

Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF100917\  
 Data File : BF099288.D  
 Acq On : 10 Oct 2017 4:06  
 Operator : SJ/JU  
 Sample : PB103201BL  
 Misc :  
 ALS Vial : 29 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 PB103106BL

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-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         | 3.981       | 317           | 322         | 328          | rBB      | 24499          | 30321         | 1.19%           | 0.156%        |
| 2         | 4.487       | 405           | 408         | 417          | rBV      | 75106          | 88227         | 3.45%           | 0.454%        |
| 3         | 5.099       | 508           | 512         | 523          | rBV      | 436317         | 536243        | 20.99%          | 2.759%        |
| 4         | 5.493       | 575           | 579         | 582          | rBV      | 2154209        | 2033800       | 79.62%          | 10.465%       |
| 5         | 6.498       | 744           | 750         | 752          | rBV      | 1830099        | 1991799       | 77.97%          | 10.249%       |
| 6         | 6.634       | 769           | 773         | 776          | rBV      | 2361049        | 2139738       | 83.76%          | 11.010%       |
| 7         | 6.863       | 808           | 812         | 815          | rBV      | 624719         | 519933        | 20.35%          | 2.675%        |
| 8         | 7.016       | 834           | 838         | 842          | rBV      | 1850741        | 1731170       | 67.77%          | 8.908%        |
| 9         | 7.428       | 902           | 908         | 911          | rBV      | 1314972        | 1290727       | 50.53%          | 6.642%        |
| 10        | 8.145       | 1025          | 1030        | 1033         | rBV      | 762104         | 718714        | 28.13%          | 3.698%        |
| 11        | 9.216       | 1207          | 1212        | 1216         | rBV      | 2556277        | 2554541       | 100.00%         | 13.145%       |
| 12        | 9.898       | 1323          | 1328        | 1337         | rBV      | 927695         | 784961        | 30.73%          | 4.039%        |
| 13        | 10.686      | 1458          | 1462        | 1482         | rBV      | 1275262        | 1258002       | 49.25%          | 6.473%        |
| 14        | 11.386      | 1577          | 1581        | 1584         | rBV      | 889388         | 733951        | 28.73%          | 3.777%        |
| 15        | 12.969      | 1845          | 1850        | 1853         | rBV      | 2203759        | 2018269       | 79.01%          | 10.385%       |
| 16        | 14.027      | 2026          | 2030        | 2041         | rBV      | 518306         | 486580        | 19.05%          | 2.504%        |
| 17        | 15.504      | 2275          | 2281        | 2293         | rBV      | 337576         | 461396        | 18.06%          | 2.374%        |
| 18        | 16.433      | 2432          | 2439        | 2445         | rBV2     | 15548          | 28616         | 1.12%           | 0.147%        |
| 19        | 17.727      | 2651          | 2659        | 2667         | rBV5     | 9118           | 26895         | 1.05%           | 0.138%        |

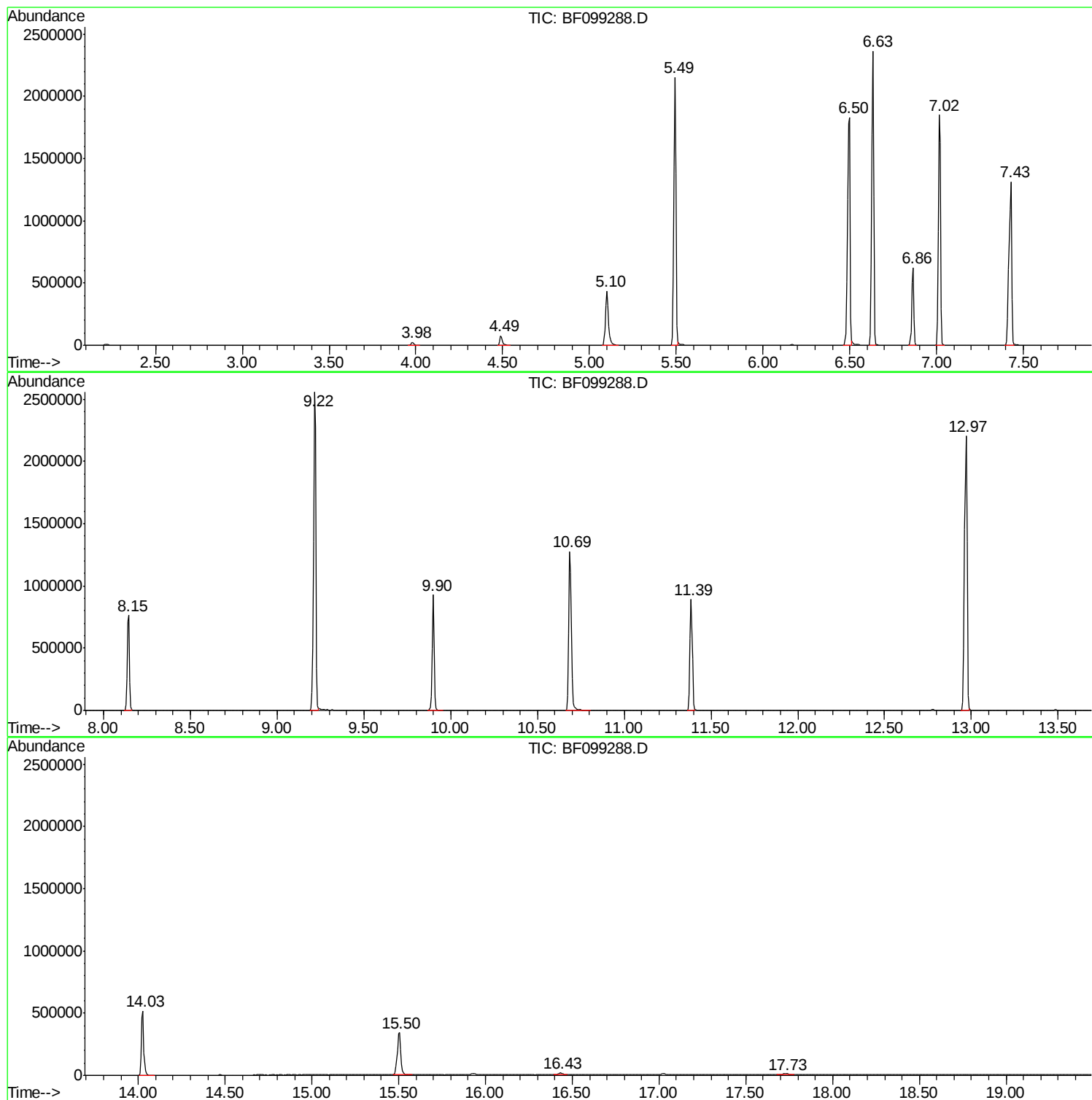
Sum of corrected areas: 19433883

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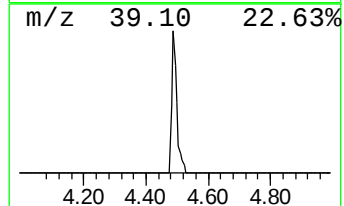
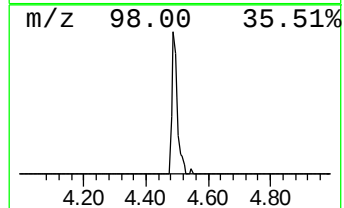
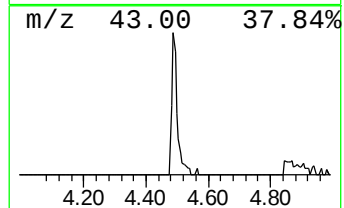
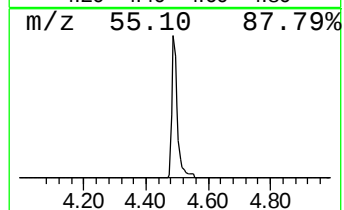
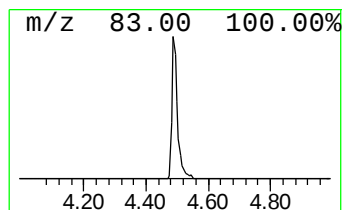
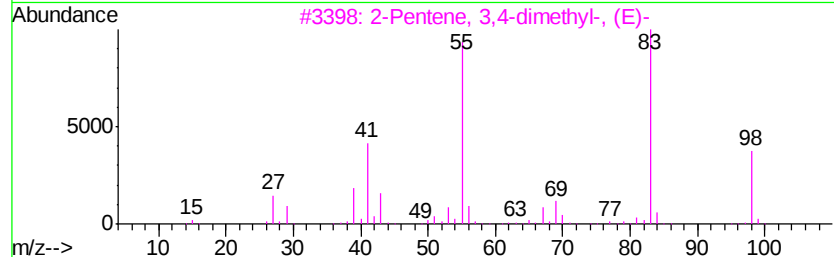
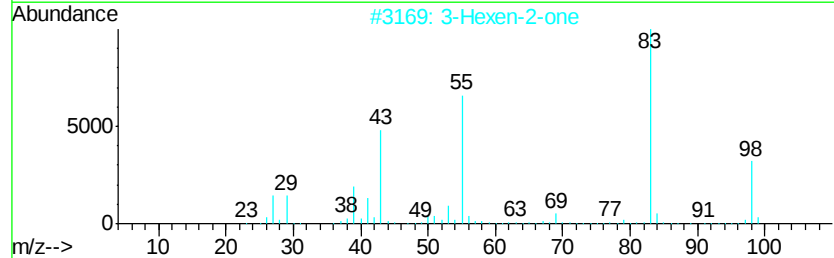
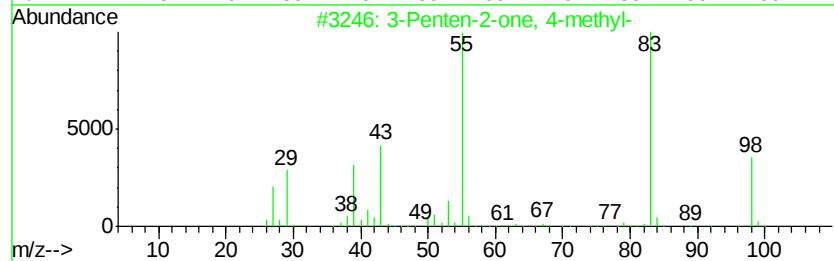
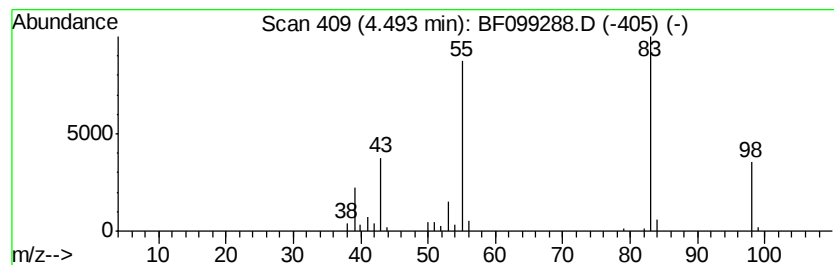
Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF092317.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

| R.T. | EstConc | Area  | Relative to ISTD       | R.T. |
|------|---------|-------|------------------------|------|
| 4.49 | 3.39 ng | 88227 | 1,4-Dichlorobenzene-d4 | 6.86 |

| Hit# | of | 5 | Tentative ID                   | MW | MolForm | CAS#        | Qual |
|------|----|---|--------------------------------|----|---------|-------------|------|
| 1    |    |   | 3-Penten-2-one, 4-methyl-      | 98 | C6H10O  | 000141-79-7 | 90   |
| 2    |    |   | 3-Hexen-2-one                  | 98 | C6H10O  | 000763-93-9 | 86   |
| 3    |    |   | 2-Pentene, 3,4-dimethyl-, (E)- | 98 | C7H14   | 004914-92-5 | 80   |
| 4    |    |   | Furan, 2-methoxy-              | 98 | C5H6O2  | 025414-22-6 | 78   |
| 5    |    |   | 2-Pentene, 3,4-dimethyl-, (Z)- | 98 | C7H14   | 004914-91-4 | 72   |



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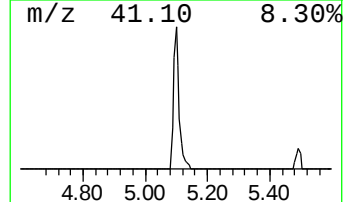
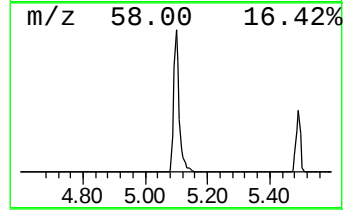
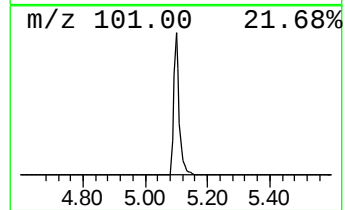
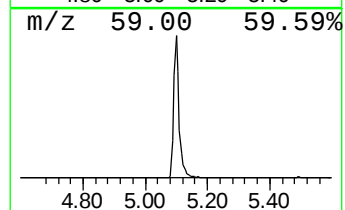
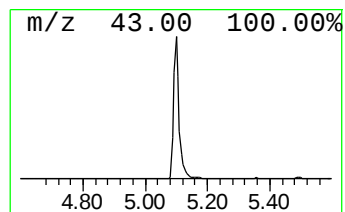
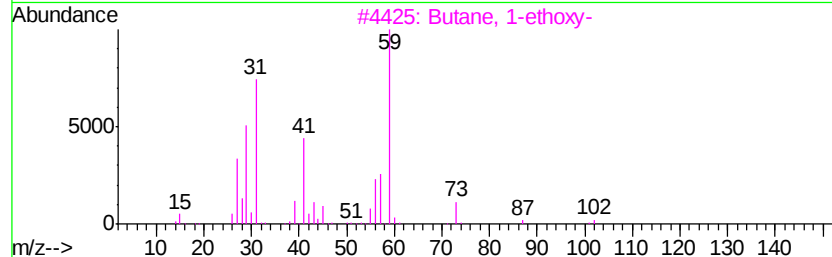
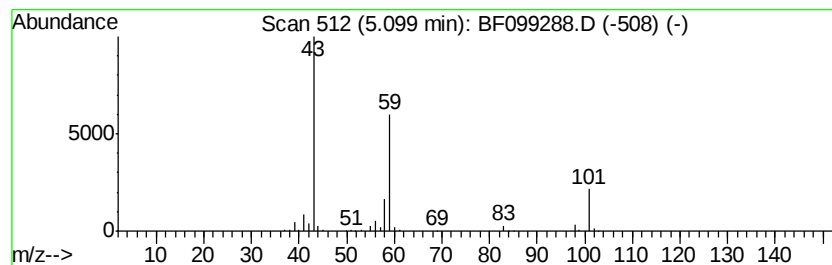
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T. | EstConc  | Area   | Relative to ISTD       | R.T. |
|------|----------|--------|------------------------|------|
| 5.10 | 20.63 ng | 536243 | 1,4-Dichlorobenzene-d4 | 6.86 |

| 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-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 23   |
| 3    |    | Butane, 1-ethoxy-                   | 102 | C6H14O   | 000628-81-9 | 9    |
| 4    |    | Morpholine, 4-methyl-               | 101 | C5H11NO  | 000109-02-4 | 9    |
| 5    |    | 2,3-Butanedione, monooxime          | 101 | C4H7NO2  | 000057-71-6 | 9    |



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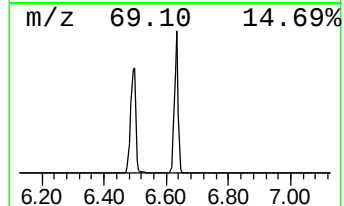
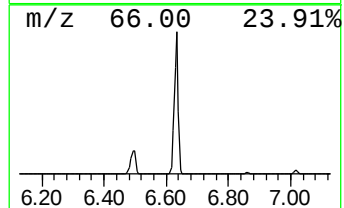
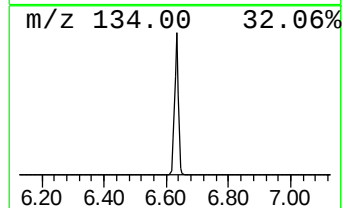
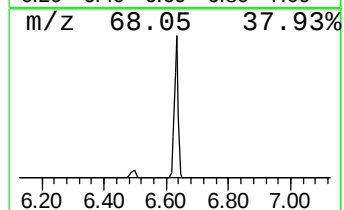
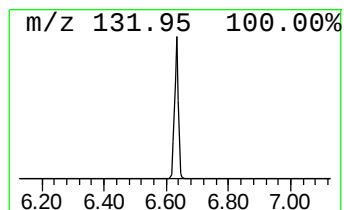
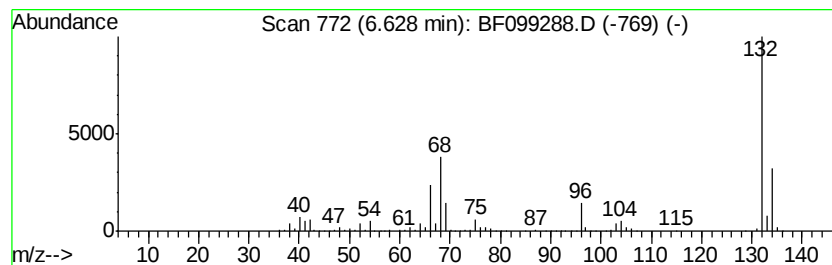
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Peak Number 3 unknown6.63 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.63 | 82.31 ng | 2139740 | 1,4-Dichlorobenzene-d4 | 6.86 |

| Hit# | of | Tentative ID                     | MW  | MolForm   | CAS#         | Qual |
|------|----|----------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 3-Chloro-6-fluoro-pyrazine       | 132 | C4H2ClFN2 | 1000146-10-7 | 35   |
| 2    |    | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO   | 031357-76-3  | 35   |
| 3    |    | 5-Aminoindole                    | 132 | C8H8N2    | 005192-03-0  | 12   |
| 4    |    | Tranylcypromine-propionyl        | 189 | C12H15NO  | 1000123-86-3 | 12   |
| 5    |    | 4-Chloro-2-fluoro-pyrimidine     | 132 | C4H2ClFN2 | 051422-00-5  | 9    |



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| TIC Top Hit name     | RT   | EstConc | Units | Response | --Internal Standard-- |      |        |      |
|----------------------|------|---------|-------|----------|-----------------------|------|--------|------|
|                      |      |         |       |          | #                     | RT   | Resp   | Conc |
| 3-Penten-2-one, 4... | 4.49 | 3.4     | ng    | 88227    | 1                     | 6.86 | 519933 | 20.0 |
| 2-Pentanone, 4-hy... | 5.10 | 20.6    | ng    | 536243   | 1                     | 6.86 | 519933 | 20.0 |
| unknown6.63          | 6.63 | 82.3    | ng    | 2139740  | 1                     | 6.86 | 519933 | 20.0 |