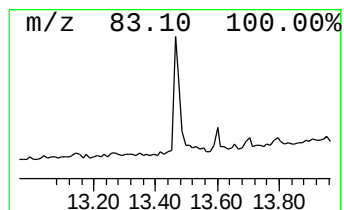
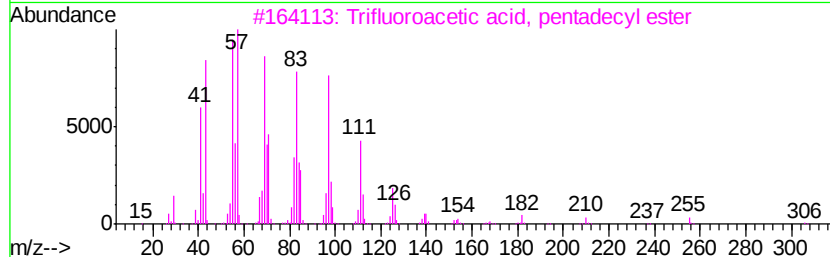
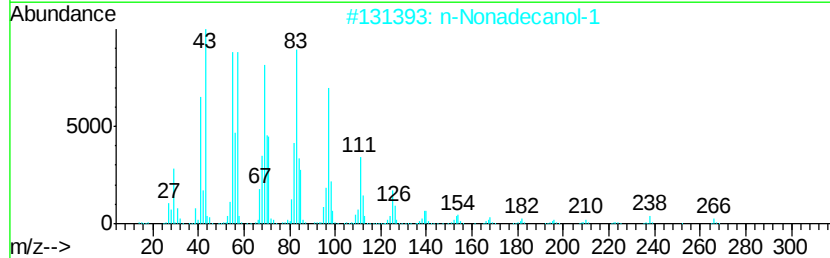
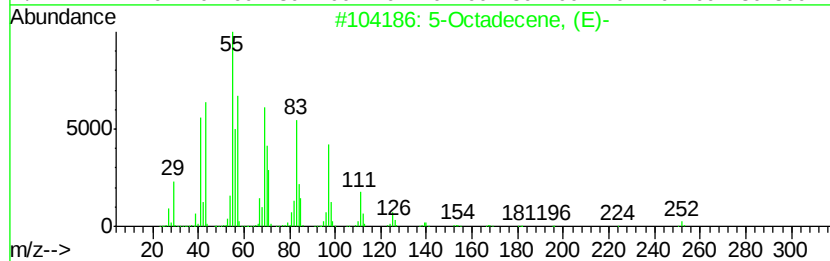
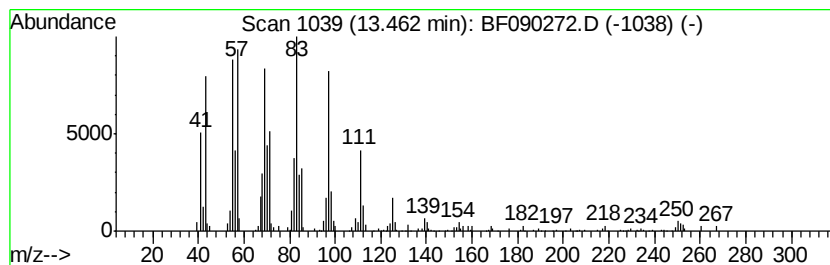
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 5 5-Octadecene, (E)- Concentration Rank 6

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 13.46 | 2.77 ng | 192690 | Chrysene-d12     | 13.58 |

| Hit# | of | Tentative ID                        | MW  | MolForm    | CAS#        | Qual |
|------|----|-------------------------------------|-----|------------|-------------|------|
| 1    | 5  | 5-Octadecene, (E)-                  | 252 | C18H36     | 007206-21-5 | 96   |
| 2    |    | n-Nonadecanol-1                     | 284 | C19H40O    | 001454-84-8 | 94   |
| 3    |    | Trifluoroacetic acid, pentadecyl... | 324 | C17H31F3O2 | 959010-23-2 | 93   |
| 4    |    | Heptafluorobutyric acid, n-tetra... | 410 | C18H29F7O2 | 007365-36-8 | 93   |
| 5    |    | Pentafluoropropionic acid, penta... | 374 | C18H31F5O2 | 959092-08-1 | 93   |



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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... | 4.56  | 15.4    | ng    | 612833   | 1                     | 6.48  | 797568  | 20.0 |
| unknown6.24          | 6.24  | 70.9    | ng    | 2828550  | 1                     | 6.48  | 797568  | 20.0 |
| 5-Octadecene, (E)-   | 13.46 | 2.8     | ng    | 192690   | 5                     | 13.58 | 1392580 | 20.0 |