

Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF062116\  
 Data File : BF088225.D  
 Acq On : 21 Jun 2016 21:13  
 Operator : UM/SJ  
 Sample : PB91462BL  
 Misc :  
 ALS Vial : 11 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 PB91462BL

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-BF060716.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       | 3             | 5           | 13           | rVV      | 463396         | 743013        | 25.96%          | 3.335%        |
| 2         | 1.758       | 13            | 15          | 61           | rVB      | 1295314        | 2862635       | 100.00%         | 12.849%       |
| 3         | 4.090       | 217           | 219         | 230          | rBB      | 105459         | 153269        | 5.35%           | 0.688%        |
| 4         | 4.799       | 279           | 281         | 296          | rBV      | 435259         | 699750        | 24.44%          | 3.141%        |
| 5         | 5.244       | 318           | 320         | 323          | rBV      | 1176781        | 1707362       | 59.64%          | 7.664%        |
| 6         | 6.307       | 411           | 413         | 415          | rBV      | 1610914        | 1708850       | 59.70%          | 7.670%        |
| 7         | 6.422       | 421           | 423         | 425          | rBV      | 1912388        | 1737588       | 60.70%          | 7.799%        |
| 8         | 6.650       | 441           | 443         | 446          | rBV      | 571828         | 478530        | 16.72%          | 2.148%        |
| 9         | 6.810       | 454           | 457         | 459          | rBV      | 1203255        | 1475995       | 51.56%          | 6.625%        |
| 10        | 7.222       | 491           | 493         | 495          | rBV      | 1166332        | 1175293       | 41.06%          | 5.276%        |
| 11        | 7.930       | 553           | 555         | 558          | rBV      | 527558         | 640326        | 22.37%          | 2.874%        |
| 12        | 9.016       | 647           | 650         | 652          | rBV      | 2130116        | 2326441       | 81.27%          | 10.443%       |
| 13        | 9.679       | 706           | 708         | 711          | rBV      | 606025         | 725620        | 25.35%          | 3.257%        |
| 14        | 10.468      | 775           | 777         | 780          | rBV2     | 916536         | 1263038       | 44.12%          | 5.669%        |
| 15        | 11.165      | 836           | 838         | 840          | rBV      | 867926         | 787349        | 27.50%          | 3.534%        |
| 16        | 12.582      | 960           | 962         | 964          | rBB      | 83614          | 73062         | 2.55%           | 0.328%        |
| 17        | 12.754      | 974           | 977         | 979          | rBV      | 1736750        | 2307536       | 80.61%          | 10.358%       |
| 18        | 13.279      | 1021          | 1023        | 1025         | rVB      | 56948          | 48232         | 1.68%           | 0.216%        |
| 19        | 13.794      | 1065          | 1068        | 1070         | rBV      | 781663         | 763415        | 26.67%          | 3.427%        |
| 20        | 15.165      | 1186          | 1188        | 1195         | rBV      | 496709         | 601002        | 20.99%          | 2.698%        |

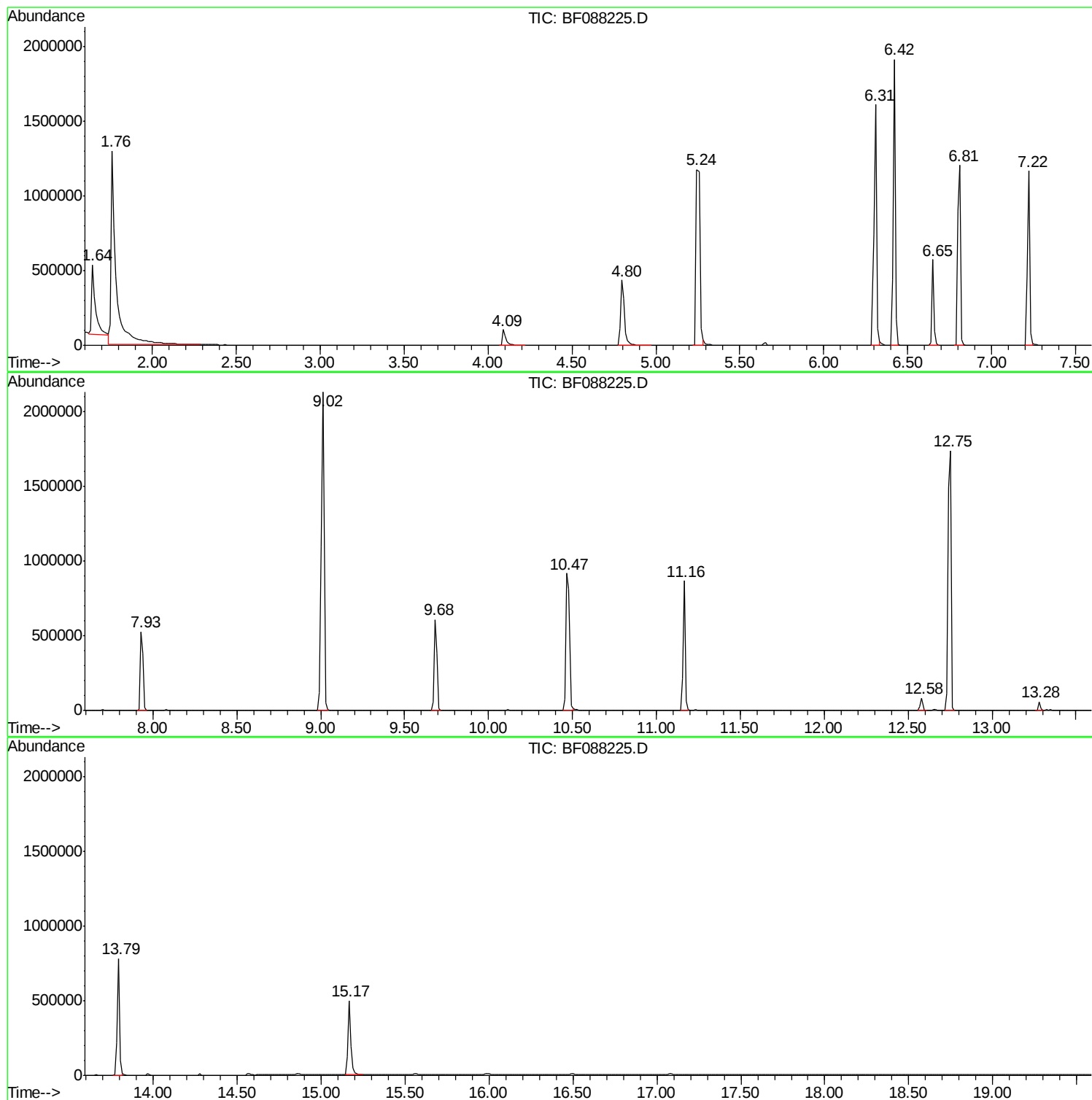
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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF060716.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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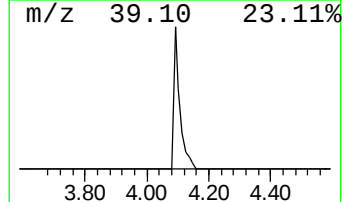
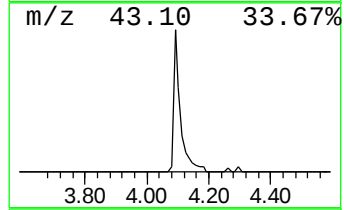
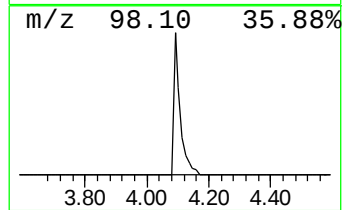
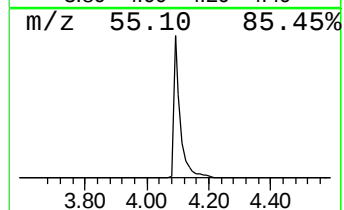
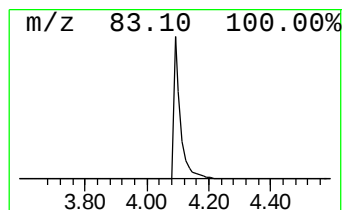
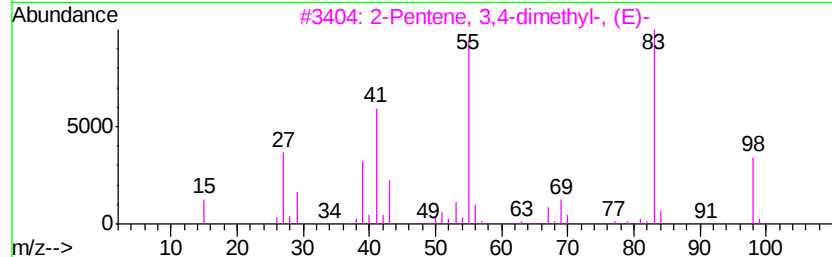
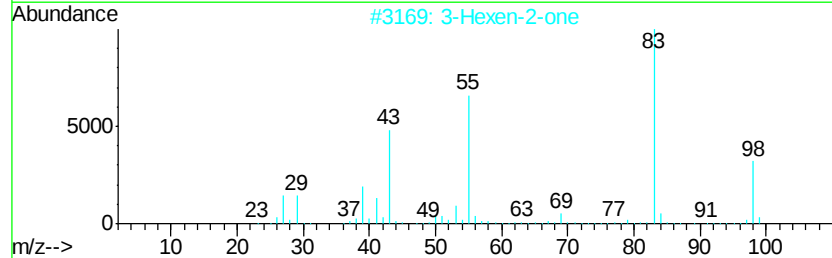
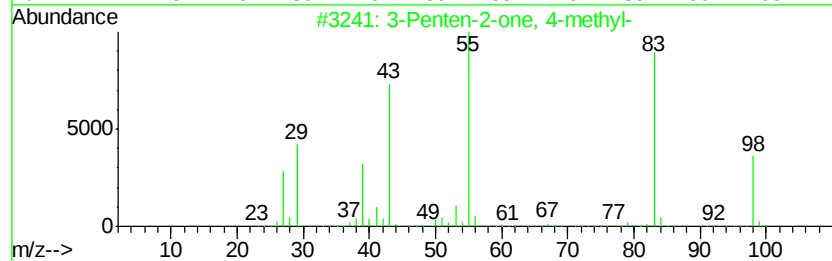
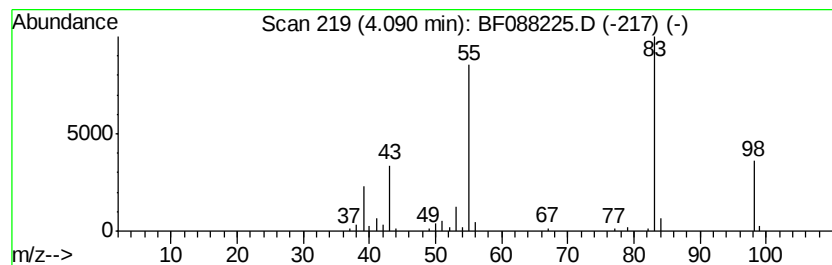
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 6

| R.T. | EstConc | Area   | Relative to ISTD       | R.T. |
|------|---------|--------|------------------------|------|
| 4.09 | 6.41 ng | 153269 | 1,4-Dichlorobenzene-d4 | 6.65 |

| Hit# | of | Tentative ID                   | MW | MolForm | CAS#        | Qual |
|------|----|--------------------------------|----|---------|-------------|------|
| 1    | 5  | 3-Penten-2-one, 4-methyl-      | 98 | C6H10O  | 000141-79-7 | 91   |
| 2    |    | 3-Hexen-2-one                  | 98 | C6H10O  | 000763-93-9 | 90   |
| 3    |    | 2-Pentene, 3,4-dimethyl-, (E)- | 98 | C7H14   | 004914-92-5 | 90   |
| 4    |    | 2-Pentene, 2,4-dimethyl-       | 98 | C7H14   | 000625-65-0 | 87   |
| 5    |    | 2-Pentene, 3,4-dimethyl-, (Z)- | 98 | C7H14   | 004914-91-4 | 86   |



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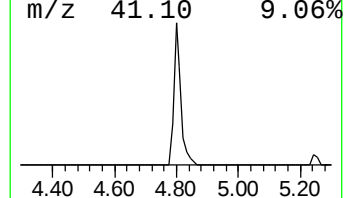
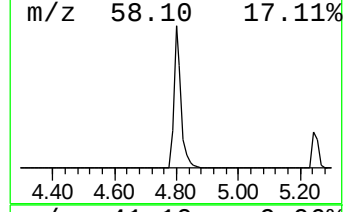
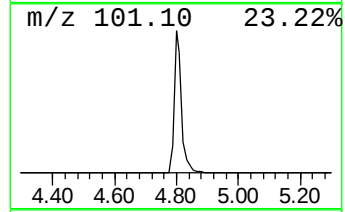
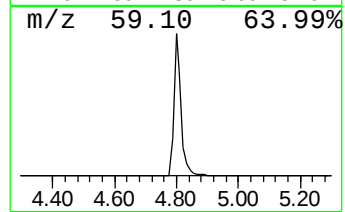
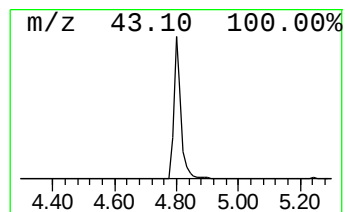
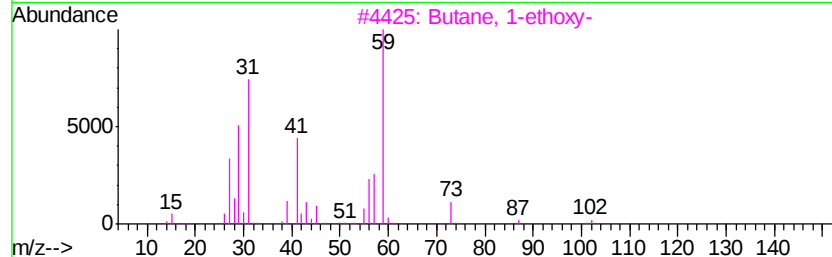
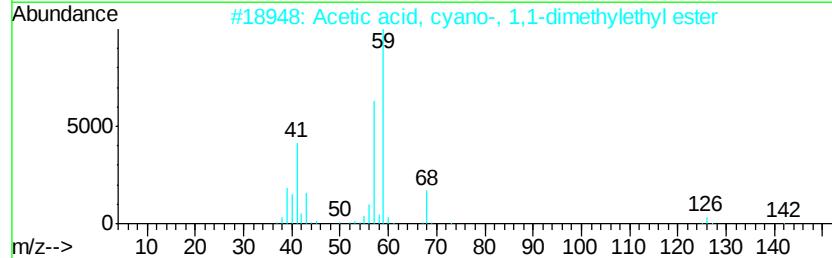
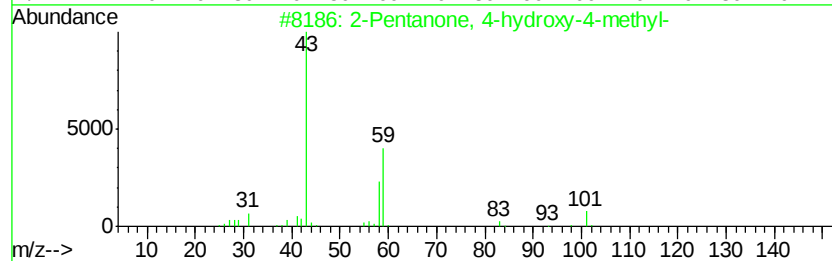
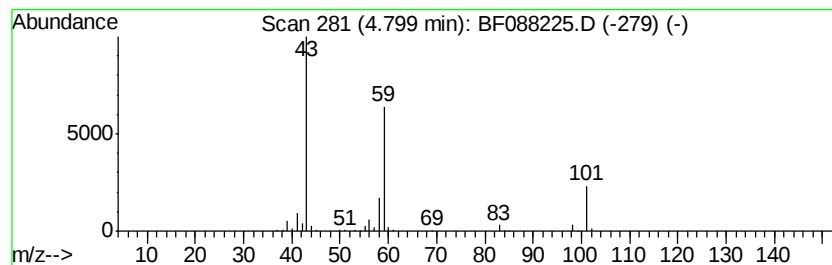
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Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

| R.T. | EstConc  | Area   | Relative to ISTD       | R.T. |
|------|----------|--------|------------------------|------|
| 4.80 | 29.25 ng | 699750 | 1,4-Dichlorobenzene-d4 | 6.65 |

| Hit# | of | Tentative ID                         | MW  | MolForm  | CAS#        | Qual |
|------|----|--------------------------------------|-----|----------|-------------|------|
| 1    | 5  | 2-Pentanone, 4-hydroxy-4-methyl-     | 116 | C6H12O2  | 000123-42-2 | 56   |
| 2    |    | Acetic acid, cyano-, 1,1-dimethyl... | 141 | C7H11NO2 | 001116-98-9 | 25   |
| 3    |    | Butane, 1-ethoxy-                    | 102 | C6H14O   | 000628-81-9 | 9    |
| 4    |    | 5-Hexen-2-one                        | 98  | C6H10O   | 000109-49-9 | 9    |
| 5    |    | (+)-4-Amino-4,5-dihydro-2(3H)-f...   | 101 | C4H7NO2  | 016504-58-8 | 9    |



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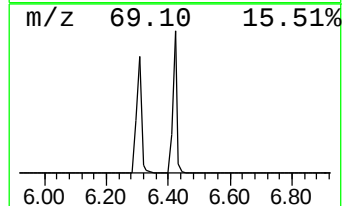
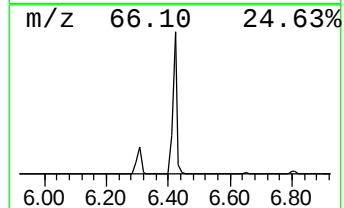
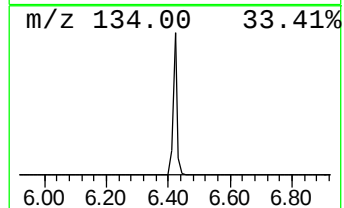
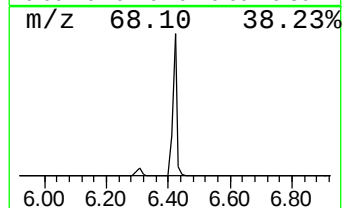
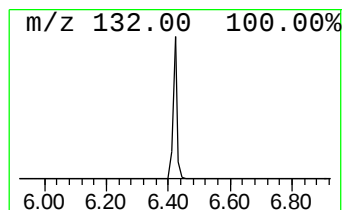
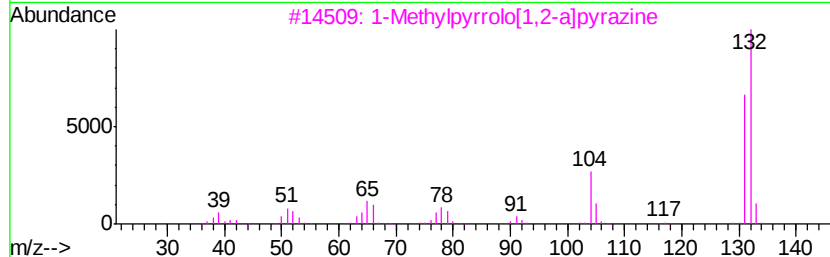
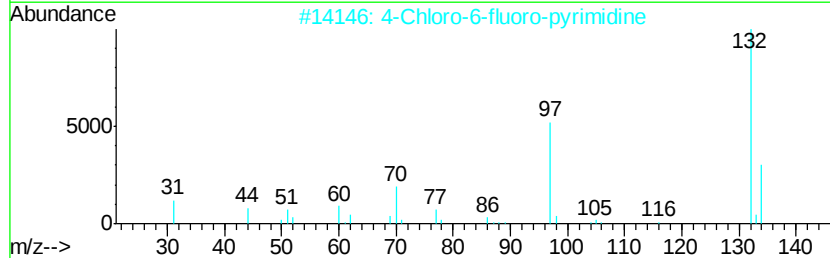
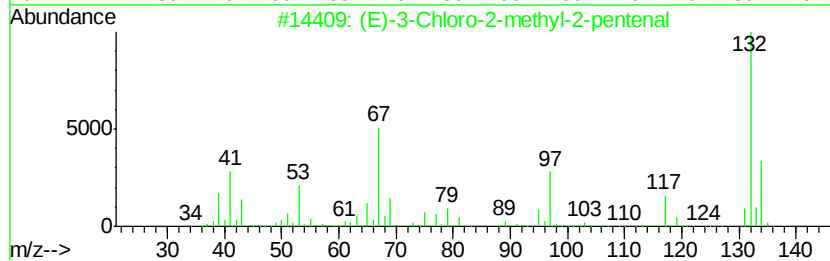
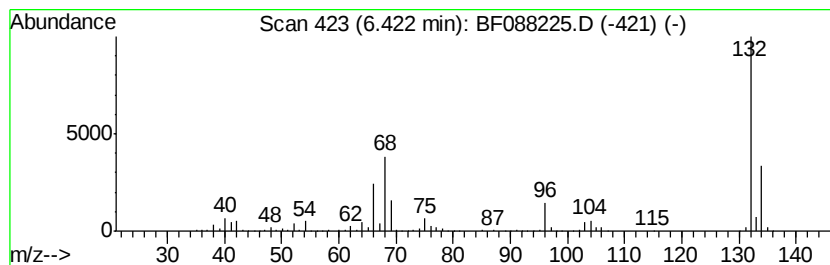
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Peak Number 5 unknown6.42 Concentration Rank 2

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.42 | 72.62 ng | 1737590 | 1,4-Dichlorobenzene-d4 | 6.65 |

| Hit# | of | Tentative ID                        | MW  | MolForm   | CAS#        | Qual |
|------|----|-------------------------------------|-----|-----------|-------------|------|
| 1    | 5  | (E)-3-Chloro-2-methyl-2-pentenal    | 132 | C6H9ClO   | 031357-76-3 | 17   |
| 2    |    | 4-Chloro-6-fluoro-pyrimidine        | 132 | C4H2ClFN2 | 051422-01-6 | 9    |
| 3    |    | 1-Methylpyrrolo[1,2-a]pyrazine      | 132 | C8H8N2    | 064608-59-9 | 9    |
| 4    |    | 2H-Cyclopenta[d]pyridazine, 2-me... | 132 | C8H8N2    | 022291-85-6 | 9    |
| 5    |    | 5-Fluoro-2-chloropyrimidine         | 132 | C4H2ClFN2 | 062802-42-0 | 9    |



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| TIC Top Hit name     | RT   | EstConc | Units | Response | --Internal Standard-- |      |        |      |
|----------------------|------|---------|-------|----------|-----------------------|------|--------|------|
|                      |      |         |       |          | #                     | RT   | Resp   | Conc |
| 3-Penten-2-one, 4... | 4.09 | 6.4     | ng    | 153269   | 1                     | 6.65 | 478530 | 20.0 |
| 2-Pentanone, 4-hy... | 4.80 | 29.3    | ng    | 699750   | 1                     | 6.65 | 478530 | 20.0 |
| unknown6.42          | 6.42 | 72.6    | ng    | 1737590  | 1                     | 6.65 | 478530 | 20.0 |