

Data Path : Z:\HPCHEM1\BNA G\DATA\BG030218\  
 Data File : BG032961.D  
 Acq On : 3 Mar 2018 00:47  
 Operator : SJ/JU  
 Sample : PB107023BL  
 Misc :  
 ALS Vial : 16 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 PB107023BL

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\_G\METHODS\8270-BG022118.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         | 3.341       | 6             | 9           | 19           | rVB      | 22666          | 34647         | 1.17%           | 0.211%        |
| 2         | 3.511       | 33            | 38          | 48           | rVB4     | 13460          | 30453         | 1.03%           | 0.185%        |
| 3         | 5.820       | 425           | 431         | 441          | rBV3     | 19415          | 33545         | 1.14%           | 0.204%        |
| 4         | 6.331       | 510           | 518         | 529          | rBV      | 777530         | 1342398       | 45.43%          | 8.157%        |
| 5         | 8.011       | 794           | 804         | 815          | rBV      | 765924         | 1429753       | 48.39%          | 8.688%        |
| 6         | 8.422       | 866           | 874         | 883          | rBV      | 756623         | 1398477       | 47.33%          | 8.498%        |
| 7         | 8.916       | 950           | 958         | 966          | rVB      | 190402         | 335295        | 11.35%          | 2.037%        |
| 8         | 9.251       | 1007          | 1015        | 1025         | rVB      | 565444         | 1040786       | 35.22%          | 6.324%        |
| 9         | 10.114      | 1151          | 1162        | 1174         | rBV      | 449272         | 836708        | 28.32%          | 5.084%        |
| 10        | 11.800      | 1440          | 1449        | 1457         | rBV      | 266565         | 497795        | 16.85%          | 3.025%        |
| 11        | 14.162      | 1842          | 1851        | 1858         | rBV      | 1184467        | 1934900       | 65.49%          | 11.757%       |
| 12        | 15.530      | 2077          | 2084        | 2092         | rVB2     | 400767         | 662722        | 22.43%          | 4.027%        |
| 13        | 16.999      | 2328          | 2334        | 2349         | rBV      | 858971         | 1346488       | 45.57%          | 8.182%        |
| 14        | 18.256      | 2541          | 2548        | 2560         | rBV2     | 535643         | 854137        | 28.91%          | 5.190%        |
| 15        | 20.776      | 2971          | 2977        | 2988         | rBV      | 2259240        | 2954694       | 100.00%         | 17.954%       |
| 16        | 22.615      | 3281          | 3290        | 3302         | rBV2     | 464083         | 905708        | 30.65%          | 5.504%        |
| 17        | 26.422      | 3925          | 3938        | 3957         | rBV2     | 211792         | 818259        | 27.69%          | 4.972%        |

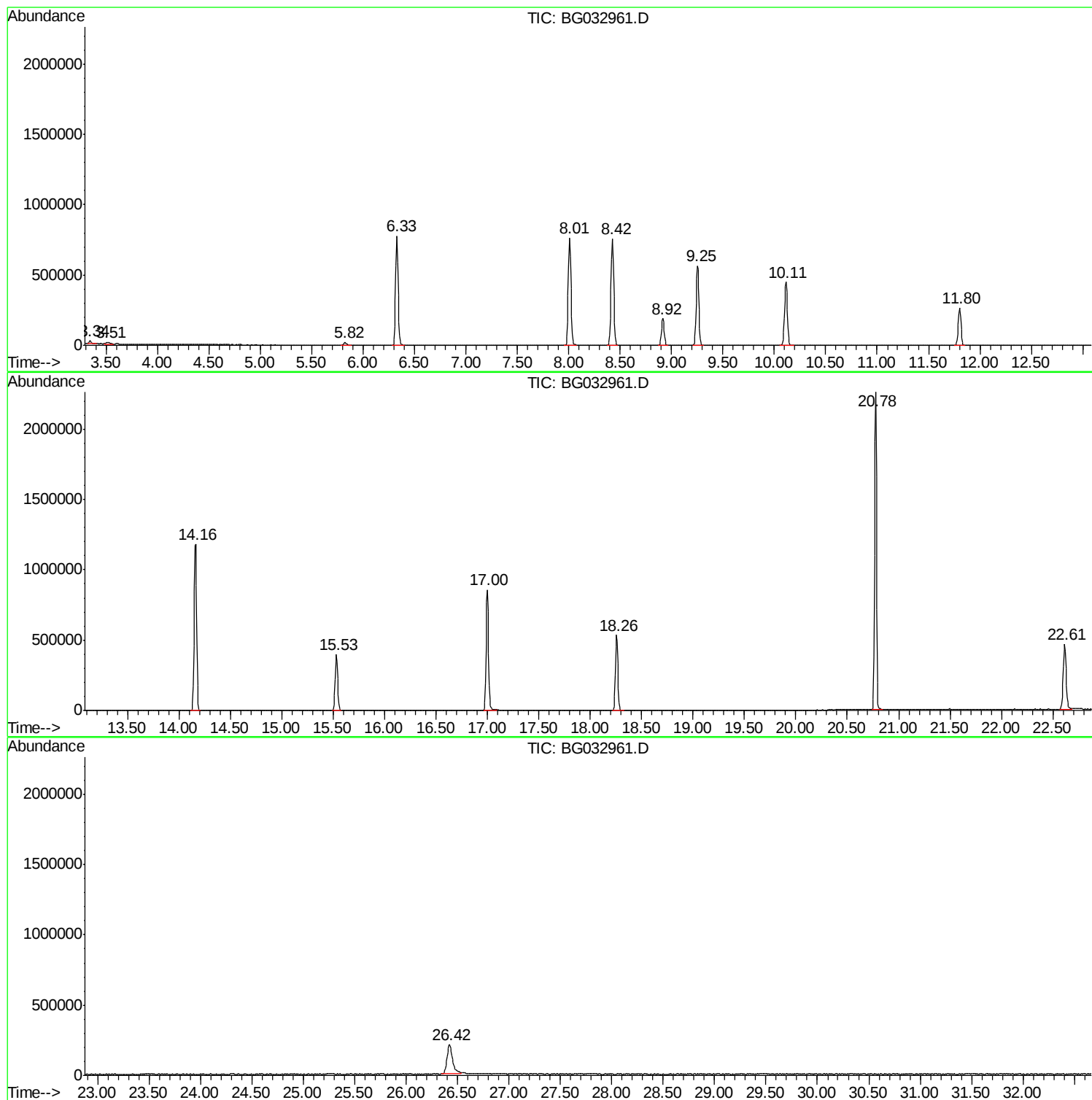
Sum of corrected areas: 16456765

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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG022118.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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ALS Vial : 16 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampled :  
PB107023BL

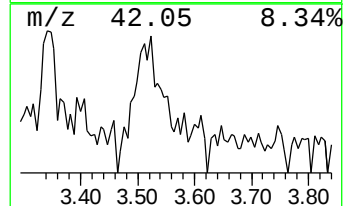
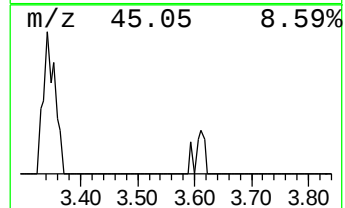
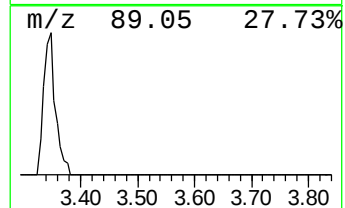
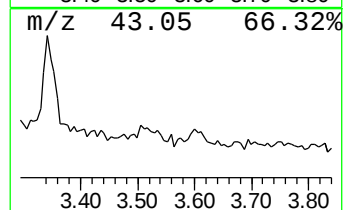
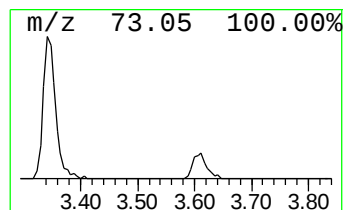
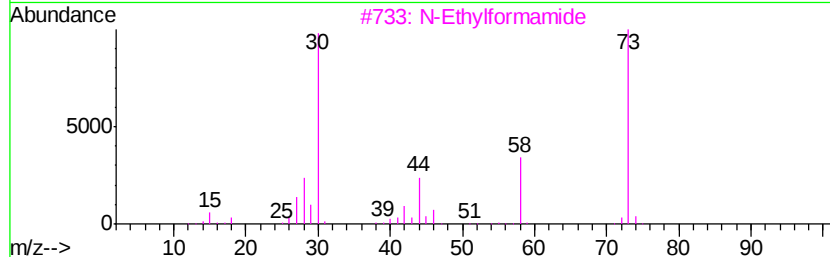
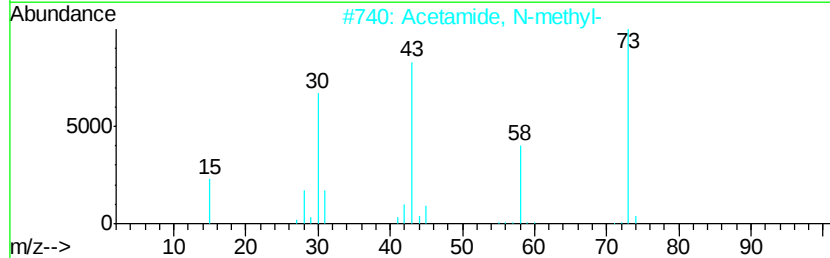
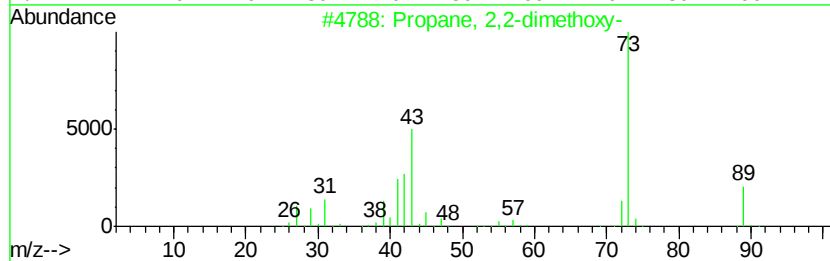
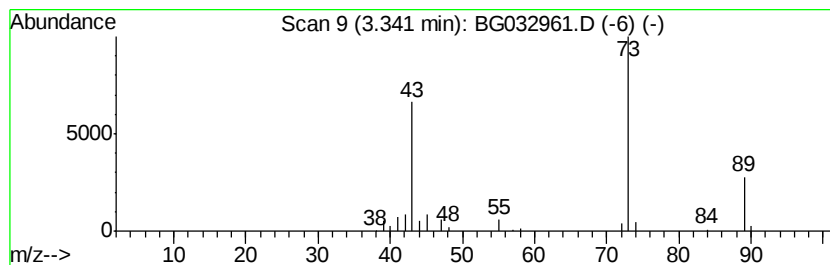
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG022118.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 3

| R.T. | EstConc | Area  | Relative to ISTD       | R.T. |
|------|---------|-------|------------------------|------|
| 3.34 | 2.07 ng | 34647 | 1,4-Dichlorobenzene-d4 | 8.92 |

| Hit# | of | Tentative ID                 | MW  | MolForm | CAS#        | Qual |
|------|----|------------------------------|-----|---------|-------------|------|
| 1    | 5  | Propane, 2,2-dimethoxy-      | 104 | C5H12O2 | 000077-76-9 | 39   |
| 2    |    | Acetamide, N-methyl-         | 73  | C3H7NO  | 000079-16-3 | 35   |
| 3    |    | N-Ethylformamide             | 73  | C3H7NO  | 000627-45-2 | 9    |
| 4    |    | Ethanol, 2-(1-methylethoxy)- | 104 | C5H12O2 | 000109-59-1 | 9    |
| 5    |    | Malic Acid                   | 134 | C4H6O5  | 006915-15-7 | 9    |



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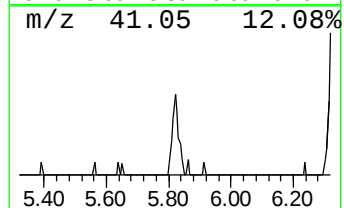
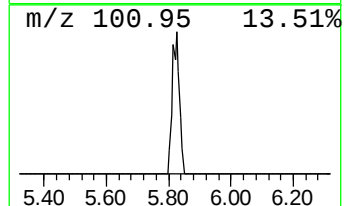
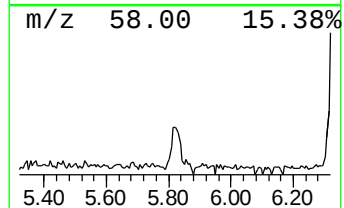
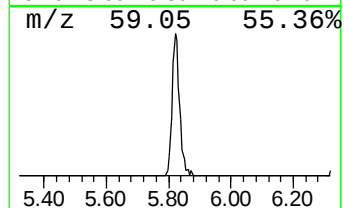
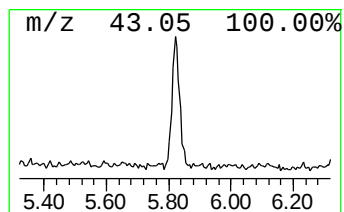
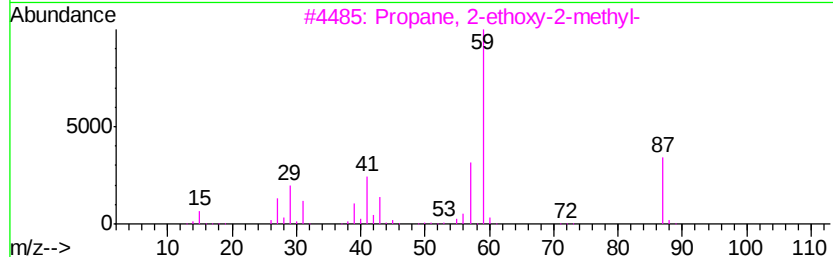
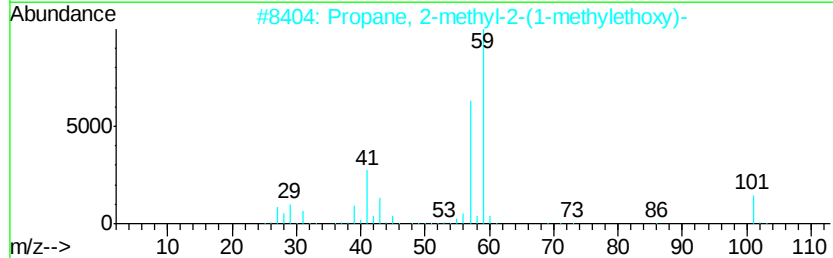
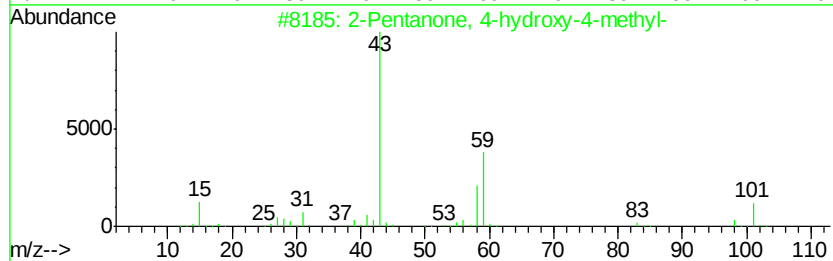
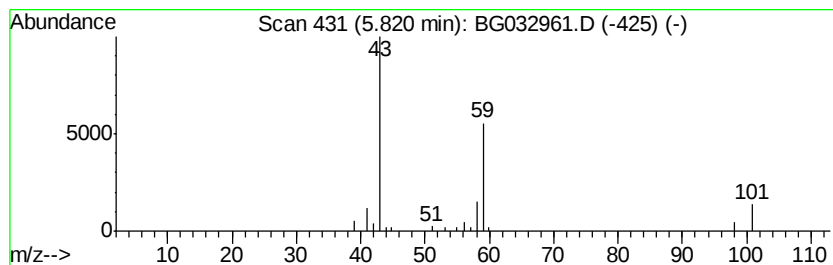
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

| R.T. | EstConc | Area  | Relative to ISTD       | R.T. |
|------|---------|-------|------------------------|------|
| 5.82 | 2.00 ng | 33545 | 1,4-Dichlorobenzene-d4 | 8.92 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|---------|-------------|------|
| 1    |    |   | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2 | 000123-42-2 | 72   |
| 2    |    |   | Propane, 2-methyl-2-(1-methyleth... | 116 | C7H16O  | 017348-59-3 | 33   |
| 3    |    |   | Propane, 2-ethoxy-2-methyl-         | 102 | C6H14O  | 000637-92-3 | 23   |
| 4    |    |   | 2,3-Butanedione, monooxime          | 101 | C4H7NO2 | 000057-71-6 | 9    |
| 5    |    |   | 5-Hexen-2-one                       | 98  | C6H10O  | 000109-49-9 | 9    |



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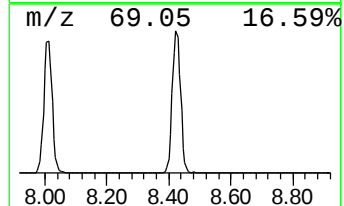
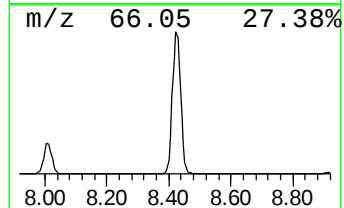
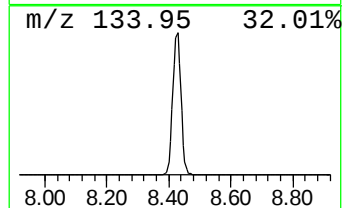
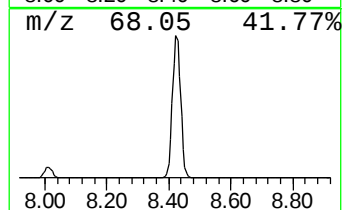
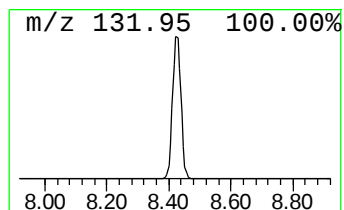
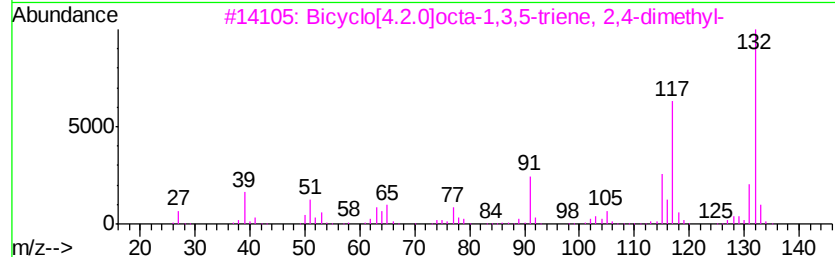
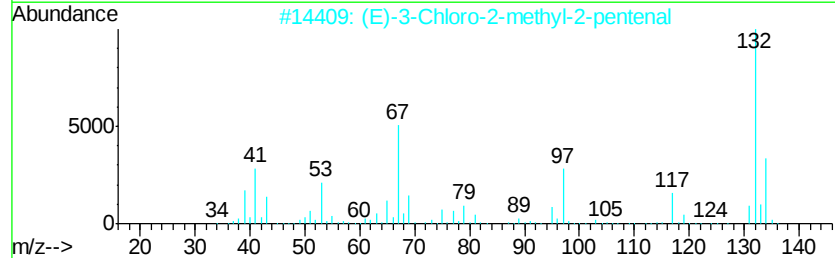
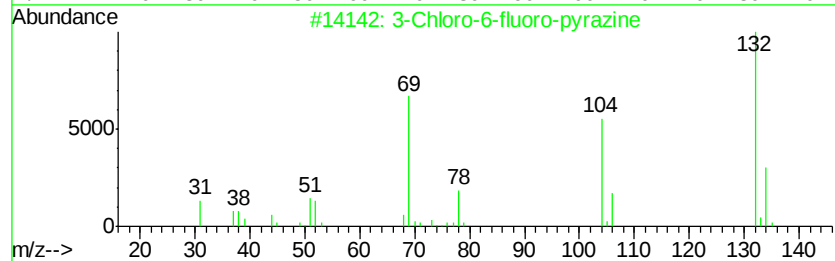
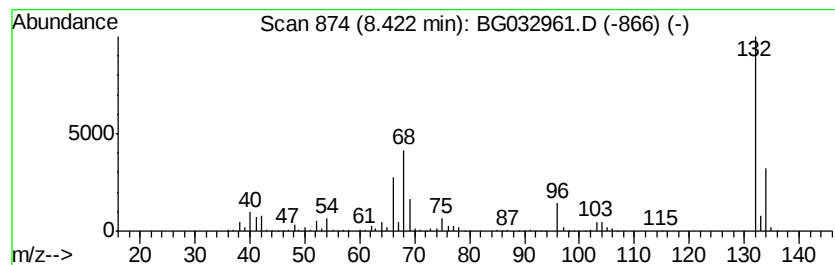
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Peak Number 3 unknown8.42 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 8.42 | 83.42 ng | 1398480 | 1,4-Dichlorobenzene-d4 | 8.92 |

| Hit# | of | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|-------------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 3-Chloro-6-fluoro-pyrazine          | 132 | C4H2ClFN2 | 1000146-10-7 | 27   |
| 2    |    | (E)-3-Chloro-2-methyl-2-pentenal    | 132 | C6H9ClO   | 031357-76-3  | 17   |
| 3    |    | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12    | 028749-81-7  | 9    |
| 4    |    | 1-Methylpyrrolo[1,2-a]pyrazine      | 132 | C8H8N2    | 064608-59-9  | 9    |
| 5    |    | 4-Methylpyrrolo[1,2-a]pyrazine      | 132 | C8H8N2    | 064608-60-2  | 9    |



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| TIC Top Hit name     | RT   | EstConc | Units | Response | --Internal Standard-- |      |        |      |
|----------------------|------|---------|-------|----------|-----------------------|------|--------|------|
|                      |      |         |       |          | #                     | RT   | Resp   | Conc |
| Propane, 2,2-dime... | 3.34 | 2.1     | ng    | 34647    | 1                     | 8.92 | 335295 | 20.0 |
| 2-Pentanone, 4-hy... | 5.82 | 2.0     | ng    | 33545    | 1                     | 8.92 | 335295 | 20.0 |
| unknown8.42          | 8.42 | 83.4    | ng    | 1398480  | 1                     | 8.92 | 335295 | 20.0 |