

Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF100817\  
 Data File : BF099227.D  
 Acq On : 8 Oct 2017 12:49  
 Operator : SJ/JU  
 Sample : PB102980BL  
 Misc :  
 ALS Vial : 6 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 PB102980BL

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-BF092317.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         | 2.269       | 28            | 31          | 40           | rVB      | 46310          | 62287         | 1.90%           | 0.260%        |
| 2         | 2.481       | 53            | 67          | 73           | rVB      | 217104         | 434487        | 13.22%          | 1.813%        |
| 3         | 5.087       | 506           | 510         | 524          | rBV      | 380595         | 472041        | 14.36%          | 1.970%        |
| 4         | 5.487       | 574           | 578         | 581          | rBV      | 2154221        | 1928887       | 58.69%          | 8.049%        |
| 5         | 6.493       | 745           | 749         | 752          | rBV      | 1930450        | 1897628       | 57.74%          | 7.919%        |
| 6         | 6.634       | 769           | 773         | 776          | rBV      | 2362055        | 2003047       | 60.95%          | 8.359%        |
| 7         | 6.863       | 808           | 812         | 816          | rBV      | 813518         | 629901        | 19.17%          | 2.629%        |
| 8         | 7.022       | 835           | 839         | 842          | rBV      | 2631881        | 2271206       | 69.11%          | 9.478%        |
| 9         | 7.428       | 903           | 908         | 911          | rBV      | 1778289        | 1786229       | 54.35%          | 7.454%        |
| 10        | 8.145       | 1026          | 1030        | 1034         | rBV      | 1045970        | 873466        | 26.58%          | 3.645%        |
| 11        | 9.222       | 1208          | 1213        | 1216         | rBV      | 3468634        | 3277832       | 99.74%          | 13.679%       |
| 12        | 9.898       | 1324          | 1328        | 1332         | rBV      | 1017611        | 971018        | 29.55%          | 4.052%        |
| 13        | 10.692      | 1459          | 1463        | 1476         | rBV      | 1401631        | 1277830       | 38.88%          | 5.333%        |
| 14        | 11.386      | 1577          | 1581        | 1585         | rBV      | 1072782        | 996364        | 30.32%          | 4.158%        |
| 15        | 12.974      | 1846          | 1851        | 1854         | rBV      | 3093501        | 3286417       | 100.00%         | 13.715%       |
| 16        | 14.027      | 2026          | 2030        | 2034         | rBV      | 999612         | 917493        | 27.92%          | 3.829%        |
| 17        | 15.504      | 2276          | 2281        | 2293         | rVB      | 632894         | 804964        | 24.49%          | 3.359%        |
| 18        | 15.939      | 2350          | 2355        | 2360         | rBV2     | 22549          | 34210         | 1.04%           | 0.143%        |
| 19        | 17.739      | 2654          | 2661        | 2666         | rBV5     | 14179          | 37588         | 1.14%           | 0.157%        |

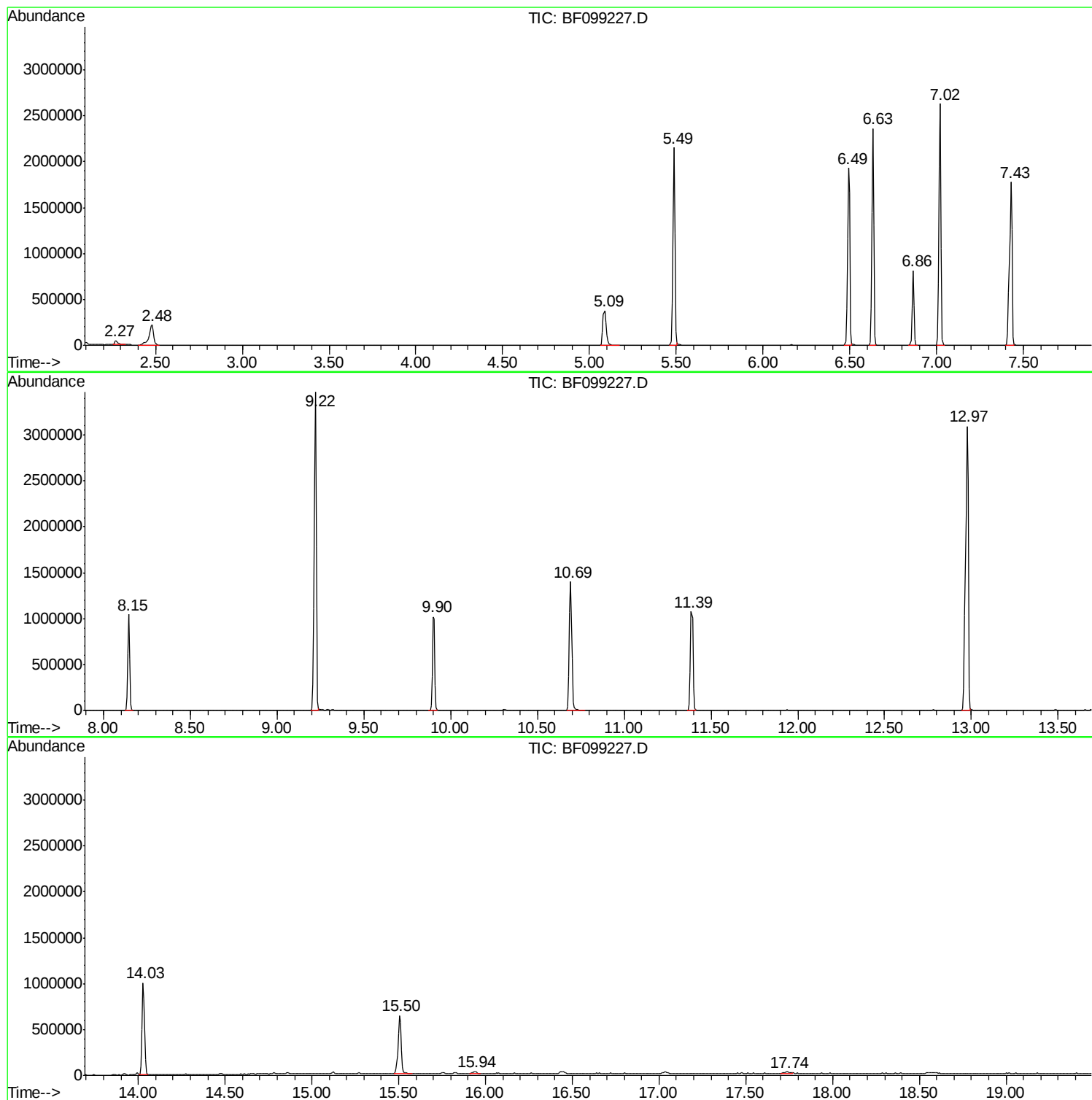
Sum of corrected areas: 23962895

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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF092317.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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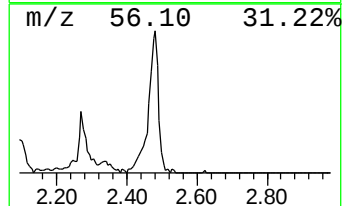
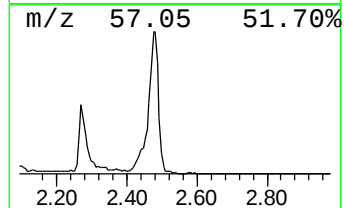
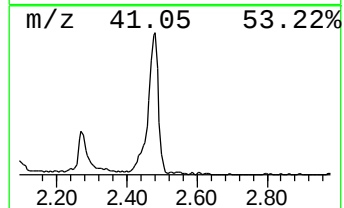
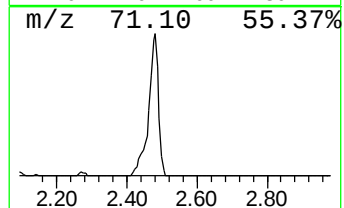
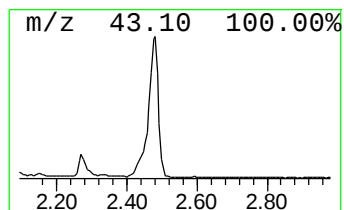
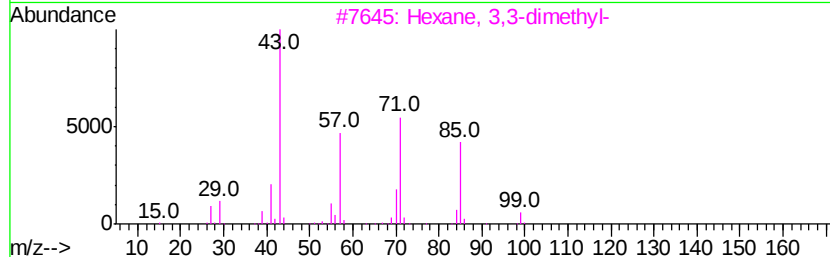
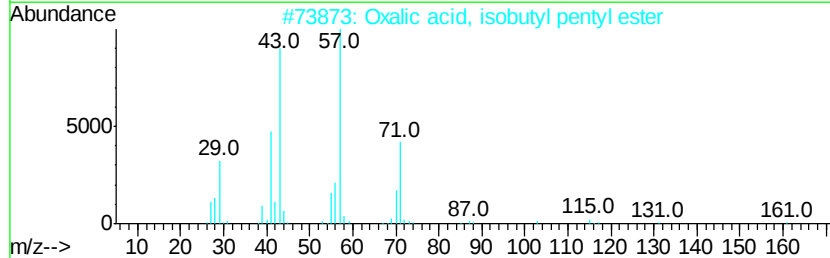
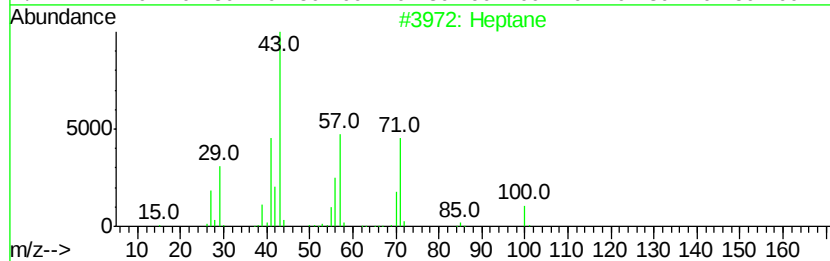
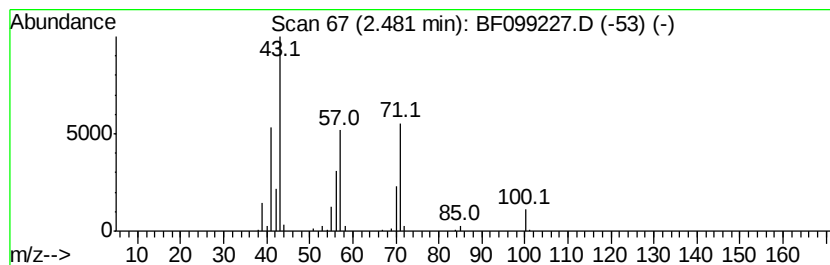
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 Heptane Concentration Rank 4

| R.T. | EstConc  | Area   | Relative to ISTD       | R.T. |
|------|----------|--------|------------------------|------|
| 2.48 | 13.80 ng | 434487 | 1,4-Dichlorobenzene-d4 | 6.86 |

| Hit# | of | Tentative ID                       | MW  | MolForm  | CAS#         | Qual |
|------|----|------------------------------------|-----|----------|--------------|------|
| 1    | 5  | Heptane                            | 100 | C7H16    | 000142-82-5  | 95   |
| 2    |    | Oxalic acid, isobutyl pentyl ester | 216 | C11H20O4 | 1000309-37-0 | 50   |
| 3    |    | Hexane, 3,3-dimethyl-              | 114 | C8H18    | 000563-16-6  | 50   |
| 4    |    | Pentane, 3,3-dimethyl-             | 100 | C7H16    | 000562-49-2  | 50   |
| 5    |    | Pentane, 2,4-dimethyl-             | 100 | C7H16    | 000108-08-7  | 38   |



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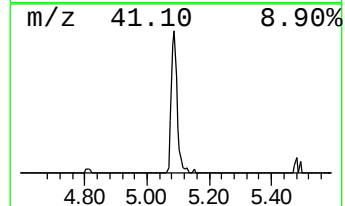
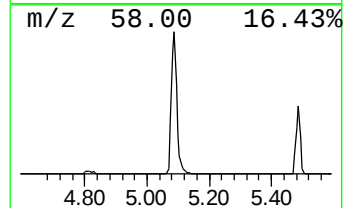
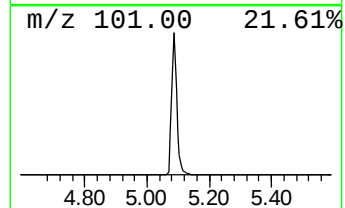
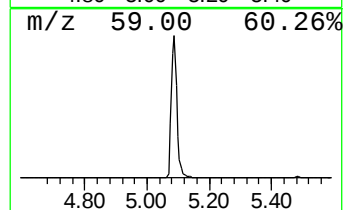
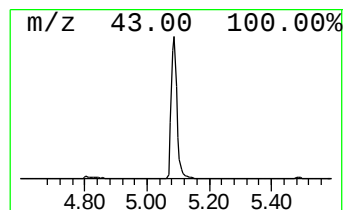
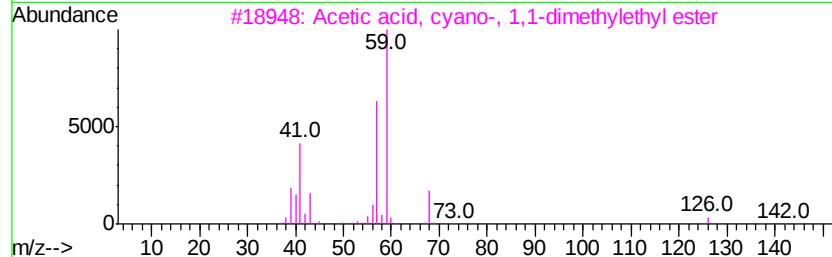
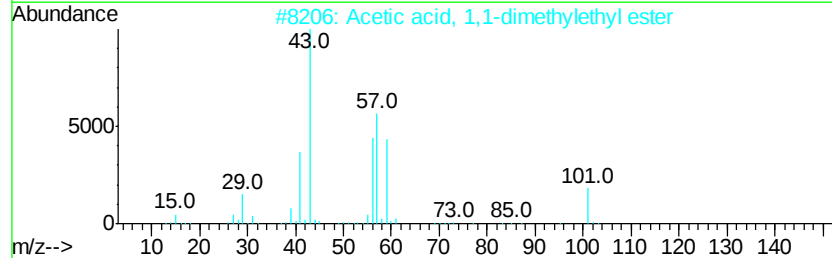
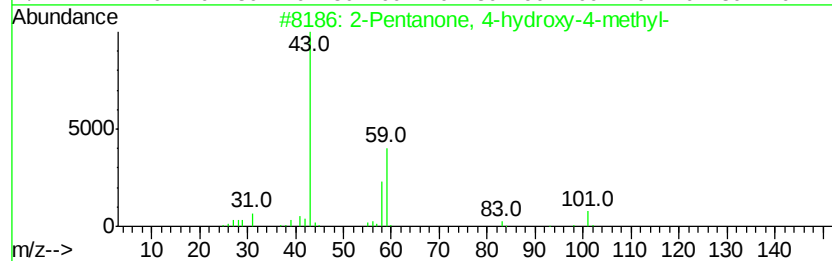
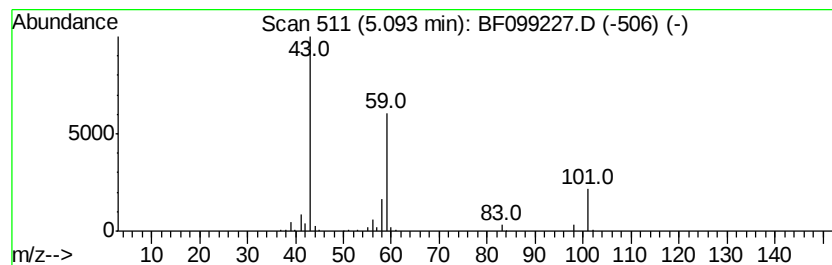
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T. | EstConc  | Area   | Relative to ISTD       | R.T. |
|------|----------|--------|------------------------|------|
| 5.09 | 14.99 ng | 472041 | 1,4-Dichlorobenzene-d4 | 6.86 |

| Hit# | of                                   | 5   | Tentative ID | MW          | MolForm | CAS# | Qual |
|------|--------------------------------------|-----|--------------|-------------|---------|------|------|
| 1    | 2-Pentanone, 4-hydroxy-4-methyl-     | 116 | C6H12O2      | 000123-42-2 | 56      |      |      |
| 2    | Acetic acid, 1,1-dimethylethyl e...  | 116 | C6H12O2      | 000540-88-5 | 39      |      |      |
| 3    | Acetic acid, cyano-, 1,1-dimethyl... | 141 | C7H11NO2     | 001116-98-9 | 17      |      |      |
| 4    | Butane, 1-ethoxy-                    | 102 | C6H14O       | 000628-81-9 | 9       |      |      |
| 5    | Acetone                              | 58  | C3H6O        | 000067-64-1 | 9       |      |      |



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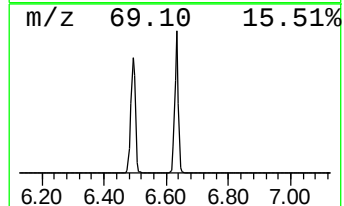
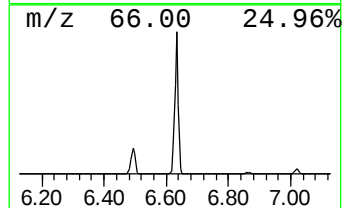
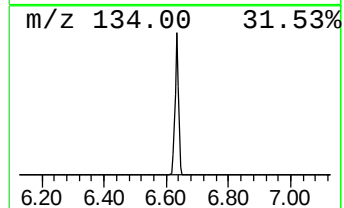
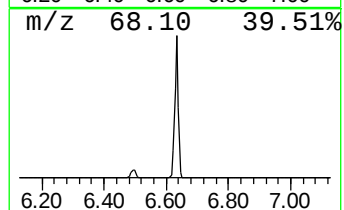
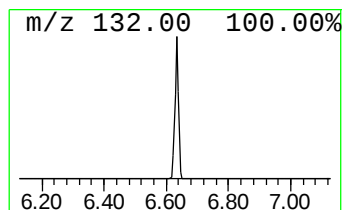
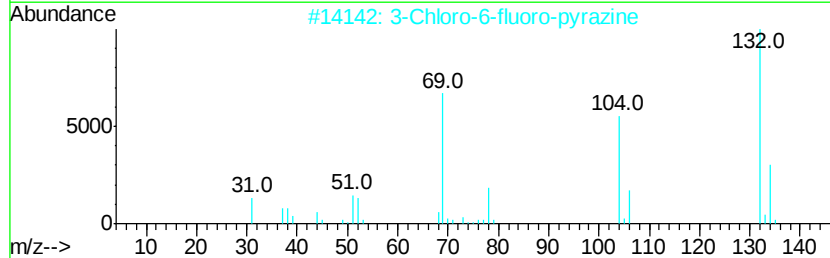
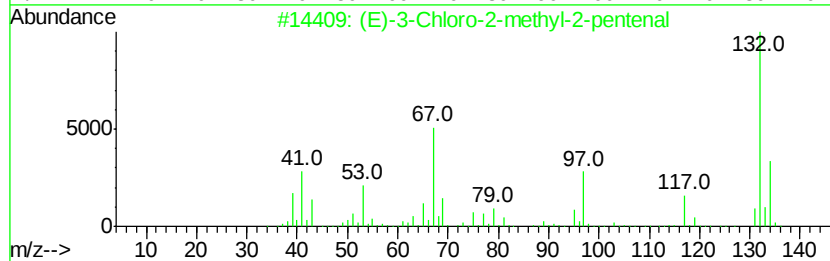
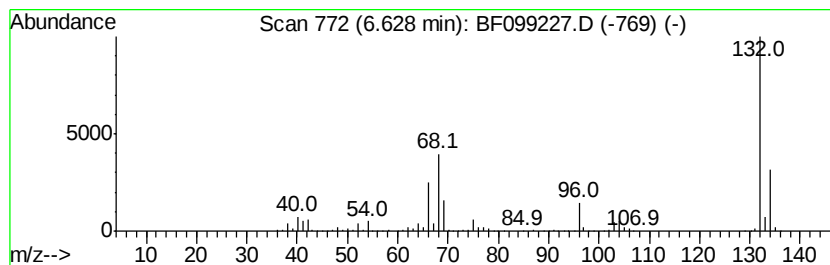
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TIC Integration Parameters: LSCINT.P

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Peak Number 3 unknown6.63 Concentration Rank 2

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.63 | 63.60 ng | 2003050 | 1,4-Dichlorobenzene-d4 | 6.86 |

| Hit# | of | Tentative ID                     | MW  | MolForm   | CAS#         | Qual |
|------|----|----------------------------------|-----|-----------|--------------|------|
| 1    | 5  | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO   | 031357-76-3  | 35   |
| 2    |    | 3-Chloro-6-fluoro-pyrazine       | 132 | C4H2ClFN2 | 1000146-10-7 | 25   |
| 3    |    | 5-Aminoindole                    | 132 | C8H8N2    | 005192-03-0  | 12   |
| 4    |    | 4-Methylpyrrolo[1,2-a]pyrazine   | 132 | C8H8N2    | 064608-60-2  | 9    |
| 5    |    | 1H-Benzimidazole, 2-methyl-      | 132 | C8H8N2    | 000615-15-6  | 9    |



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| TIC Top Hit name     | RT   | EstConc | Units | Response | --Internal Standard-- |      |        |      |
|----------------------|------|---------|-------|----------|-----------------------|------|--------|------|
|                      |      |         |       |          | #                     | RT   | Resp   | Conc |
| Heptane              | 2.48 | 13.8    | ng    | 434487   | 1                     | 6.86 | 629901 | 20.0 |
| 2-Pentanone, 4-hy... | 5.09 | 15.0    | ng    | 472041   | 1                     | 6.86 | 629901 | 20.0 |
| unknown6.63          | 6.63 | 63.6    | ng    | 2003050  | 1                     | 6.86 | 629901 | 20.0 |