

Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF101716\  
 Data File : BF090617.D  
 Acq On : 17 Oct 2016 19:39  
 Operator : UM/SJ  
 Sample : H5227-03 5X  
 Misc :  
 ALS Vial : 16 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 3

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-BF101316.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         | 5.068       | 237           | 239         | 247          | rBV      | 127319         | 190437        | 9.81%           | 1.053%        |
| 2         | 5.503       | 275           | 277         | 290          | rBV      | 625596         | 733919        | 37.82%          | 4.056%        |
| 3         | 6.531       | 365           | 367         | 377          | rBV      | 634615         | 780287        | 40.21%          | 4.312%        |
| 4         | 6.669       | 377           | 379         | 388          | rVV      | 811660         | 853599        | 43.98%          | 4.718%        |
| 5         | 6.909       | 398           | 400         | 402          | rBV      | 1157806        | 1179165       | 60.76%          | 6.517%        |
| 6         | 7.057       | 411           | 413         | 416          | rBV      | 571486         | 596944        | 30.76%          | 3.299%        |
| 7         | 7.469       | 446           | 449         | 455          | rBV      | 293144         | 421960        | 21.74%          | 2.332%        |
| 8         | 8.189       | 510           | 512         | 515          | rBV      | 1416567        | 1733560       | 89.32%          | 9.581%        |
| 9         | 9.275       | 604           | 607         | 609          | rBV      | 532574         | 738504        | 38.05%          | 4.082%        |
| 10        | 9.663       | 639           | 641         | 645          | rVB      | 177556         | 154216        | 7.95%           | 0.852%        |
| 11        | 9.812       | 652           | 654         | 656          | rBV      | 46192          | 42756         | 2.20%           | 0.236%        |
| 12        | 9.949       | 664           | 666         | 668          | rBV      | 2272364        | 1940753       | 100.00%         | 10.726%       |
| 13        | 9.983       | 668           | 669         | 674          | rVB4     | 37565          | 40242         | 2.07%           | 0.222%        |
| 14        | 10.738      | 732           | 735         | 742          | rBV      | 373062         | 416260        | 21.45%          | 2.301%        |
| 15        | 10.852      | 744           | 745         | 750          | rVB      | 23117          | 43159         | 2.22%           | 0.239%        |
| 16        | 11.309      | 781           | 785         | 786          | rBV2     | 16414          | 25162         | 1.30%           | 0.139%        |
| 17        | 11.435      | 794           | 796         | 802          | rBV2     | 1456754        | 1724487       | 88.86%          | 9.531%        |
| 18        | 11.515      | 802           | 803         | 805          | rVB      | 36913          | 34815         | 1.79%           | 0.192%        |
| 19        | 11.663      | 813           | 816         | 821          | rBV5     | 19115          | 46840         | 2.41%           | 0.259%        |
| 20        | 11.938      | 838           | 840         | 841          | rBV      | 29518          | 28437         | 1.47%           | 0.157%        |
| 21        | 11.972      | 841           | 843         | 844          | rVV      | 23361          | 32699         | 1.68%           | 0.181%        |
| 22        | 12.052      | 848           | 850         | 854          | rVB2     | 49636          | 81430         | 4.20%           | 0.450%        |
| 23        | 12.486      | 886           | 888         | 890          | rBV      | 33971          | 41951         | 2.16%           | 0.232%        |
| 24        | 12.521      | 890           | 891         | 894          | rVB3     | 18909          | 27895         | 1.44%           | 0.154%        |
| 25        | 12.566      | 894           | 895         | 898          | rBV2     | 15114          | 25231         | 1.30%           | 0.139%        |
| 26        | 12.646      | 900           | 902         | 905          | rBV      | 312810         | 314451        | 16.20%          | 1.738%        |
| 27        | 12.875      | 918           | 922         | 926          | rBV      | 307593         | 382431        | 19.71%          | 2.114%        |
| 28        | 13.024      | 932           | 935         | 939          | rBV      | 482283         | 574519        | 29.60%          | 3.175%        |
| 29        | 13.092      | 939           | 941         | 945          | rVB3     | 24538          | 46623         | 2.40%           | 0.258%        |
| 30        | 13.206      | 947           | 951         | 953          | rBV      | 43781          | 80758         | 4.16%           | 0.446%        |
| 31        | 13.309      | 958           | 960         | 964          | rVV2     | 36483          | 55795         | 2.87%           | 0.308%        |
| 32        | 14.075      | 1024          | 1027        | 1035         | rBV2     | 1250825        | 1909866       | 98.41%          | 10.555%       |
| 33        | 15.115      | 1115          | 1118        | 1123         | rBV      | 192948         | 444092        | 22.88%          | 2.454%        |
| 34        | 15.412      | 1142          | 1144        | 1147         | rVB      | 125352         | 172204        | 8.87%           | 0.952%        |

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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-BF101316.M  
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

|    |        |      |      |      |      |         |         |        |        |
|----|--------|------|------|------|------|---------|---------|--------|--------|
| 35 | 15.469 | 1147 | 1149 | 1152 | rBV  | 117604  | 207704  | 10.70% | 1.148% |
| 36 | 15.538 | 1152 | 1155 | 1165 | rVB  | 1072707 | 1798791 | 92.69% | 9.942% |
| 37 | 16.235 | 1214 | 1216 | 1220 | rVB2 | 91747   | 171796  | 8.85%  | 0.949% |

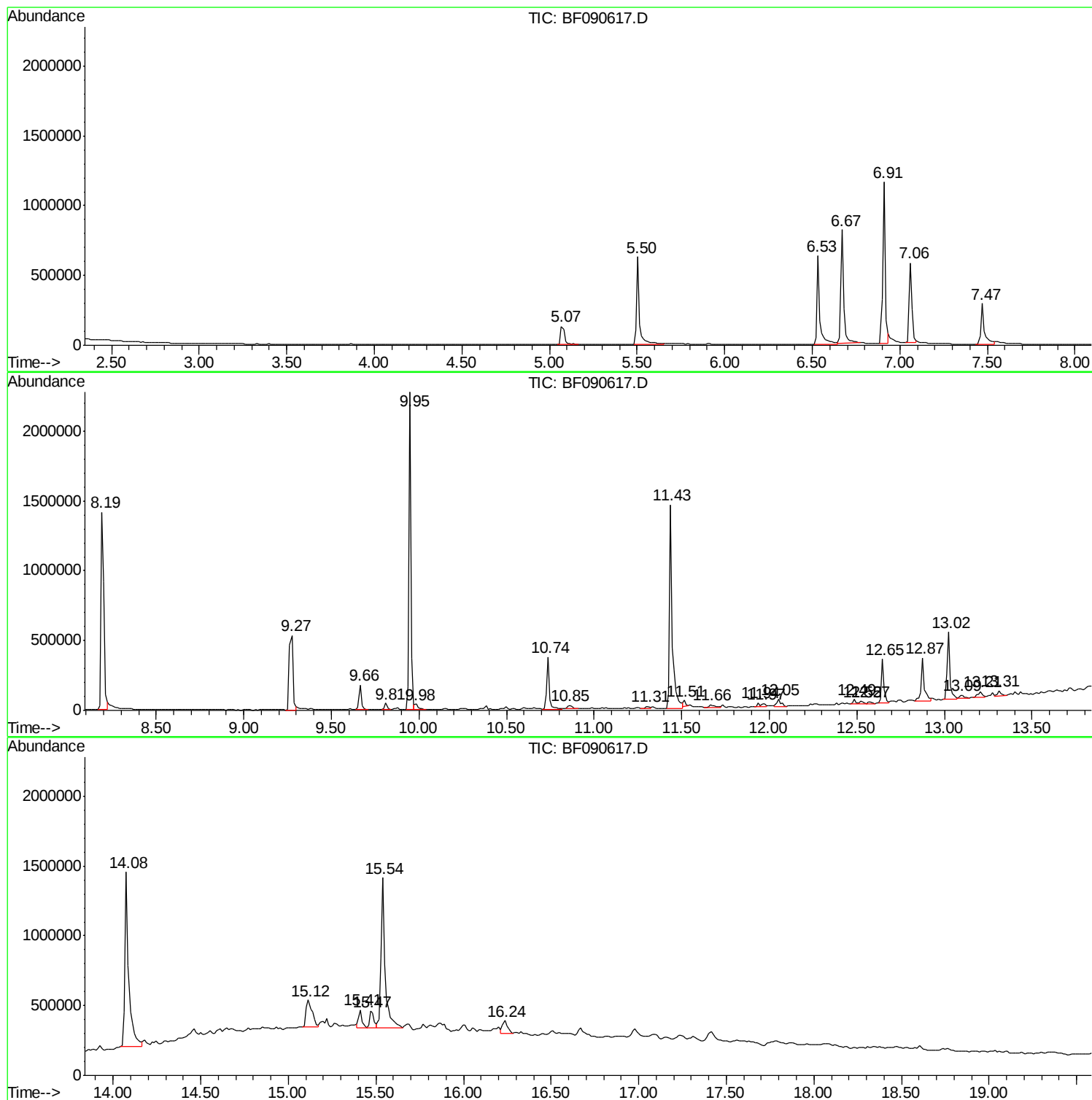
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BNA\_F  
ClientSampled :  
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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF101316.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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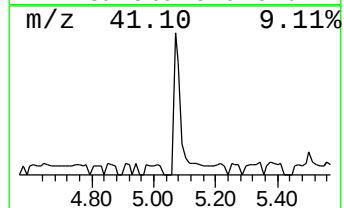
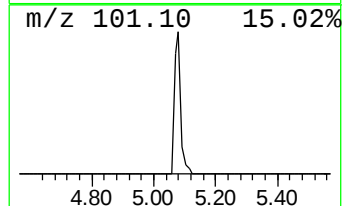
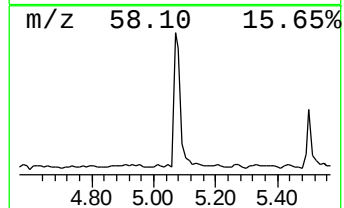
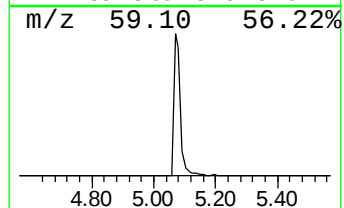
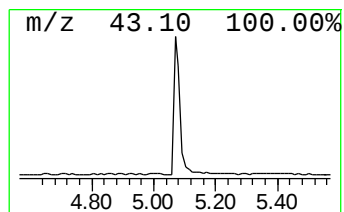
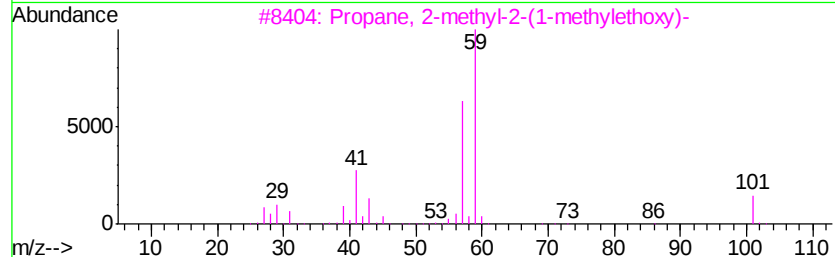
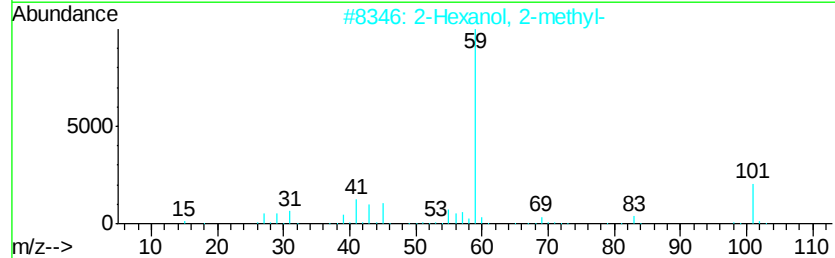
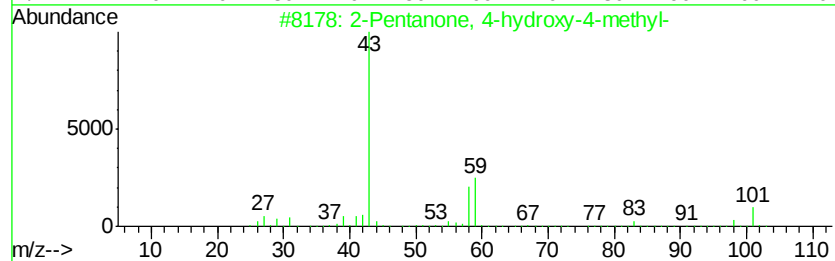
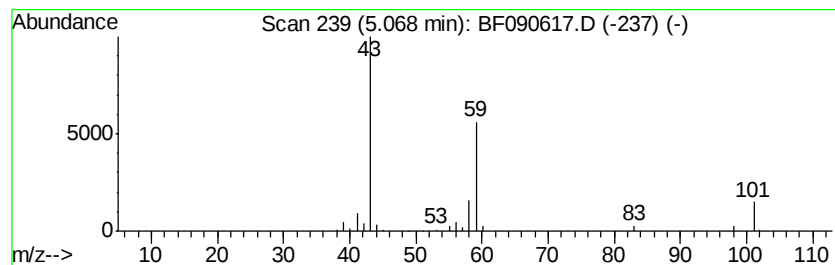
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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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. |
|------|---------|--------|------------------------|------|
| 5.07 | 3.23 ng | 190437 | 1,4-Dichlorobenzene-d4 | 6.91 |

| Hit# of | 5                                     | Tentative ID | MW      | MolForm     | CAS# | Qual |
|---------|---------------------------------------|--------------|---------|-------------|------|------|
| 1       | 2-Pentanone, 4-hydroxy-4-methyl-      | 116          | C6H12O2 | 000123-42-2 | 59   |      |
| 2       | 2-Hexanol, 2-methyl-                  | 116          | C7H16O  | 000625-23-0 | 40   |      |
| 3       | Propane, 2-methyl-2-(1-methylethoxy)- | 116          | C7H16O  | 017348-59-3 | 36   |      |
| 4       | 3-Hexanol                             | 102          | C6H14O  | 000623-37-0 | 33   |      |
| 5       | 2-Pentanol, 2,4-dimethyl-             | 116          | C7H16O  | 000625-06-9 | 33   |      |



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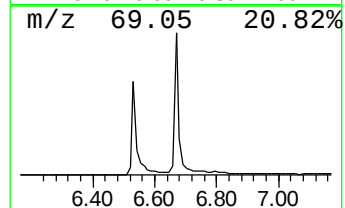
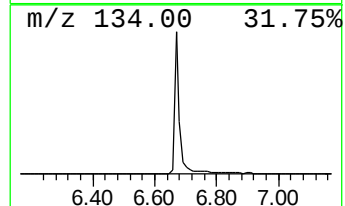
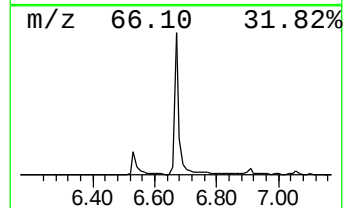
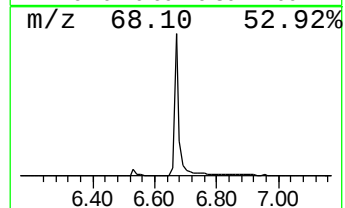
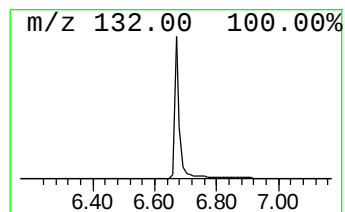
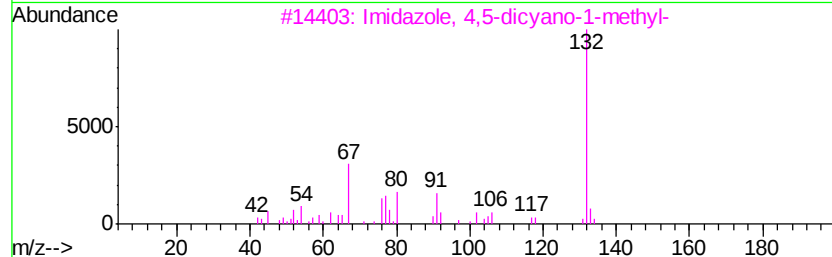
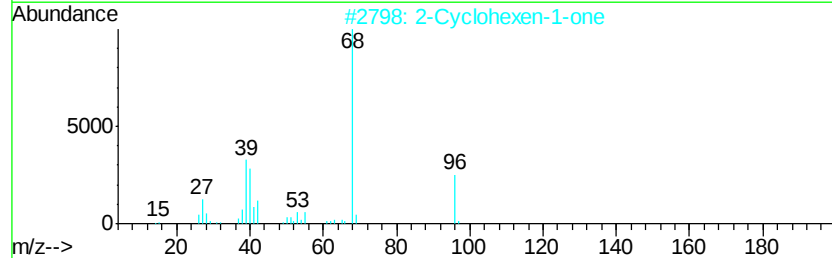
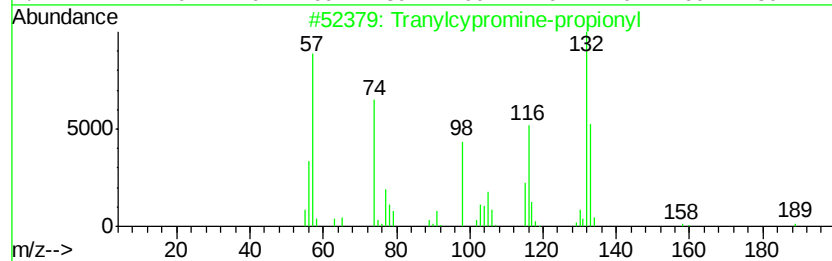
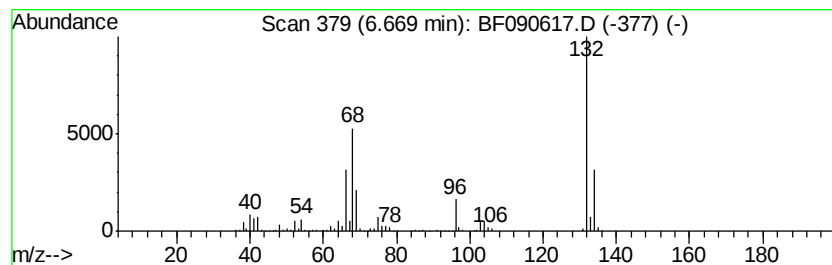
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Peak Number 2 unknown6.67 Concentration Rank 1

| R.T. | EstConc  | Area   | Relative to ISTD       | R.T. |
|------|----------|--------|------------------------|------|
| 6.67 | 14.48 ng | 853599 | 1,4-Dichlorobenzene-d4 | 6.91 |

| Hit# | of | Tentative ID                     | MW  | MolForm  | CAS#         | Qual |
|------|----|----------------------------------|-----|----------|--------------|------|
| 1    | 5  | Tranylcypromine-propionyl        | 189 | C12H15NO | 1000123-86-3 | 10   |
| 2    |    | 2-Cyclohexen-1-one               | 96  | C6H8O    | 000930-68-7  | 10   |
| 3    |    | Imidazole, 4,5-dicyano-1-methyl- | 132 | C6H4N4   | 019485-35-9  | 9    |
| 4    |    | Bicyclo[3.1.0]hexan-3-one        | 96  | C6H8O    | 001755-04-0  | 9    |
| 5    |    | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO  | 031357-76-3  | 9    |



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| TIC Top Hit name     | RT   | EstConc | Units | Response | --Internal Standard-- |      |         |      |
|----------------------|------|---------|-------|----------|-----------------------|------|---------|------|
|                      |      |         |       |          | #                     | RT   | Resp    | Conc |
| 2-Pentanone, 4-hy... | 5.07 | 3.2     | ng    | 190437   | 1                     | 6.91 | 1179170 | 20.0 |
| unknown6.67          | 6.67 | 14.5    | ng    | 853599   | 1                     | 6.91 | 1179170 | 20.0 |